



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 23, 2026 – 03:36 AM UTC

PDB ID : 4BIT / pdb\_00004bit  
BMRB ID : 19164  
Title : solution structure of cerebral dopamine neurotrophic factor (CDNF)  
Authors : Latge, C.; Cabral, K.M.S.; Raymundo, D.P.; Foguel, D.; Herrmann, T.; Almeida, M.S.  
Deposited on : 2013-04-13

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

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 : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

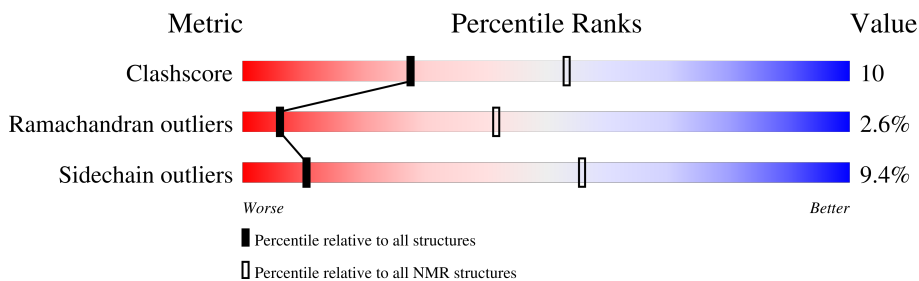
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 92%.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	161	

## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:11-A:100 (90)	1.43	12
2	A:106-A:130, A:137-A:153 (42)	0.73	18

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 5 clusters and 3 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2580 atoms, of which 1301 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CEREBRAL DOPAMINE NEUROTROPHIC FACTOR.

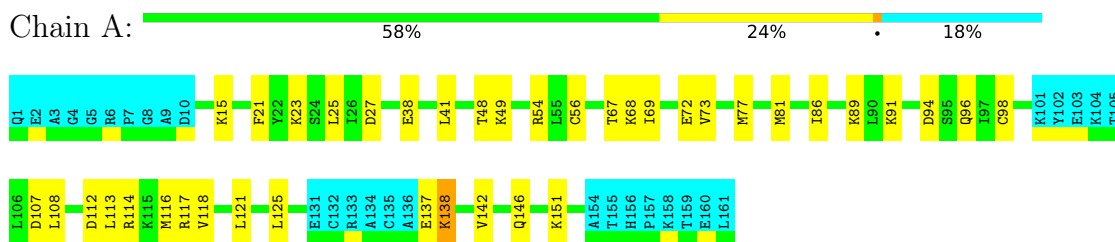
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	161	2580	806	1301	218	243	12	0

## 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: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR

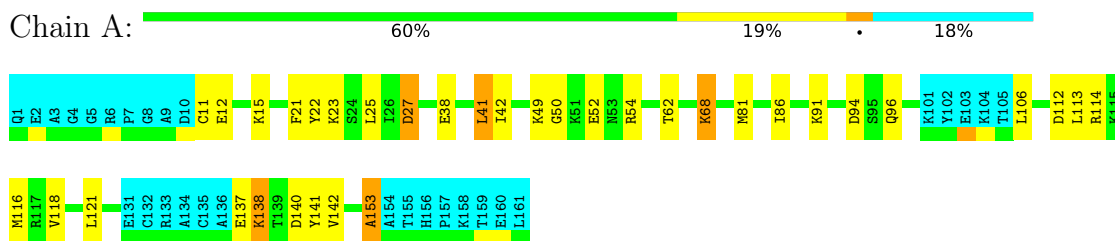


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

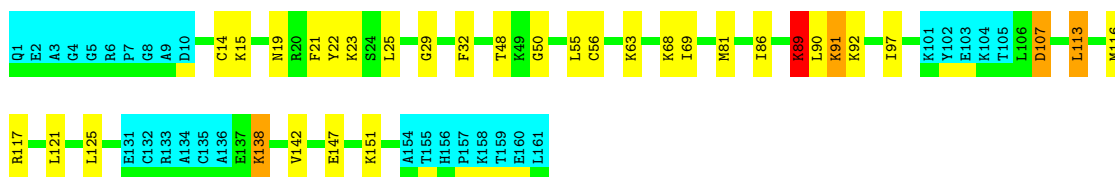
- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR



#### 4.2.2 Score per residue for model 2

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR

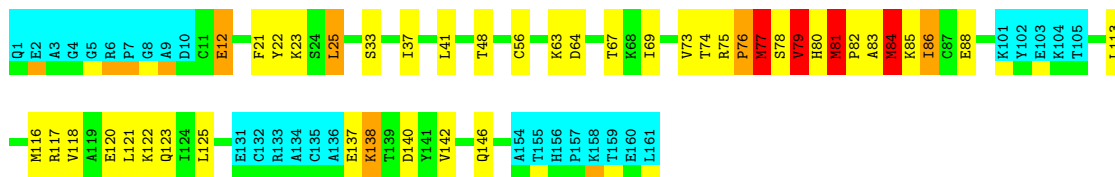




#### 4.2.3 Score per residue for model 3

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR

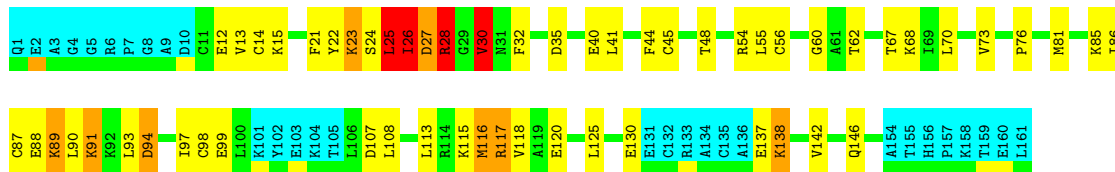
Chain A: 55% 21% 18%



#### 4.2.4 Score per residue for model 4

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR

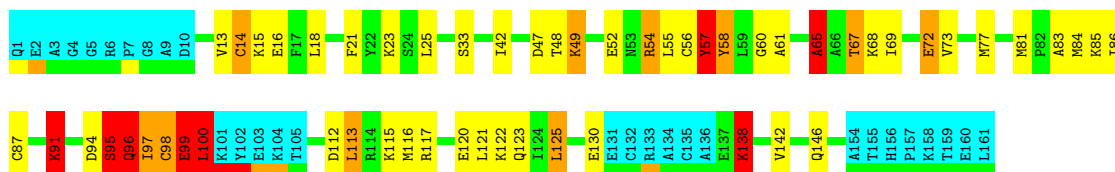
Chain A: 47% 28% 5% 18%



#### 4.2.5 Score per residue for model 5

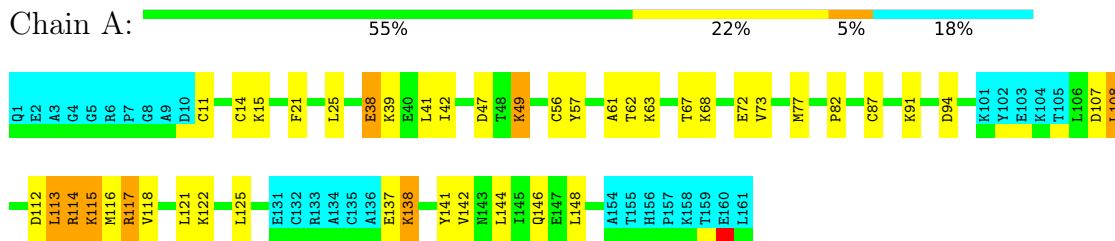
- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR

Chain A: 47% 24% 6% 5% 18%



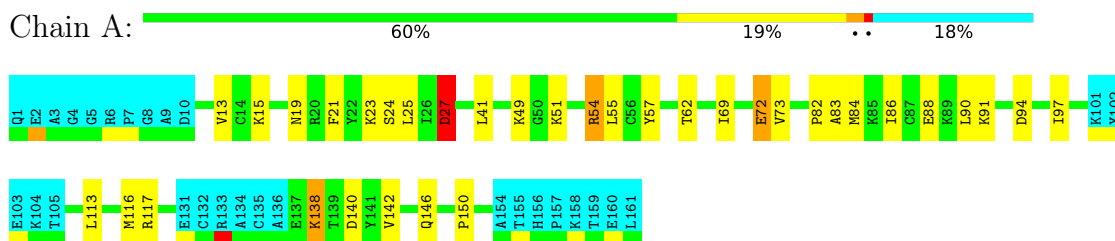
#### 4.2.6 Score per residue for model 6

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR



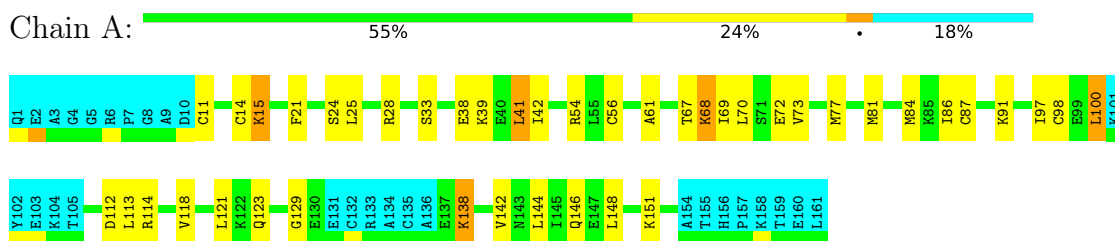
### 4.2.7 Score per residue for model 7

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR



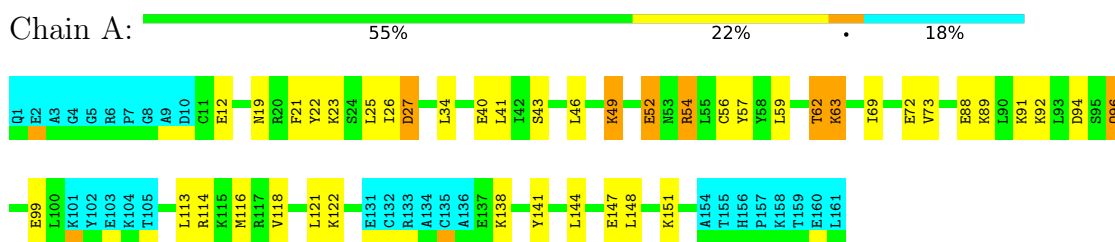
### 4.2.8 Score per residue for model 8

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR



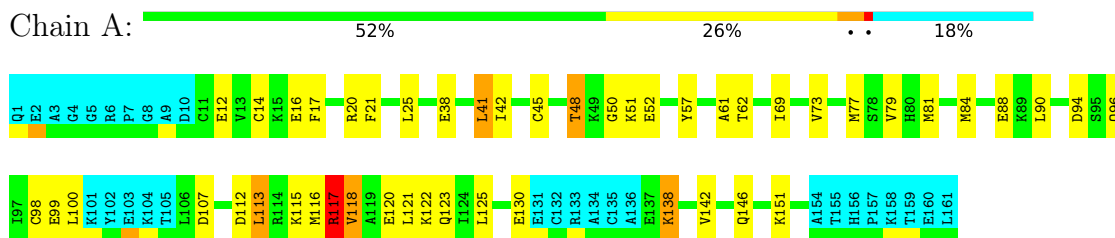
### 4.2.9 Score per residue for model 9

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR



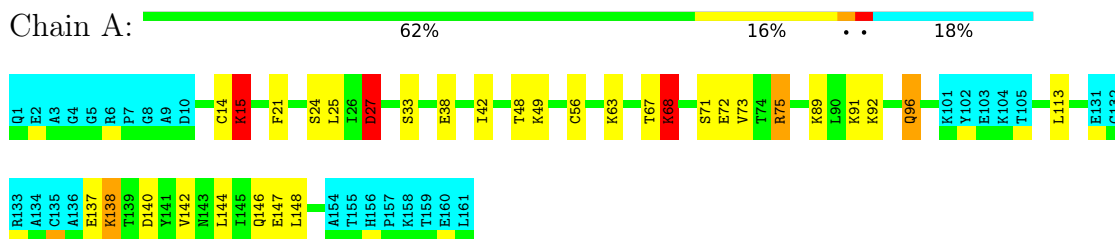
#### 4.2.10 Score per residue for model 10

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR



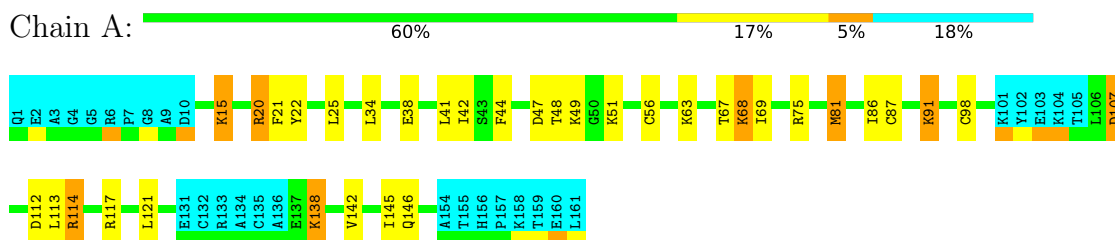
#### 4.2.11 Score per residue for model 11

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR



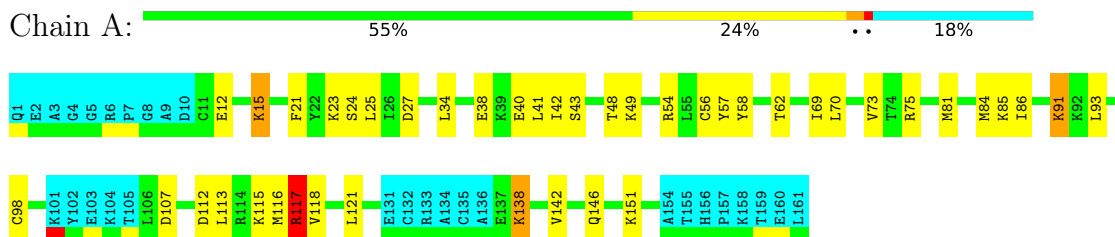
#### 4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR



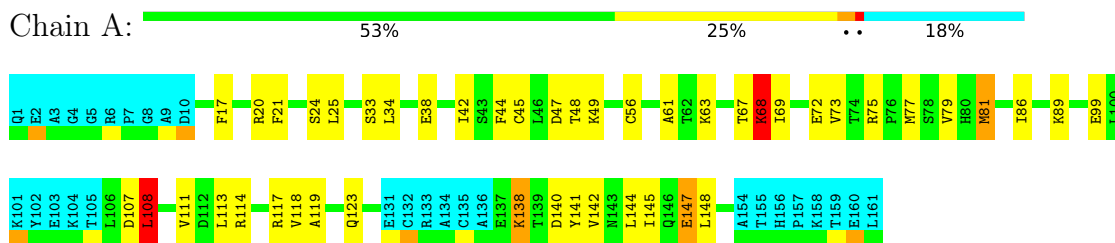
#### 4.2.13 Score per residue for model 13

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR



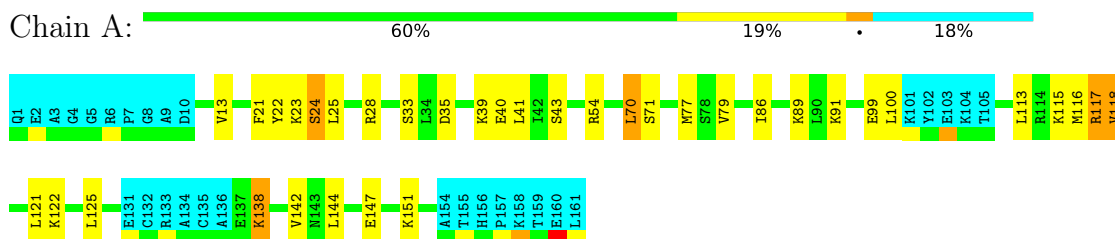
## 4.2.14 Score per residue for model 14

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR



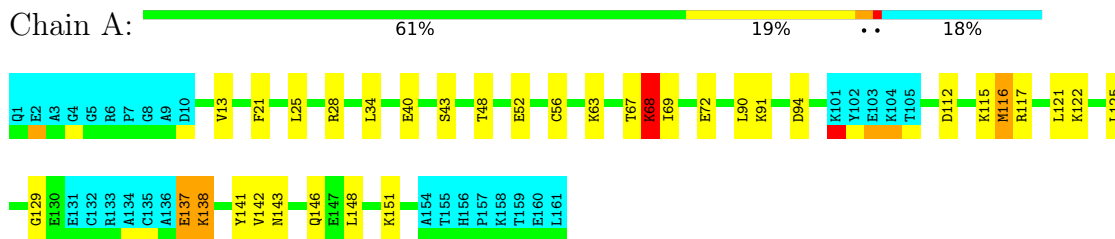
## 4.2.15 Score per residue for model 15

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR



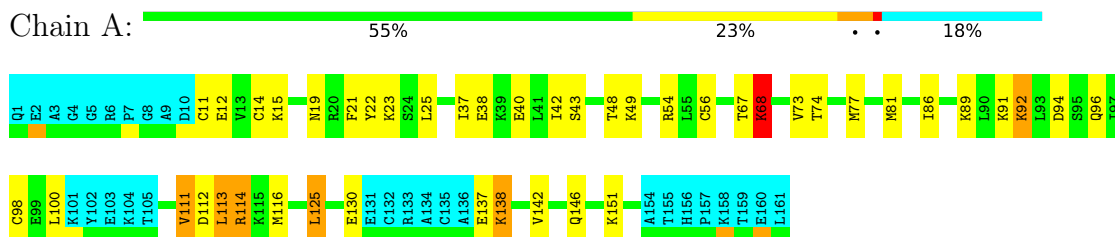
## 4.2.16 Score per residue for model 16

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR



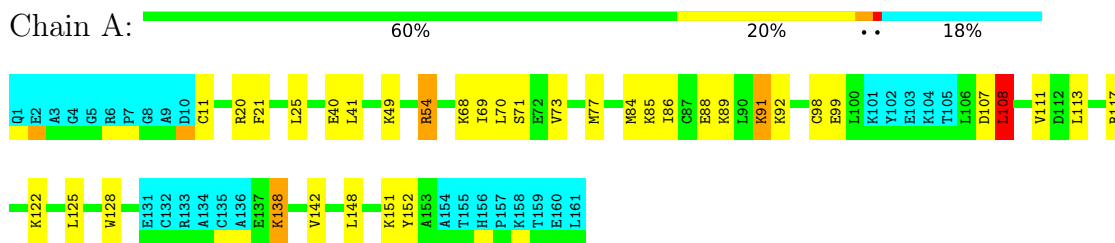
## 4.2.17 Score per residue for model 17

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR



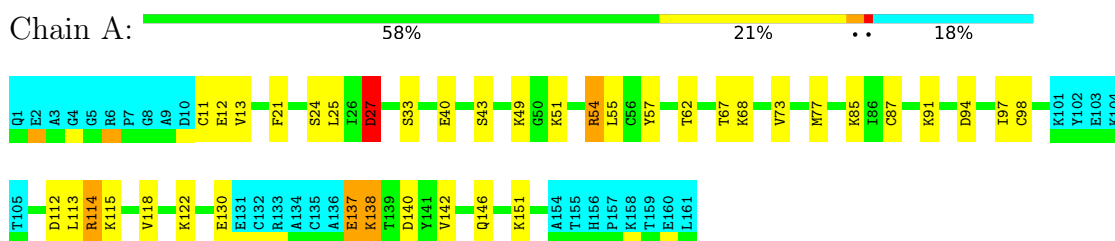
### 4.2.18 Score per residue for model 18

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR



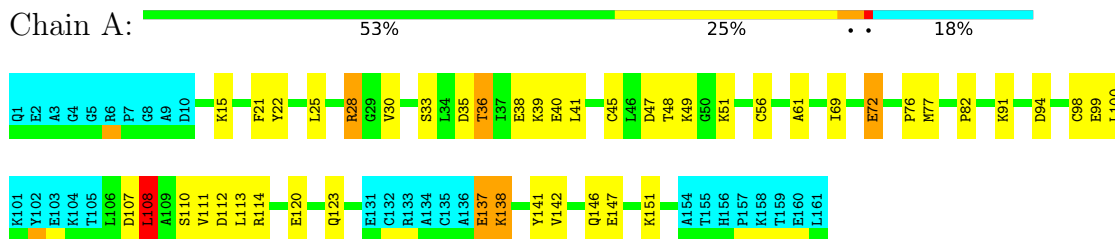
### 4.2.19 Score per residue for model 19

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR



### 4.2.20 Score per residue for model 20

- Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *CNS USING RECOORD SCRIPTS*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
CNS	refinement	1.3
UNIO	structure solution	10
CNS	structure solution	1.3

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	2014
Number of shifts mapped to atoms	2014
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

## 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	1.24±0.08	4±3/1078 ( 0.3± 0.3%)	1.19±0.06	2±3/1448 ( 0.1± 0.2%)
All	All	1.24	75/21560 ( 0.3%)	1.19	39/28960 ( 0.1%)

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

Mol	Chain	Chirality	Planarity
1	A	0.1±0.3	0.7±0.6
All	All	2	13

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	91	LYS	CA-C	-11.38	1.37	1.52	2	2
1	A	30	VAL	C-N	-9.35	1.19	1.33	4	1
1	A	81	MET	N-CA	-9.13	1.33	1.46	3	1
1	A	91	LYS	C-O	-8.54	1.13	1.24	2	2
1	A	27	ASP	N-CA	-8.45	1.36	1.46	4	1
1	A	116	MET	N-CA	-8.18	1.35	1.45	4	1
1	A	107	ASP	N-CA	-6.81	1.37	1.46	13	2
1	A	94	ASP	C-N	-6.79	1.24	1.33	5	1
1	A	48	THR	C-N	-6.74	1.27	1.33	10	1
1	A	84	MET	CA-C	-6.42	1.44	1.52	3	1
1	A	107	ASP	C-N	-6.39	1.24	1.33	18	6
1	A	77	MET	N-CA	6.25	1.54	1.46	3	1
1	A	75	ARG	CA-C	6.17	1.59	1.52	3	1
1	A	118	VAL	C-O	-6.14	1.16	1.24	15	1
1	A	95	SER	N-CA	-6.13	1.38	1.46	5	1
1	A	79	VAL	N-CA	-6.11	1.38	1.46	15	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	24	SER	N-CA	-6.06	1.38	1.46	14	4
1	A	36	THR	N-CA	-6.00	1.39	1.46	20	1
1	A	58	TYR	N-CA	5.97	1.53	1.46	5	1
1	A	92	LYS	CA-CB	-5.89	1.44	1.53	11	1
1	A	25	LEU	N-CA	-5.88	1.38	1.46	4	2
1	A	92	LYS	C-N	-5.74	1.26	1.33	11	1
1	A	115	LYS	N-CA	-5.73	1.39	1.46	16	3
1	A	77	MET	C-N	-5.72	1.25	1.33	3	1
1	A	94	ASP	CA-CB	5.68	1.59	1.54	5	1
1	A	79	VAL	C-N	-5.66	1.26	1.33	15	2
1	A	108	LEU	CA-CB	-5.59	1.44	1.53	14	4
1	A	72	GLU	N-CA	-5.57	1.39	1.46	11	3
1	A	111	VAL	N-CA	-5.56	1.40	1.46	17	1
1	A	28	ARG	CA-C	5.53	1.60	1.53	4	1
1	A	117	ARG	CA-C	-5.52	1.46	1.52	15	3
1	A	57	TYR	CA-C	5.50	1.59	1.52	5	1
1	A	122	LYS	N-CA	-5.49	1.39	1.46	10	4
1	A	98	CYS	N-CA	-5.49	1.39	1.46	18	1
1	A	91	LYS	N-CA	5.46	1.53	1.46	18	1
1	A	92	LYS	N-CA	-5.44	1.39	1.46	2	1
1	A	81	MET	CA-CB	-5.41	1.47	1.53	10	3
1	A	112	ASP	C-N	-5.38	1.26	1.33	16	1
1	A	100	LEU	C-N	5.32	1.40	1.33	5	1
1	A	58	TYR	CA-CB	5.31	1.61	1.53	5	1
1	A	79	VAL	CA-CB	5.30	1.61	1.54	3	1
1	A	65	ALA	CA-C	5.24	1.59	1.52	5	1
1	A	117	ARG	NE-CZ	5.18	1.38	1.33	13	2
1	A	65	ALA	C-N	5.18	1.41	1.33	5	1
1	A	83	ALA	CA-CB	-5.09	1.46	1.53	3	1

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	95	SER	N-CA-C	7.39	126.53	110.80	5	1
1	A	94	ASP	CA-C-N	7.25	135.38	121.54	5	1
1	A	94	ASP	C-N-CA	7.25	135.38	121.54	5	1
1	A	32	PHE	CA-CB-CG	6.67	120.47	113.80	2	1
1	A	94	ASP	CA-C-O	6.56	124.92	120.19	5	1
1	A	96	GLN	CB-CA-C	-6.56	97.36	110.42	5	1
1	A	57	TYR	CB-CA-C	6.46	119.35	109.34	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	112	ASP	CA-CB-CG	6.40	119.00	112.60	13	1
1	A	138	LYS	N-CA-C	-6.34	105.67	113.41	5	1
1	A	91	LYS	N-CA-CB	5.97	120.58	110.49	2	1
1	A	27	ASP	CA-CB-CG	5.96	118.56	112.60	9	4
1	A	91	LYS	N-CA-C	-5.91	105.74	113.12	5	2
1	A	47	ASP	CA-CB-CG	5.89	118.49	112.60	12	1
1	A	26	ILE	CA-C-N	5.88	128.08	120.44	9	2
1	A	26	ILE	C-N-CA	5.88	128.08	120.44	9	2
1	A	110	SER	N-CA-C	-5.85	106.27	113.41	20	1
1	A	57	TYR	CA-CB-CG	5.74	124.24	113.90	5	1
1	A	30	VAL	N-CA-C	5.72	121.24	109.34	4	1
1	A	98	CYS	CA-C-N	5.63	132.29	121.54	5	1
1	A	98	CYS	C-N-CA	5.63	132.29	121.54	5	1
1	A	90	LEU	N-CA-C	5.47	116.92	111.07	10	1
1	A	81	MET	N-CA-CB	-5.43	100.71	110.37	3	1
1	A	89	LYS	N-CA-C	5.41	120.03	113.38	2	1
1	A	24	SER	N-CA-C	-5.35	106.43	113.12	13	2
1	A	116	MET	N-CA-C	5.25	117.63	110.55	1	2
1	A	93	LEU	N-CA-C	-5.25	106.94	113.55	13	1
1	A	28	ARG	N-CA-C	5.22	119.17	109.56	4	1
1	A	115	LYS	N-CA-CB	-5.06	102.54	110.44	19	1
1	A	29	GLY	N-CA-C	-5.05	106.61	113.37	2	1
1	A	89	LYS	CA-C-N	-5.05	111.90	121.54	4	1
1	A	89	LYS	C-N-CA	-5.05	111.90	121.54	4	1

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

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	91	LYS	CA	1
1	A	95	SER	CA	1

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	114	ARG	Sidechain	5
1	A	28	ARG	Sidechain	4
1	A	20	ARG	Sidechain	3
1	A	75	ARG	Sidechain	1

## 6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1062	1094	1094	21±9
All	All	21240	21880	21880	419

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:LEU:HA	1:A:116:MET:SD	0.81	2.16	10	6
1:A:76:PRO:HG2	1:A:81:MET:SD	0.78	2.18	3	1
1:A:55:LEU:HA	1:A:99:GLU:O	0.78	1.79	5	1
1:A:54:ARG:O	1:A:57:TYR:HB3	0.75	1.82	5	2
1:A:22:TYR:HB3	1:A:28:ARG:HA	0.73	1.60	4	1
1:A:79:VAL:HA	1:A:86:ILE:HB	0.73	1.58	3	1
1:A:55:LEU:HD12	1:A:99:GLU:HB2	0.71	1.62	5	1
1:A:57:TYR:CE1	1:A:65:ALA:HA	0.70	2.21	5	1
1:A:91:LYS:HE2	1:A:98:CYS:SG	0.70	2.27	8	1
1:A:91:LYS:HG2	1:A:98:CYS:SG	0.69	2.26	13	1
1:A:87:CYS:HB2	1:A:98:CYS:SG	0.69	2.28	5	1
1:A:14:CYS:SG	1:A:97:ILE:HG21	0.68	2.28	2	1
1:A:57:TYR:CD1	1:A:65:ALA:HA	0.67	2.24	5	1
1:A:79:VAL:CA	1:A:86:ILE:HB	0.67	2.19	3	1
1:A:112:ASP:OD1	1:A:114:ARG:HG2	0.66	1.90	20	3
1:A:58:TYR:HB2	1:A:99:GLU:HA	0.66	1.67	5	1
1:A:26:ILE:HG13	1:A:30:VAL:HG23	0.66	1.66	4	1
1:A:55:LEU:CD1	1:A:99:GLU:HB2	0.65	2.21	5	1
1:A:72:GLU:O	1:A:76:PRO:HD2	0.64	1.91	20	1
1:A:15:LYS:HE3	1:A:84:MET:SD	0.64	2.32	8	1
1:A:116:MET:HG3	1:A:121:LEU:HD11	0.63	1.70	6	3
1:A:87:CYS:HB3	1:A:98:CYS:SG	0.63	2.34	12	1
1:A:144:LEU:O	1:A:148:LEU:HG	0.63	1.94	9	4
1:A:58:TYR:O	1:A:69:ILE:HG13	0.62	1.95	5	1
1:A:79:VAL:C	1:A:81:MET:H	0.62	2.03	3	1
1:A:54:ARG:O	1:A:100:LEU:HA	0.61	1.94	5	1
1:A:22:TYR:O	1:A:25:LEU:HB2	0.61	1.94	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:ILE:HD13	1:A:28:ARG:H	0.61	1.54	4	1
1:A:45:CYS:HA	1:A:48:THR:OG1	0.61	1.95	10	3
1:A:21:PHE:O	1:A:25:LEU:HD23	0.61	1.96	4	20
1:A:48:THR:HG21	1:A:56:CYS:SG	0.60	2.35	2	9
1:A:11:CYS:SG	1:A:14:CYS:HB3	0.60	2.36	6	2
1:A:84:MET:HA	1:A:84:MET:HE2	0.60	1.73	3	1
1:A:58:TYR:CD2	1:A:100:LEU:N	0.60	2.69	5	1
1:A:138:LYS:O	1:A:142:VAL:HG23	0.60	1.97	10	18
1:A:112:ASP:OD2	1:A:114:ARG:HG2	0.60	1.96	17	2
1:A:79:VAL:CB	1:A:86:ILE:HB	0.59	2.27	3	1
1:A:50:GLY:O	1:A:54:ARG:HD3	0.59	1.98	1	1
1:A:56:CYS:SG	1:A:61:ALA:HB3	0.58	2.38	20	4
1:A:13:VAL:HG23	1:A:100:LEU:HD11	0.58	1.75	5	1
1:A:36:THR:O	1:A:40:GLU:HG2	0.58	1.98	20	1
1:A:79:VAL:HB	1:A:86:ILE:HB	0.58	1.76	3	1
1:A:120:GLU:HA	1:A:123:GLN:NE2	0.57	2.13	3	3
1:A:95:SER:HA	1:A:97:ILE:HD12	0.57	1.76	5	1
1:A:26:ILE:CD1	1:A:27:ASP:H	0.57	2.12	4	1
1:A:58:TYR:CE2	1:A:97:ILE:HA	0.56	2.34	5	1
1:A:138:LYS:H	1:A:138:LYS:HD3	0.56	1.60	19	4
1:A:96:GLN:HE21	1:A:96:GLN:HA	0.56	1.60	9	2
1:A:68:LYS:HE3	1:A:68:LYS:HA	0.56	1.77	11	1
1:A:138:LYS:HD3	1:A:138:LYS:H	0.56	1.61	4	7
1:A:25:LEU:HB3	1:A:30:VAL:N	0.55	2.17	4	1
1:A:23:LYS:HZ2	1:A:27:ASP:CG	0.55	2.11	1	1
1:A:78:SER:HB2	1:A:86:ILE:HG13	0.55	1.79	3	1
1:A:117:ARG:O	1:A:121:LEU:HD12	0.55	2.01	13	2
1:A:58:TYR:HD2	1:A:100:LEU:N	0.54	2.00	5	1
1:A:26:ILE:HD11	1:A:30:VAL:H	0.54	1.62	4	1
1:A:91:LYS:HA	1:A:94:ASP:O	0.54	2.03	16	7
1:A:13:VAL:HG12	1:A:55:LEU:HD22	0.54	1.78	19	2
1:A:38:GLU:O	1:A:42:ILE:HG13	0.54	2.02	8	5
1:A:73:VAL:O	1:A:77:MET:HG2	0.54	2.03	19	1
1:A:73:VAL:O	1:A:77:MET:HG3	0.53	2.03	10	6
1:A:14:CYS:HB3	1:A:98:CYS:SG	0.53	2.43	10	1
1:A:86:ILE:O	1:A:89:LYS:HG3	0.53	2.04	2	1
1:A:81:MET:O	1:A:86:ILE:HD11	0.53	2.04	2	9
1:A:58:TYR:HB2	1:A:100:LEU:H	0.53	1.64	5	1
1:A:73:VAL:O	1:A:76:PRO:HG2	0.52	2.03	4	1
1:A:91:LYS:HD2	1:A:98:CYS:SG	0.52	2.43	20	1
1:A:95:SER:HA	1:A:97:ILE:CD1	0.52	2.34	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:ARG:O	1:A:121:LEU:HD13	0.52	2.04	6	2
1:A:11:CYS:SG	1:A:87:CYS:HB3	0.52	2.44	8	2
1:A:112:ASP:OD2	1:A:115:LYS:HG2	0.52	2.03	10	2
1:A:85:LYS:NZ	1:A:85:LYS:HB3	0.52	2.19	18	1
1:A:86:ILE:O	1:A:90:LEU:HG	0.52	2.04	7	1
1:A:49:LYS:N	1:A:49:LYS:HE2	0.52	2.19	9	1
1:A:12:GLU:HG3	1:A:98:CYS:O	0.51	2.05	17	1
1:A:19:ASN:O	1:A:23:LYS:HG3	0.51	2.06	2	3
1:A:78:SER:CB	1:A:86:ILE:HG13	0.51	2.36	3	1
1:A:15:LYS:HB2	1:A:15:LYS:NZ	0.51	2.21	11	1
1:A:55:LEU:HA	1:A:99:GLU:C	0.50	2.31	5	1
1:A:148:LEU:HD22	1:A:151:LYS:NZ	0.50	2.21	8	1
1:A:24:SER:HA	1:A:27:ASP:OD1	0.50	2.05	11	2
1:A:26:ILE:H	1:A:26:ILE:HD12	0.50	1.67	4	1
1:A:81:MET:HB2	1:A:82:PRO:CD	0.50	2.37	3	1
1:A:40:GLU:HA	1:A:43:SER:OG	0.49	2.07	9	6
1:A:18:LEU:HB2	1:A:83:ALA:HB2	0.49	1.84	5	1
1:A:20:ARG:HD3	1:A:44:PHE:CZ	0.49	2.42	12	1
1:A:141:TYR:O	1:A:145:ILE:HG12	0.49	2.08	14	1
1:A:54:ARG:HA	1:A:54:ARG:NE	0.49	2.22	18	2
1:A:11:CYS:HB2	1:A:98:CYS:O	0.49	2.08	19	1
1:A:94:ASP:OD1	1:A:96:GLN:HG2	0.49	2.07	10	2
1:A:15:LYS:HE2	1:A:16:GLU:OE2	0.49	2.08	5	1
1:A:58:TYR:CB	1:A:100:LEU:H	0.49	2.21	5	1
1:A:49:LYS:N	1:A:49:LYS:HD3	0.49	2.22	13	1
1:A:142:VAL:O	1:A:146:GLN:HG3	0.49	2.08	13	11
1:A:27:ASP:OD1	1:A:28:ARG:HG3	0.49	2.07	4	1
1:A:11:CYS:SG	1:A:91:LYS:HE2	0.49	2.48	1	1
1:A:54:ARG:NE	1:A:54:ARG:HA	0.49	2.23	15	1
1:A:11:CYS:O	1:A:15:LYS:HG2	0.49	2.08	6	1
1:A:138:LYS:HD2	1:A:138:LYS:H	0.48	1.66	5	1
1:A:24:SER:HA	1:A:27:ASP:OD2	0.48	2.07	7	1
1:A:48:THR:HB	1:A:52:GLU:HB2	0.48	1.85	10	1
1:A:120:GLU:O	1:A:123:GLN:HG2	0.48	2.08	10	1
1:A:58:TYR:HB2	1:A:99:GLU:CA	0.48	2.36	5	1
1:A:59:LEU:O	1:A:69:ILE:HB	0.48	2.08	9	1
1:A:26:ILE:CD1	1:A:30:VAL:H	0.48	2.21	4	1
1:A:35:ASP:O	1:A:39:LYS:HG3	0.48	2.09	15	1
1:A:90:LEU:HB2	1:A:93:LEU:HG	0.48	1.86	4	1
1:A:21:PHE:CE2	1:A:41:LEU:HG	0.48	2.43	8	1
1:A:21:PHE:CE1	1:A:41:LEU:HG	0.48	2.43	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:GLN:O	1:A:100:LEU:HG	0.48	2.09	17	1
1:A:22:TYR:OH	1:A:77:MET:HG2	0.47	2.09	20	3
1:A:137:GLU:O	1:A:140:ASP:HB3	0.47	2.09	1	3
1:A:81:MET:CB	1:A:82:PRO:CD	0.47	2.92	3	1
1:A:81:MET:HB2	1:A:82:PRO:HD3	0.47	1.84	3	1
1:A:121:LEU:HD12	1:A:121:LEU:H	0.47	1.70	16	4
1:A:86:ILE:O	1:A:89:LYS:HG2	0.47	2.09	15	4
1:A:55:LEU:HD12	1:A:99:GLU:CB	0.47	2.38	5	1
1:A:116:MET:SD	1:A:121:LEU:HD11	0.47	2.50	5	3
1:A:137:GLU:H	1:A:137:GLU:CD	0.47	2.18	16	1
1:A:43:SER:HA	1:A:46:LEU:HG	0.47	1.87	9	1
1:A:94:ASP:OD2	1:A:96:GLN:HG2	0.47	2.10	9	1
1:A:116:MET:SD	1:A:121:LEU:HG	0.47	2.49	13	1
1:A:49:LYS:HD3	1:A:49:LYS:N	0.47	2.24	11	1
1:A:76:PRO:HB2	1:A:79:VAL:HG12	0.46	1.87	3	1
1:A:58:TYR:CB	1:A:99:GLU:HA	0.46	2.37	5	1
1:A:58:TYR:O	1:A:69:ILE:HG12	0.46	2.09	13	1
1:A:38:GLU:O	1:A:42:ILE:HD13	0.46	2.11	13	3
1:A:12:GLU:O	1:A:15:LYS:HG2	0.46	2.10	4	1
1:A:78:SER:C	1:A:86:ILE:HG13	0.46	2.36	3	1
1:A:97:ILE:HG22	1:A:98:CYS:N	0.46	2.26	5	1
1:A:84:MET:O	1:A:88:GLU:HG2	0.46	2.11	10	2
1:A:94:ASP:OD2	1:A:97:ILE:HG13	0.46	2.10	19	1
1:A:23:LYS:HD2	1:A:27:ASP:O	0.46	2.11	4	1
1:A:87:CYS:O	1:A:91:LYS:HG3	0.46	2.10	19	1
1:A:121:LEU:HD11	1:A:138:LYS:HB2	0.45	1.89	2	1
1:A:144:LEU:O	1:A:147:GLU:HG3	0.45	2.11	11	1
1:A:145:ILE:HG22	1:A:146:GLN:OE1	0.45	2.11	12	1
1:A:147:GLU:O	1:A:151:LYS:HE2	0.45	2.12	15	3
1:A:122:LYS:HG2	1:A:141:TYR:OH	0.45	2.11	6	2
1:A:28:ARG:O	1:A:28:ARG:HD2	0.45	2.11	20	1
1:A:54:ARG:C	1:A:100:LEU:HA	0.45	2.37	5	1
1:A:68:LYS:HB2	1:A:72:GLU:OE2	0.45	2.11	16	1
1:A:116:MET:HB2	1:A:121:LEU:HD11	0.45	1.89	16	1
1:A:85:LYS:HA	1:A:88:GLU:HG3	0.45	1.89	3	1
1:A:117:ARG:HG2	1:A:120:GLU:OE2	0.45	2.12	4	1
1:A:19:ASN:O	1:A:23:LYS:HG2	0.45	2.11	9	1
1:A:138:LYS:H	1:A:138:LYS:HD2	0.45	1.71	2	2
1:A:118:VAL:HG12	1:A:138:LYS:N	0.45	2.26	8	2
1:A:118:VAL:O	1:A:122:LYS:HG3	0.45	2.11	6	3
1:A:79:VAL:C	1:A:81:MET:N	0.45	2.75	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:LYS:NZ	1:A:68:LYS:HB2	0.45	2.26	12	1
1:A:125:LEU:HA	1:A:130:GLU:OE1	0.45	2.11	17	1
1:A:116:MET:HA	1:A:120:GLU:OE2	0.45	2.12	4	1
1:A:68:LYS:HB3	1:A:70:LEU:CD2	0.45	2.42	8	1
1:A:108:LEU:HA	1:A:111:VAL:CG1	0.45	2.41	14	3
1:A:68:LYS:HB2	1:A:68:LYS:NZ	0.45	2.27	14	1
1:A:37:ILE:HB	1:A:74:THR:CG2	0.44	2.42	3	1
1:A:81:MET:HG3	1:A:82:PRO:HD2	0.44	1.90	3	1
1:A:96:GLN:HE21	1:A:96:GLN:CA	0.44	2.24	9	1
1:A:119:ALA:O	1:A:123:GLN:HG2	0.44	2.11	14	1
1:A:57:TYR:HA	1:A:62:THR:OG1	0.44	2.12	13	5
1:A:21:PHE:CZ	1:A:25:LEU:HD21	0.44	2.48	14	1
1:A:115:LYS:NZ	1:A:116:MET:HG2	0.44	2.27	4	1
1:A:14:CYS:HA	1:A:55:LEU:HD11	0.44	1.88	5	1
1:A:47:ASP:O	1:A:49:LYS:HE3	0.44	2.13	14	2
1:A:96:GLN:HA	1:A:99:GLU:OE2	0.44	2.13	9	1
1:A:148:LEU:O	1:A:151:LYS:HB2	0.44	2.13	16	2
1:A:84:MET:HE2	1:A:84:MET:HA	0.44	1.88	18	1
1:A:58:TYR:HB2	1:A:100:LEU:N	0.44	2.26	5	1
1:A:30:VAL:HG11	1:A:40:GLU:HG3	0.44	1.89	20	1
1:A:112:ASP:OD1	1:A:114:ARG:HG3	0.44	2.13	8	2
1:A:22:TYR:OH	1:A:82:PRO:HB2	0.44	2.13	3	1
1:A:23:LYS:HB3	1:A:23:LYS:NZ	0.44	2.28	13	1
1:A:34:LEU:O	1:A:38:GLU:HB2	0.44	2.13	13	1
1:A:52:GLU:H	1:A:52:GLU:CD	0.44	2.21	16	1
1:A:14:CYS:SG	1:A:55:LEU:HD11	0.44	2.53	4	2
1:A:125:LEU:HD12	1:A:125:LEU:C	0.44	2.38	6	3
1:A:121:LEU:HD12	1:A:121:LEU:N	0.44	2.27	16	3
1:A:137:GLU:O	1:A:141:TYR:HD1	0.43	1.96	1	2
1:A:13:VAL:HB	1:A:98:CYS:O	0.43	2.14	5	1
1:A:148:LEU:HD22	1:A:151:LYS:HZ3	0.43	1.73	8	1
1:A:16:GLU:OE1	1:A:20:ARG:HD3	0.43	2.13	10	1
1:A:34:LEU:CD2	1:A:75:ARG:HA	0.43	2.43	12	2
1:A:14:CYS:HB2	1:A:97:ILE:O	0.43	2.13	8	1
1:A:79:VAL:HG22	1:A:80:HIS:H	0.43	1.74	3	1
1:A:91:LYS:HG2	1:A:96:GLN:CB	0.43	2.44	5	1
1:A:89:LYS:O	1:A:92:LYS:HG2	0.43	2.13	17	1
1:A:72:GLU:OE1	1:A:75:ARG:HD2	0.43	2.14	14	1
1:A:73:VAL:HG22	1:A:93:LEU:HD22	0.43	1.91	4	1
1:A:94:ASP:OD1	1:A:97:ILE:HG13	0.43	2.13	7	1
1:A:12:GLU:CD	1:A:51:LYS:HZ2	0.43	2.21	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:TYR:OH	1:A:78:SER:HA	0.43	2.14	3	1
1:A:88:GLU:O	1:A:92:LYS:HG2	0.43	2.13	9	1
1:A:125:LEU:HB2	1:A:130:GLU:CD	0.43	2.39	10	1
1:A:17:PHE:CE1	1:A:48:THR:HG21	0.43	2.47	14	1
1:A:125:LEU:HD13	1:A:130:GLU:OE2	0.43	2.14	5	1
1:A:68:LYS:HA	1:A:68:LYS:CE	0.43	2.44	8	1
1:A:142:VAL:HG12	1:A:146:GLN:NE2	0.43	2.29	16	2
1:A:63:LYS:HZ3	1:A:64:ASP:CG	0.42	2.22	3	1
1:A:20:ARG:HD3	1:A:44:PHE:CE2	0.42	2.49	12	1
1:A:37:ILE:HB	1:A:74:THR:HG23	0.42	1.90	17	1
1:A:26:ILE:CD1	1:A:28:ARG:H	0.42	2.25	4	1
1:A:63:LYS:HD3	1:A:63:LYS:H	0.42	1.74	9	1
1:A:13:VAL:HG21	1:A:100:LEU:HB2	0.42	1.91	15	1
1:A:106:LEU:N	1:A:153:ALA:HB1	0.42	2.29	1	1
1:A:60:GLY:O	1:A:68:LYS:HG3	0.42	2.14	4	1
1:A:17:PHE:CE2	1:A:48:THR:HG21	0.42	2.48	10	1
1:A:76:PRO:O	1:A:78:SER:N	0.42	2.52	3	1
1:A:23:LYS:O	1:A:27:ASP:HB2	0.42	2.14	13	2
1:A:125:LEU:C	1:A:125:LEU:HD12	0.42	2.40	18	1
1:A:48:THR:HB	1:A:52:GLU:C	0.42	2.39	5	1
1:A:78:SER:HB3	1:A:85:LYS:H	0.42	1.74	3	1
1:A:147:GLU:OE1	1:A:148:LEU:HD23	0.42	2.15	14	1
1:A:88:GLU:CD	1:A:88:GLU:H	0.42	2.23	18	1
1:A:15:LYS:O	1:A:19:ASN:HB2	0.41	2.15	2	1
1:A:91:LYS:HD3	1:A:91:LYS:O	0.41	2.15	2	1
1:A:75:ARG:N	1:A:75:ARG:HD2	0.41	2.30	13	1
1:A:45:CYS:HA	1:A:48:THR:HG23	0.41	1.92	4	1
1:A:116:MET:O	1:A:138:LYS:HG3	0.41	2.15	7	1
1:A:14:CYS:SG	1:A:97:ILE:HD13	0.41	2.55	2	1
1:A:86:ILE:C	1:A:88:GLU:H	0.41	2.23	4	1
1:A:138:LYS:N	1:A:138:LYS:HD2	0.41	2.31	8	1
1:A:69:ILE:CG2	1:A:72:GLU:HB2	0.41	2.45	9	1
1:A:11:CYS:SG	1:A:91:LYS:HG2	0.41	2.55	18	1
1:A:68:LYS:O	1:A:69:ILE:HG12	0.41	2.15	5	1
1:A:21:PHE:HB2	1:A:44:PHE:CE2	0.41	2.51	14	1
1:A:22:TYR:HH	1:A:78:SER:HA	0.41	1.75	3	1
1:A:70:LEU:HG	1:A:71:SER:H	0.41	1.76	15	1
1:A:16:GLU:CD	1:A:16:GLU:H	0.41	2.24	5	1
1:A:54:ARG:HG2	1:A:100:LEU:HD21	0.41	1.92	8	1
1:A:118:VAL:HA	1:A:121:LEU:HD13	0.41	1.93	10	1
1:A:42:ILE:HA	1:A:61:ALA:HB1	0.41	1.91	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ASP:O	1:A:49:LYS:HG3	0.41	2.16	6	1
1:A:151:LYS:HD2	1:A:151:LYS:O	0.41	2.16	13	1
1:A:24:SER:O	1:A:28:ARG:HG2	0.41	2.15	15	1
1:A:51:LYS:HD2	1:A:100:LEU:O	0.41	2.16	20	1
1:A:79:VAL:N	1:A:86:ILE:HD12	0.41	2.31	3	1
1:A:52:GLU:CD	1:A:52:GLU:H	0.41	2.24	9	1
1:A:138:LYS:HD3	1:A:138:LYS:N	0.40	2.31	1	1
1:A:56:CYS:HB2	1:A:62:THR:HG23	0.40	1.93	9	1
1:A:89:LYS:NZ	1:A:89:LYS:HB2	0.40	2.31	9	1
1:A:125:LEU:HB2	1:A:130:GLU:CG	0.40	2.45	10	1
1:A:128:TRP:HB3	1:A:152:TYR:CE2	0.40	2.51	18	1
1:A:51:LYS:O	1:A:54:ARG:HB2	0.40	2.16	19	1
1:A:21:PHE:CD2	1:A:44:PHE:CD1	0.40	3.09	4	1
1:A:72:GLU:OE2	1:A:72:GLU:HA	0.40	2.16	7	1
1:A:14:CYS:O	1:A:15:LYS:HG3	0.40	2.16	11	1
1:A:68:LYS:HG3	1:A:68:LYS:O	0.40	2.15	17	1
1:A:70:LEU:HD12	1:A:71:SER:N	0.40	2.31	18	1
1:A:122:LYS:O	1:A:125:LEU:HG	0.40	2.16	18	1
1:A:87:CYS:O	1:A:94:ASP:HB3	0.40	2.16	4	1
1:A:148:LEU:HA	1:A:151:LYS:HE2	0.40	1.93	9	1
1:A:71:SER:HA	1:A:75:ARG:CG	0.40	2.46	11	1
1:A:42:ILE:CD1	1:A:61:ALA:HA	0.40	2.46	10	1

## 6.3 Torsion angles [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	132/161 (82%)	117±5 (89±4%)	12±4 (9±3%)	3±2 (3±2%)	6	42
All	All	2640/3220 (82%)	2338 (89%)	234 (9%)	68 (3%)	6	42

All 28 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	69	ILE	9
1	A	15	LYS	7
1	A	68	LYS	6
1	A	73	VAL	6
1	A	108	LEU	5
1	A	67	THR	3
1	A	99	GLU	3
1	A	82	PRO	3
1	A	50	GLY	2
1	A	13	VAL	2
1	A	70	LEU	2
1	A	72	GLU	2
1	A	100	LEU	2
1	A	129	GLY	2
1	A	153	ALA	1
1	A	90	LEU	1
1	A	77	MET	1
1	A	79	VAL	1
1	A	81	MET	1
1	A	25	LEU	1
1	A	30	VAL	1
1	A	14	CYS	1
1	A	65	ALA	1
1	A	95	SER	1
1	A	96	GLN	1
1	A	97	ILE	1
1	A	51	LYS	1
1	A	83	ALA	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	120/141 (85%)	109±3 (91±3%)	11±3 (9±3%)	10	56
All	All	2400/2820 (85%)	2175 (91%)	225 (9%)	10	56

All 59 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	138	LYS	20
1	A	113	LEU	18
1	A	41	LEU	13
1	A	68	LYS	10
1	A	117	ARG	10
1	A	49	LYS	9
1	A	33	SER	8
1	A	67	THR	8
1	A	54	ARG	8
1	A	63	LYS	7
1	A	137	GLU	7
1	A	118	VAL	6
1	A	125	LEU	6
1	A	91	LYS	6
1	A	99	GLU	5
1	A	22	TYR	4
1	A	27	ASP	4
1	A	23	LYS	4
1	A	85	LYS	4
1	A	12	GLU	3
1	A	62	THR	3
1	A	107	ASP	3
1	A	84	MET	3
1	A	96	GLN	3
1	A	38	GLU	3
1	A	39	LYS	3
1	A	115	LYS	3
1	A	151	LYS	3
1	A	15	LYS	3
1	A	52	GLU	2
1	A	89	LYS	2
1	A	35	ASP	2
1	A	40	GLU	2
1	A	72	GLU	2
1	A	34	LEU	2
1	A	147	GLU	2
1	A	92	LYS	2
1	A	69	ILE	1
1	A	76	PRO	1
1	A	77	MET	1
1	A	86	ILE	1
1	A	121	LEU	1
1	A	26	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	28	ARG	1
1	A	30	VAL	1
1	A	32	PHE	1
1	A	94	ASP	1
1	A	97	ILE	1
1	A	130	GLU	1
1	A	57	TYR	1
1	A	140	ASP	1
1	A	100	LEU	1
1	A	123	GLN	1
1	A	114	ARG	1
1	A	70	LEU	1
1	A	90	LEU	1
1	A	143	ASN	1
1	A	111	VAL	1
1	A	47	ASP	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	4-A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
4	A	30:VAL	C	31:ASN	N	1.19

## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 91% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list*

#### 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	2014
Number of shifts mapped to atoms	2014
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	159	$-0.24 \pm 0.09$	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	152	$0.38 \pm 0.05$	None needed (< 0.5 ppm)
$^{13}\text{C}'$	136	$-0.19 \pm 0.05$	None needed (< 0.5 ppm)
$^{15}\text{N}$	139	$0.82 \pm 0.32$	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 92%, i.e. 1712 atoms were assigned a chemical shift out of a possible 1867. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	617/658 (94%)	254/265 (96%)	246/264 (93%)	117/129 (91%)
Sidechain	1003/1098 (91%)	683/713 (96%)	312/345 (90%)	8/40 (20%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	92/111 (83%)	46/54 (85%)	45/54 (83%)	1/3 (33%)
Overall	1712/1867 (92%)	983/1032 (95%)	603/663 (91%)	126/172 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 2014 atoms were assigned a chemical shift out of a possible 2225. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	742/802 (93%)	308/324 (95%)	295/322 (92%)	139/156 (89%)
Sidechain	1170/1296 (90%)	797/839 (95%)	364/407 (89%)	9/50 (18%)
Aromatic	102/127 (80%)	51/62 (82%)	50/61 (82%)	1/4 (25%)
Overall	2014/2225 (91%)	1156/1225 (94%)	709/790 (90%)	149/210 (71%)

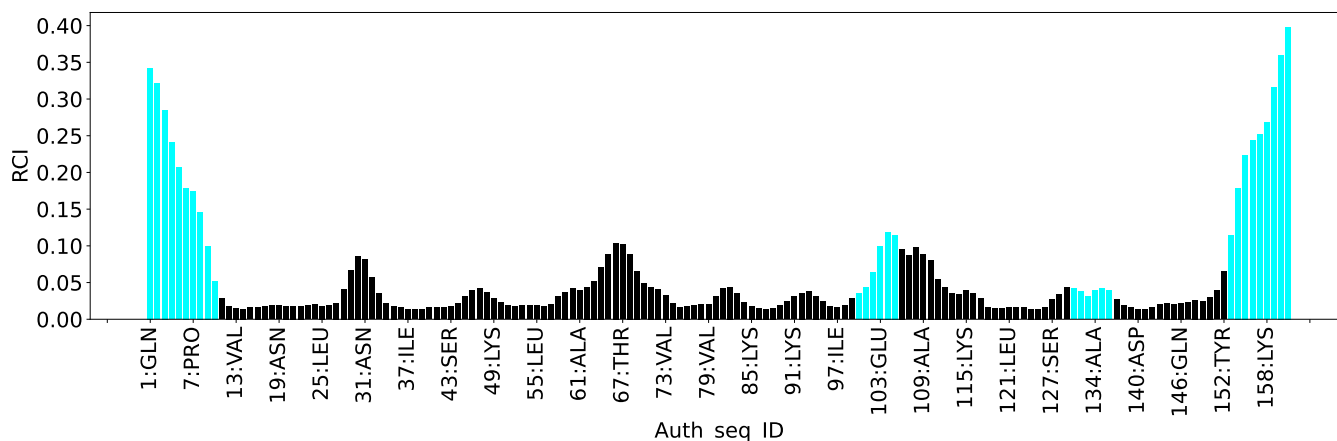
#### 7.1.4 Statistically unusual chemical shifts [i](#)

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	2017
Intra-residue ( $ i-j =0$ )	746
Sequential ( $ i-j =1$ )	551
Medium range ( $ i-j >1$ and $ i-j <5$ )	387
Long range ( $ i-j \geq 5$ )	333
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	160
Number of unmapped restraints	0
Number of restraints per residue	13.5
Number of long range restraints per residue <sup>1</sup>	2.1

<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)	65.5	0.2
0.2-0.5 (Medium)	113.8	0.5
>0.5 (Large)	164.7	5.75

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	4.4	9.96
10.0-20.0 (Medium)	1.2	18.86
>20.0 (Large)	0.1	30.82

## 9 Distance violation analysis

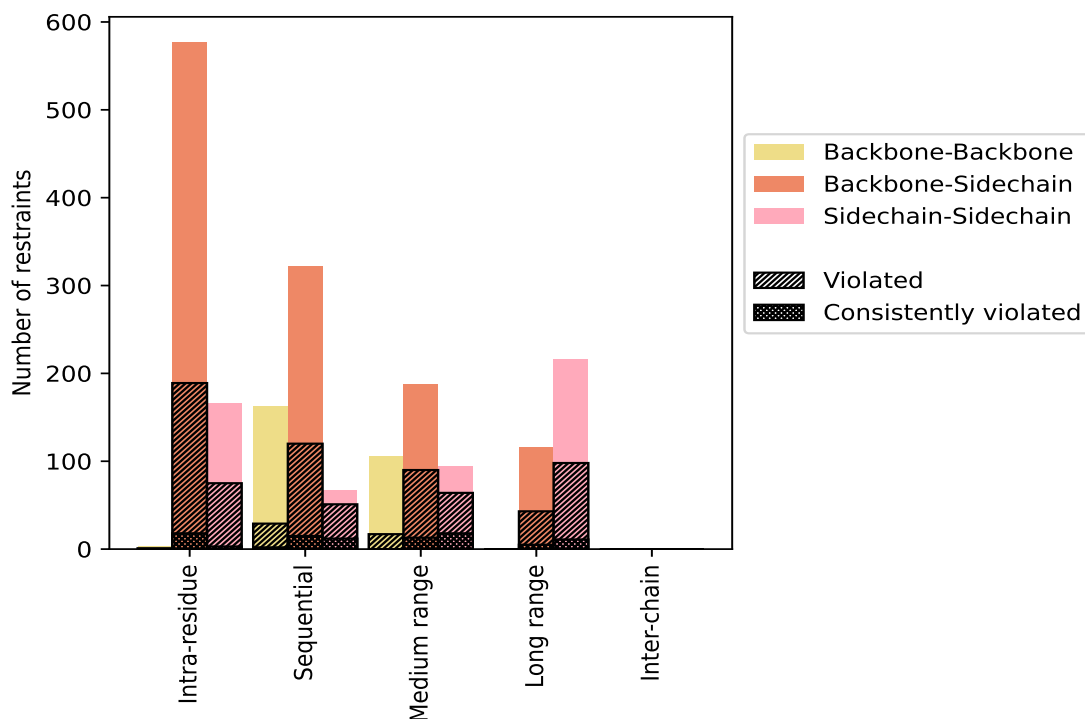
### 9.1 Summary of distance violations

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>746</b>	<b>37.0</b>	<b>265</b>	<b>35.5</b>	<b>13.1</b>	<b>21</b>	<b>2.8</b>	<b>1.0</b>
Backbone-Backbone	3	0.1	1	33.3	0.0	0	0.0	0.0
Backbone-Sidechain	577	28.6	189	32.8	9.4	18	3.1	0.9
Sidechain-Sidechain	166	8.2	75	45.2	3.7	3	1.8	0.1
<b>Sequential (<math> i-j =1</math>)</b>	<b>551</b>	<b>27.3</b>	<b>200</b>	<b>36.3</b>	<b>9.9</b>	<b>29</b>	<b>5.3</b>	<b>1.4</b>
Backbone-Backbone	162	8.0	29	17.9	1.4	2	1.2	0.1
Backbone-Sidechain	322	16.0	120	37.3	5.9	15	4.7	0.7
Sidechain-Sidechain	67	3.3	51	76.1	2.5	12	17.9	0.6
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>387</b>	<b>19.2</b>	<b>171</b>	<b>44.2</b>	<b>8.5</b>	<b>31</b>	<b>8.0</b>	<b>1.5</b>
Backbone-Backbone	105	5.2	17	16.2	0.8	0	0.0	0.0
Backbone-Sidechain	188	9.3	90	47.9	4.5	13	6.9	0.6
Sidechain-Sidechain	94	4.7	64	68.1	3.2	18	19.1	0.9
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>333</b>	<b>16.5</b>	<b>141</b>	<b>42.3</b>	<b>7.0</b>	<b>16</b>	<b>4.8</b>	<b>0.8</b>
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	116	5.8	43	37.1	2.1	5	4.3	0.2
Sidechain-Sidechain	216	10.7	98	45.4	4.9	11	5.1	0.5
<b>Inter-chain</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>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
<b>Hydrogen 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>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>2017</b>	<b>100.0</b>	<b>777</b>	<b>38.5</b>	<b>38.5</b>	<b>97</b>	<b>4.8</b>	<b>4.8</b>
Backbone-Backbone	271	13.4	47	17.3	2.3	2	0.7	0.1
Backbone-Sidechain	1203	59.6	442	36.7	21.9	51	4.2	2.5
Sidechain-Sidechain	543	26.9	288	53.0	14.3	44	8.1	2.2

<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	102	104	89	57	0	352	0.7	3.18	0.62	0.47
2	100	98	89	56	0	343	0.69	3.23	0.61	0.48
3	109	98	93	74	0	374	0.77	5.75	0.79	0.47
4	109	103	102	62	0	376	0.68	4.67	0.65	0.44
5	107	104	99	62	0	372	0.72	5.04	0.65	0.46
6	102	104	78	54	0	338	0.65	3.05	0.54	0.48
7	111	95	86	56	0	348	0.68	3.33	0.6	0.48
8	102	90	81	53	0	326	0.68	3.2	0.56	0.48
9	106	97	88	60	0	351	0.71	3.28	0.59	0.53
10	116	101	92	51	0	360	0.67	3.56	0.62	0.45

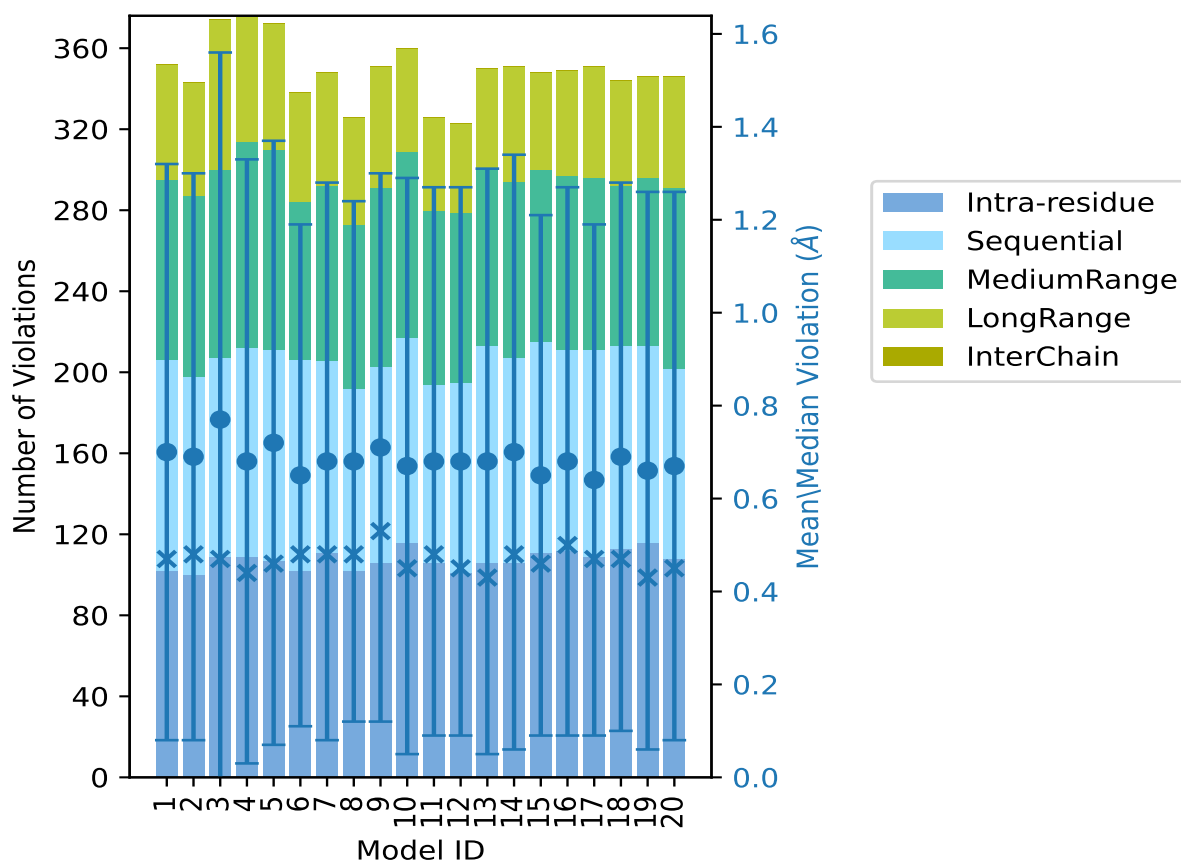
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>					
11	106	88	86	46	0	326	0.68	3.09	0.59	0.48
12	101	94	84	44	0	323	0.68	3.18	0.59	0.45
13	106	107	88	49	0	350	0.68	3.56	0.63	0.43
14	106	101	87	57	0	351	0.7	3.67	0.64	0.48
15	111	104	85	48	0	348	0.65	3.11	0.56	0.46
16	112	99	86	52	0	349	0.68	3.17	0.59	0.5
17	109	102	85	55	0	351	0.64	3.42	0.55	0.47
18	113	100	79	52	0	344	0.69	3.0	0.59	0.47
19	116	97	83	50	0	346	0.66	3.35	0.6	0.43
20	108	94	89	55	0	346	0.67	3.63	0.59	0.45

<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

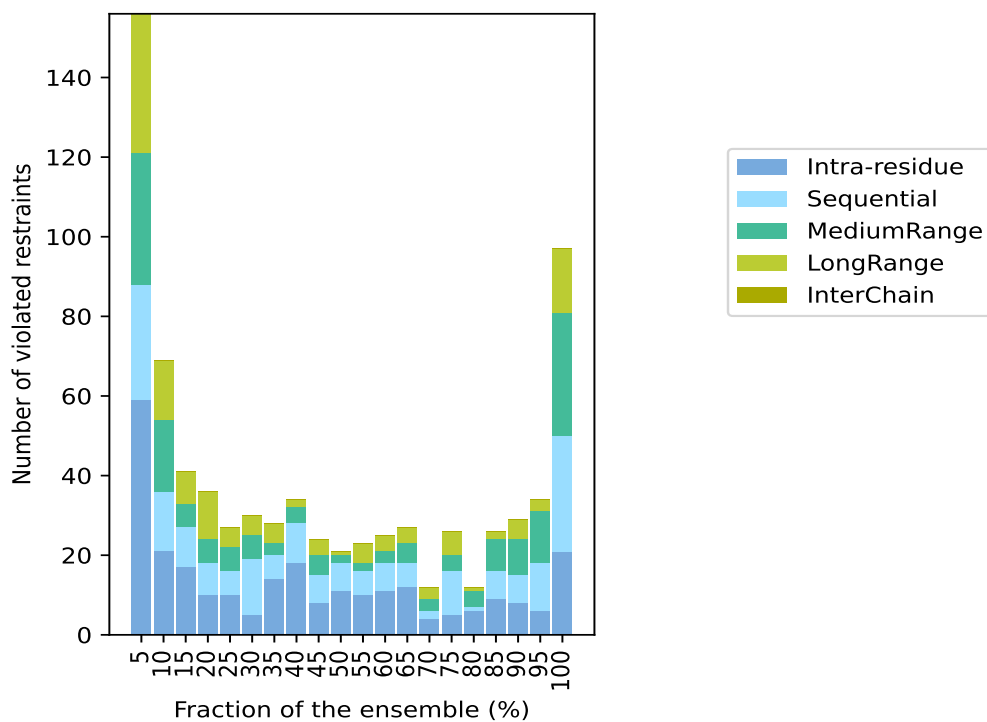
### 9.3 Distance violation statistics for the ensemble

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, 1240(IR:481, SQ:351, MR:216, LR:192, IC:0) 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>	%
59	29	33	35	0	156	1	5.0
21	15	18	15	0	69	2	10.0
17	10	6	8	0	41	3	15.0
10	8	6	12	0	36	4	20.0
10	6	6	5	0	27	5	25.0
5	14	6	5	0	30	6	30.0
14	6	3	5	0	28	7	35.0
18	10	4	2	0	34	8	40.0
8	7	5	4	0	24	9	45.0
11	7	2	1	0	21	10	50.0
10	6	2	5	0	23	11	55.0
11	7	3	4	0	25	12	60.0
12	6	5	4	0	27	13	65.0
4	2	3	3	0	12	14	70.0
5	11	4	6	0	26	15	75.0
6	1	4	1	0	12	16	80.0
9	7	8	2	0	26	17	85.0
8	7	9	5	0	29	18	90.0
6	12	13	3	0	34	19	95.0
21	29	31	16	0	97	20	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

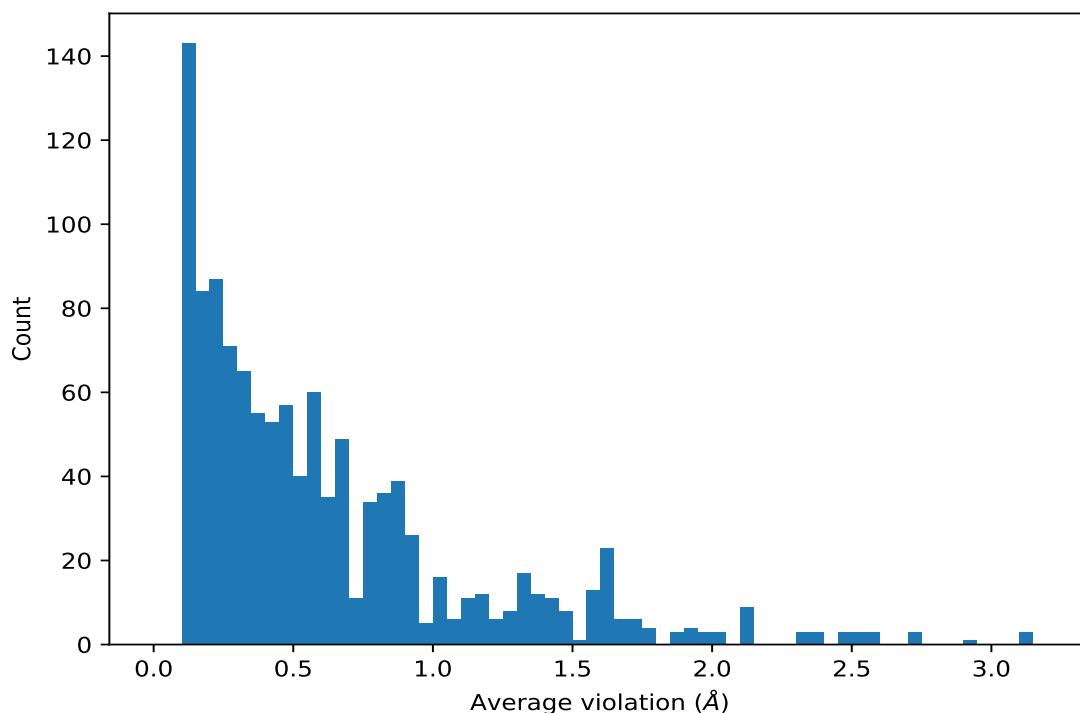
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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)
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	20	3.11	0.29	3.14
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	20	3.11	0.29	3.14
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	20	3.11	0.29	3.14
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	20	2.73	0.54	2.9
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	20	2.73	0.54	2.9
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	20	2.73	0.54	2.9
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	20	2.57	0.86	2.87
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	20	2.57	0.86	2.87
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	20	2.57	0.86	2.87
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	20	2.55	0.25	2.51
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	20	2.55	0.25	2.51
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	20	2.55	0.25	2.51
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	20	2.47	0.4	2.5
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	20	2.47	0.4	2.5
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	20	2.47	0.4	2.5
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	20	2.39	0.38	2.5

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	20	2.39	0.38	2.5
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	20	2.39	0.38	2.5
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	20	2.32	0.33	2.34
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	20	2.32	0.33	2.34
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	20	2.32	0.33	2.34
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	20	2.14	0.36	2.17
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	20	2.14	0.36	2.17
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	20	2.14	0.36	2.17
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	20	1.97	0.36	2.02
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	20	1.97	0.36	2.02
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	20	1.97	0.36	2.02
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	20	1.95	0.41	1.96
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	20	1.91	0.89	1.8
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	20	1.91	0.89	1.8
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	20	1.91	0.89	1.8
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	20	1.89	0.32	1.95
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	20	1.89	0.32	1.95
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	20	1.89	0.32	1.95
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	20	1.74	0.32	1.74
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	20	1.74	0.32	1.74
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	20	1.74	0.32	1.74
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	20	1.7	0.24	1.62
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	20	1.7	0.24	1.62
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	20	1.7	0.24	1.62
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	20	1.66	0.29	1.64
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	20	1.66	0.29	1.64
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	20	1.66	0.29	1.64
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	20	1.63	0.43	1.61
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	20	1.63	0.43	1.61
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	20	1.63	0.43	1.61
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	20	1.61	0.76	2.08
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	20	1.61	0.76	2.08
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	20	1.61	0.76	2.08
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	20	1.61	0.76	2.08
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	20	1.61	0.76	2.08
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	20	1.61	0.76	2.08
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	20	1.6	0.65	1.68
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	20	1.6	0.65	1.68
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	20	1.6	0.65	1.68
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	20	1.6	0.65	1.68
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	20	1.6	0.65	1.68
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	20	1.6	0.65	1.68

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	20	1.6	0.68	1.68
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	20	1.6	0.68	1.68
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	20	1.6	0.68	1.68
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	20	1.56	0.52	1.46
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	20	1.56	0.52	1.46
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	20	1.56	0.52	1.46
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	20	1.56	0.05	1.58
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	20	1.56	0.05	1.58
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	20	1.56	0.05	1.58
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	20	1.55	0.7	1.75
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	20	1.55	0.7	1.75
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	20	1.55	0.7	1.75
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	20	1.55	0.72	1.46
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	20	1.55	0.72	1.46
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	20	1.55	0.72	1.46
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	20	1.52	0.26	1.53
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	20	1.49	0.39	1.66
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	20	1.49	0.39	1.66
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	20	1.49	0.39	1.66
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	20	1.49	0.37	1.59
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	20	1.48	0.18	1.54
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	20	1.46	0.19	1.52
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	20	1.46	0.19	1.52
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	20	1.46	0.19	1.52
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	20	1.44	0.21	1.48
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	20	1.44	0.21	1.48
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	20	1.44	0.21	1.48
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	20	1.41	0.03	1.42
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	20	1.41	0.03	1.42
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	20	1.41	0.03	1.42
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	20	1.37	0.04	1.38
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	20	1.37	0.04	1.38
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	20	1.37	0.04	1.38
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	20	1.36	0.1	1.37
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	20	1.36	0.1	1.37
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	20	1.36	0.1	1.37
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	20	1.32	0.08	1.3
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	20	1.32	0.08	1.3
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	20	1.32	0.08	1.3
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	20	1.32	0.19	1.38
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	20	1.32	0.19	1.38
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	20	1.32	0.19	1.38

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	20	1.32	0.13	1.34
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	20	1.32	0.13	1.34
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	20	1.32	0.13	1.34
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	20	1.32	0.13	1.34
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	20	1.32	0.13	1.34
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	20	1.32	0.13	1.34
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	20	1.3	0.14	1.28
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	20	1.3	0.14	1.28
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	20	1.3	0.14	1.28
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	20	1.27	0.27	1.32
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	20	1.27	0.06	1.27
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	20	1.27	0.06	1.27
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	20	1.27	0.06	1.27
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	20	1.25	0.11	1.29
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	20	1.25	0.11	1.29
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	20	1.25	0.11	1.29
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	20	1.24	0.23	1.3
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	20	1.24	0.23	1.3
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	20	1.24	0.23	1.3
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	20	1.24	0.2	1.18
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	20	1.18	0.31	1.11
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	20	1.18	0.31	1.11
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	20	1.18	0.31	1.11
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	20	1.17	0.43	1.27
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	20	1.17	0.43	1.27
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	20	1.17	0.43	1.27
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	20	1.16	0.27	1.09
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	20	1.15	0.21	1.22
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	20	1.15	0.21	1.22
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	20	1.15	0.21	1.22
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	20	1.1	0.09	1.12
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	20	1.1	0.09	1.12
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	20	1.1	0.09	1.12
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	20	1.03	0.65	0.94
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	20	1.03	0.65	0.94
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	20	1.03	0.65	0.94
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	20	1.02	0.12	1.02
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	20	0.98	0.17	0.99
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	20	0.95	0.02	0.94
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	20	0.94	0.33	1.02
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	20	0.94	0.33	1.02
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	20	0.94	0.33	1.02

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	20	0.94	0.33	1.02
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	20	0.94	0.33	1.02
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	20	0.94	0.33	1.02
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	20	0.94	0.33	1.02
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	20	0.94	0.33	1.02
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	20	0.94	0.33	1.02
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	20	0.93	0.39	0.94
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	20	0.92	0.1	0.92
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	20	0.92	0.1	0.92
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	20	0.88	0.44	1.01
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	20	0.88	0.44	1.01
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	20	0.88	0.44	1.01
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	20	0.86	0.14	0.87
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	20	0.86	0.14	0.87
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	20	0.86	0.14	0.87
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	20	0.83	0.01	0.84
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	20	0.83	0.01	0.84
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	20	0.83	0.01	0.84
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	20	0.83	0.4	0.82
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	20	0.82	0.1	0.78
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	20	0.82	0.1	0.78
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	20	0.77	0.07	0.76
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	20	0.77	0.07	0.76
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	20	0.77	0.07	0.76
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	20	0.77	0.03	0.78
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	20	0.77	0.03	0.78
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	20	0.77	0.03	0.78
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	20	0.75	0.09	0.7
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	20	0.73	0.14	0.72
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	20	0.73	0.14	0.72
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	20	0.73	0.14	0.72
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	20	0.7	0.18	0.7
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	20	0.7	0.18	0.7
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	20	0.7	0.29	0.7
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	20	0.7	0.29	0.7
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	20	0.68	0.26	0.64
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	20	0.68	0.26	0.64
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	20	0.68	0.26	0.64
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	20	0.68	0.26	0.65
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	20	0.68	0.19	0.66
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	20	0.68	0.19	0.66
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	20	0.68	0.19	0.66

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	20	0.67	0.35	0.62
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	20	0.67	0.35	0.62
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	20	0.67	0.35	0.62
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	20	0.65	0.1	0.68
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	20	0.65	0.1	0.68
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	20	0.65	0.1	0.68
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	20	0.64	0.15	0.68
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	20	0.64	0.15	0.68
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	20	0.64	0.15	0.68
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	20	0.64	0.15	0.68
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	20	0.64	0.15	0.68
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	20	0.64	0.15	0.68
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	20	0.64	0.15	0.68
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	20	0.64	0.15	0.68
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	20	0.64	0.15	0.68
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	20	0.57	0.28	0.55
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	20	0.57	0.28	0.55
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	20	0.57	0.28	0.55
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	20	0.57	0.28	0.55
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	20	0.57	0.28	0.55
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	20	0.57	0.28	0.55
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	20	0.57	0.28	0.55
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	20	0.57	0.28	0.55
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	20	0.57	0.28	0.55
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	20	0.54	0.09	0.55
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	20	0.54	0.09	0.55
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	20	0.54	0.09	0.55
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	20	0.47	0.03	0.48
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	20	0.47	0.26	0.52
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	20	0.47	0.31	0.38
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	20	0.47	0.31	0.38
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	20	0.47	0.31	0.38
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	20	0.47	0.15	0.42
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	20	0.44	0.12	0.42
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	20	0.44	0.12	0.42
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	20	0.44	0.12	0.42
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	20	0.43	0.09	0.41
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	20	0.42	0.14	0.42
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	20	0.42	0.01	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	20	0.42	0.01	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	20	0.42	0.01	0.41
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	20	0.39	0.03	0.39

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	20	0.38	0.01	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	20	0.38	0.01	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	20	0.38	0.01	0.38
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	20	0.36	0.01	0.37
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	20	0.36	0.05	0.37
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	20	0.33	0.1	0.32
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	20	0.29	0.07	0.27
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	20	0.28	0.03	0.28
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	20	0.26	0.02	0.26
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	20	0.26	0.02	0.26
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	20	0.26	0.02	0.26
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	20	0.23	0.06	0.24
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	20	0.22	0.02	0.22
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	20	0.22	0.02	0.22
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	20	0.22	0.02	0.22
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	20	0.22	0.04	0.22
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	20	0.21	0.06	0.2
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	20	0.21	0.06	0.2
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	20	0.21	0.06	0.2
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	20	0.2	0.01	0.2
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	20	0.2	0.01	0.2
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	20	0.2	0.01	0.2
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	20	0.18	0.05	0.18
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	20	0.18	0.03	0.18
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	20	0.16	0.03	0.17
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	20	0.15	0.02	0.15
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	19	2.13	0.34	2.32
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	19	2.13	0.34	2.32
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	19	2.13	0.34	2.32
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	19	2.1	0.78	2.32
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	19	2.1	0.78	2.32
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	19	2.1	0.78	2.32
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	19	1.79	0.1	1.82
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	19	1.79	0.43	2.03
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	19	1.79	0.43	2.03
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	19	1.79	0.43	2.03
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	19	1.72	0.66	2.08
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	19	1.72	0.66	2.08
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	19	1.72	0.66	2.08
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	19	1.65	0.14	1.69
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	19	1.65	0.14	1.69
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	19	1.65	0.14	1.69

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	19	1.61	0.15	1.66
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	19	1.61	0.15	1.66
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	19	1.36	0.08	1.39
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	19	1.36	0.08	1.39
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	19	1.36	0.08	1.39
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	19	1.17	0.58	0.83
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	19	1.17	0.58	0.83
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	19	1.17	0.58	0.83
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	19	1.04	0.28	1.0
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	19	1.04	0.28	1.0
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	19	1.04	0.28	1.0
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	19	1.03	0.38	0.95
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	19	1.03	0.38	0.95
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	19	1.03	0.38	0.95
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	19	0.91	0.3	0.85
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	19	0.91	0.3	0.85
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	19	0.91	0.3	0.85
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	19	0.91	0.05	0.91
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	19	0.91	0.05	0.91
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	19	0.91	0.05	0.91
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	19	0.89	0.73	0.55
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	19	0.85	0.28	0.75
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	19	0.85	0.28	0.75
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	19	0.85	0.28	0.75
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	19	0.8	0.13	0.84
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	19	0.76	0.25	0.81
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	19	0.76	0.34	0.54
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	19	0.74	0.35	0.86
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	19	0.61	0.11	0.64
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	19	0.61	0.11	0.64
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	19	0.61	0.11	0.64
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	19	0.57	0.06	0.57
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	19	0.56	0.24	0.57
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	19	0.56	0.24	0.57
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	19	0.56	0.24	0.57
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	19	0.55	0.35	0.48
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	19	0.51	0.17	0.51
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	19	0.51	0.17	0.51
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	19	0.51	0.17	0.51
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	19	0.5	0.14	0.52
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	19	0.45	0.07	0.44
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	19	0.4	0.11	0.45

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	19	0.35	0.13	0.35
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	19	0.33	0.08	0.35
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	19	0.32	0.12	0.34
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	19	0.28	0.07	0.26
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	19	0.22	0.02	0.22
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	19	0.22	0.02	0.22
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	19	0.22	0.02	0.22
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	19	0.22	0.02	0.22
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	19	0.2	0.05	0.2
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	18	1.44	0.2	1.49
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	18	1.43	0.35	1.44
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	18	1.13	0.52	1.17
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	18	1.09	0.09	1.12
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	18	1.07	0.45	1.11
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	18	1.07	0.45	1.11
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	18	1.07	0.45	1.11
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	18	0.98	0.13	1.01
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	18	0.87	0.39	0.94
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	18	0.87	0.39	0.94
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	18	0.87	0.39	0.94
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	18	0.83	0.45	0.86
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	18	0.82	0.23	0.88
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	18	0.82	0.06	0.83
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	18	0.82	0.03	0.82
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	18	0.78	0.58	0.56
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	18	0.76	0.39	0.76
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	18	0.76	0.39	0.76
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	18	0.76	0.39	0.76
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	18	0.69	0.06	0.7
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	18	0.69	0.29	0.74
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	18	0.62	0.32	0.77
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	18	0.62	0.32	0.77
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	18	0.62	0.32	0.77
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	18	0.59	0.03	0.59
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	18	0.58	0.11	0.58
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	18	0.58	0.11	0.58
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	18	0.49	0.22	0.5
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	18	0.49	0.22	0.5
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	18	0.49	0.22	0.5
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	18	0.49	0.09	0.51
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	18	0.47	0.2	0.5
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	18	0.44	0.08	0.44

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	18	0.37	0.01	0.37
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	18	0.32	0.16	0.26
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	18	0.25	0.05	0.24
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	18	0.22	0.03	0.22
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	18	0.22	0.12	0.18
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	18	0.19	0.3	0.12
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	18	0.19	0.02	0.2
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	17	1.23	0.77	0.77
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	17	1.17	0.76	0.95
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	17	1.11	0.41	1.12
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	17	0.93	0.4	1.0
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	17	0.83	0.41	0.77
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	17	0.83	0.41	0.77
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	17	0.83	0.41	0.77
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	17	0.82	0.4	0.9
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	17	0.82	0.4	0.9
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	17	0.82	0.4	0.9
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	17	0.79	0.55	0.78
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	17	0.7	0.44	0.51
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	17	0.7	0.44	0.51
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	17	0.7	0.44	0.51
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	17	0.61	0.3	0.58
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	17	0.61	0.3	0.58
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	17	0.61	0.3	0.58
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	17	0.59	0.24	0.67
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	17	0.59	0.24	0.67
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	17	0.59	0.24	0.67
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	17	0.52	0.18	0.52
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	17	0.49	0.04	0.48
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	17	0.44	0.19	0.36
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	17	0.41	0.14	0.43
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	17	0.41	0.14	0.43
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	17	0.41	0.14	0.43
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	17	0.36	0.22	0.27
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	17	0.35	0.07	0.32
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	17	0.35	0.07	0.32
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	17	0.35	0.07	0.32
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	17	0.35	0.02	0.35
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	17	0.34	0.16	0.33
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	17	0.34	0.17	0.32
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	17	0.29	0.14	0.22
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	17	0.25	0.02	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	17	0.21	0.08	0.23
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	17	0.19	0.04	0.19
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	17	0.18	0.02	0.19
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	17	0.18	0.03	0.19
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	17	0.16	0.03	0.16
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	17	0.16	0.03	0.16
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	17	0.16	0.03	0.16
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG11	16	0.88	0.6	0.74
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG12	16	0.88	0.6	0.74
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG13	16	0.88	0.6	0.74
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD11	16	0.81	0.55	0.76
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD12	16	0.81	0.55	0.76
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD13	16	0.81	0.55	0.76
(1,324)	1:142:A:VAL:HG21	1:114:A:ARG:HB2	16	0.64	0.34	0.63
(1,324)	1:142:A:VAL:HG22	1:114:A:ARG:HB2	16	0.64	0.34	0.63
(1,324)	1:142:A:VAL:HG23	1:114:A:ARG:HB2	16	0.64	0.34	0.63
(1,193)	1:123:A:GLN:HA	1:123:A:GLN:HG3	16	0.45	0.07	0.43
(1,194)	1:123:A:GLN:HG3	1:123:A:GLN:H	16	0.39	0.16	0.34
(1,543)	1:35:A:ASP:H	1:33:A:SER:HB3	16	0.35	0.03	0.36
(1,1423)	1:121:A:LEU:H	1:121:A:LEU:HG	16	0.26	0.17	0.22
(1,1161)	1:119:A:ALA:HA	1:122:A:LYS:HG2	16	0.26	0.08	0.25
(1,323)	1:114:A:ARG:HB3	1:115:A:LYS:H	16	0.23	0.08	0.23
(1,1052)	1:92:A:LYS:HA	1:92:A:LYS:HB2	16	0.23	0.01	0.23
(1,1656)	1:122:A:LYS:H	1:122:A:LYS:HG2	16	0.2	0.1	0.18
(1,1872)	1:8:A:GLY:H	1:8:A:GLY:HA2	16	0.13	0.03	0.12
(1,11)	1:8:A:GLY:HA3	1:15:A:LYS:HE3	15	1.55	1.03	1.12
(1,3)	1:15:A:LYS:HD3	1:8:A:GLY:HA2	15	1.22	0.57	1.39
(1,1147)	1:83:A:ALA:HA	1:86:A:ILE:HG12	15	1.1	0.71	0.87
(1,611)	1:111:A:VAL:HA	1:110:A:SER:HB2	15	1.0	0.45	1.26
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG21	15	0.89	0.31	0.9
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG22	15	0.89	0.31	0.9
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG23	15	0.89	0.31	0.9
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG21	15	0.89	0.31	0.9
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG22	15	0.89	0.31	0.9
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG23	15	0.89	0.31	0.9
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG21	15	0.89	0.31	0.9
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG22	15	0.89	0.31	0.9
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG23	15	0.89	0.31	0.9
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG21	15	0.89	0.31	0.9
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG22	15	0.89	0.31	0.9
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG23	15	0.89	0.31	0.9
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG21	15	0.89	0.31	0.9

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG22	15	0.89	0.31	0.9
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG23	15	0.89	0.31	0.9
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG21	15	0.89	0.31	0.9
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG22	15	0.89	0.31	0.9
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG23	15	0.89	0.31	0.9
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB2	15	0.8	0.27	0.8
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB3	15	0.8	0.27	0.8
(1,183)	1:101:A:LYS:HB2	1:102:A:TYR:HA	15	0.76	0.4	0.64
(1,1106)	1:104:A:LYS:HG3	1:103:A:GLU:HA	15	0.74	0.44	0.62
(1,911)	1:9:A:ALA:HB1	1:15:A:LYS:HD2	15	0.7	0.46	0.58
(1,911)	1:9:A:ALA:HB2	1:15:A:LYS:HD2	15	0.7	0.46	0.58
(1,911)	1:9:A:ALA:HB3	1:15:A:LYS:HD2	15	0.7	0.46	0.58
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG21	15	0.65	0.31	0.62
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG22	15	0.65	0.31	0.62
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG23	15	0.65	0.31	0.62
(1,263)	1:86:A:ILE:H	1:85:A:LYS:HB2	15	0.64	0.17	0.63
(1,1019)	1:84:A:MET:HE1	1:15:A:LYS:HD2	15	0.64	0.55	0.32
(1,1019)	1:84:A:MET:HE2	1:15:A:LYS:HD2	15	0.64	0.55	0.32
(1,1019)	1:84:A:MET:HE3	1:15:A:LYS:HD2	15	0.64	0.55	0.32
(1,605)	1:107:A:ASP:HB3	1:110:A:SER:HB3	15	0.59	0.17	0.65
(1,1319)	1:8:A:GLY:HA3	1:9:A:ALA:H	15	0.57	0.18	0.64
(1,1380)	1:158:A:LYS:HB2	1:158:A:LYS:H	15	0.55	0.07	0.53
(1,716)	1:148:A:LEU:HD21	1:147:A:GLU:HG2	15	0.49	0.15	0.52
(1,716)	1:148:A:LEU:HD22	1:147:A:GLU:HG2	15	0.49	0.15	0.52
(1,716)	1:148:A:LEU:HD23	1:147:A:GLU:HG2	15	0.49	0.15	0.52
(1,484)	1:142:A:VAL:HG11	1:139:A:THR:HA	15	0.45	0.15	0.4
(1,484)	1:142:A:VAL:HG12	1:139:A:THR:HA	15	0.45	0.15	0.4
(1,484)	1:142:A:VAL:HG13	1:139:A:THR:HA	15	0.45	0.15	0.4
(1,1522)	1:131:A:GLU:H	1:130:A:GLU:HB3	15	0.37	0.17	0.36
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE1	15	0.37	0.19	0.35
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE2	15	0.37	0.19	0.35
(1,1102)	1:158:A:LYS:HG2	1:158:A:LYS:HA	15	0.37	0.2	0.28
(1,927)	1:23:A:LYS:HA	1:22:A:TYR:HB2	15	0.37	0.23	0.25
(1,196)	1:123:A:GLN:HB3	1:123:A:GLN:HG2	15	0.31	0.03	0.32
(1,385)	1:121:A:LEU:HB3	1:118:A:VAL:HA	15	0.3	0.15	0.23
(1,797)	1:138:A:LYS:HA	1:138:A:LYS:HG2	15	0.24	0.14	0.2
(1,46)	1:46:A:LEU:HB2	1:47:A:ASP:HA	15	0.17	0.05	0.17
(1,1511)	1:25:A:LEU:H	1:25:A:LEU:HG	15	0.15	0.02	0.14
(1,1993)	1:130:A:GLU:HB2	1:128:A:TRP:HE3	14	1.02	0.27	1.03
(1,243)	1:81:A:MET:HG3	1:85:A:LYS:HB2	14	0.86	0.78	0.68
(1,243)	1:81:A:MET:HG2	1:85:A:LYS:HB2	14	0.86	0.78	0.68
(1,558)	1:158:A:LYS:HG2	1:158:A:LYS:HE2	14	0.85	0.2	0.76

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1085)	1:56:A:CYS:HB3	1:53:A:ASN:HA	14	0.69	0.27	0.72
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD11	14	0.69	0.01	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD12	14	0.69	0.01	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD13	14	0.69	0.01	0.69
(1,9)	1:8:A:GLY:HA2	1:15:A:LYS:HE2	14	0.65	0.5	0.46
(1,9)	1:8:A:GLY:HA3	1:15:A:LYS:HE2	14	0.65	0.5	0.46
(1,1017)	1:84:A:MET:HE1	1:15:A:LYS:HE2	14	0.53	0.28	0.45
(1,1017)	1:84:A:MET:HE2	1:15:A:LYS:HE2	14	0.53	0.28	0.45
(1,1017)	1:84:A:MET:HE3	1:15:A:LYS:HE2	14	0.53	0.28	0.45
(1,589)	1:63:A:LYS:HB3	1:63:A:LYS:HG3	14	0.36	0.01	0.37
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB1	14	0.34	0.24	0.22
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB2	14	0.34	0.24	0.22
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB3	14	0.34	0.24	0.22
(1,95)	1:35:A:ASP:HB3	1:34:A:LEU:HB3	14	0.32	0.08	0.32
(1,1835)	1:114:A:ARG:H	1:114:A:ARG:HD2	14	0.26	0.12	0.2
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD11	14	0.19	0.04	0.2
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD12	14	0.19	0.04	0.2
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD13	14	0.19	0.04	0.2
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD11	14	0.19	0.04	0.2
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD12	14	0.19	0.04	0.2
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD13	14	0.19	0.04	0.2
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD11	14	0.19	0.04	0.2
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD12	14	0.19	0.04	0.2
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD13	14	0.19	0.04	0.2
(1,559)	1:158:A:LYS:HE3	1:158:A:LYS:HG2	13	0.97	0.38	1.25
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE1	13	0.93	0.46	0.93
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE2	13	0.93	0.46	0.93
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE3	13	0.93	0.46	0.93
(1,138)	1:42:A:ILE:HD11	1:38:A:GLU:HG2	13	0.83	0.39	0.91
(1,138)	1:42:A:ILE:HD12	1:38:A:GLU:HG2	13	0.83	0.39	0.91
(1,138)	1:42:A:ILE:HD13	1:38:A:GLU:HG2	13	0.83	0.39	0.91
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB1	13	0.79	0.45	0.7
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB2	13	0.79	0.45	0.7
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB3	13	0.79	0.45	0.7
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD11	13	0.67	0.37	0.49
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD12	13	0.67	0.37	0.49
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD13	13	0.67	0.37	0.49
(1,506)	1:93:A:LEU:H	1:92:A:LYS:HG2	13	0.64	0.13	0.62
(1,164)	1:2:A:GLU:HG3	1:2:A:GLU:HA	13	0.6	0.02	0.6
(1,1586)	1:143:A:ASN:HB3	1:142:A:VAL:H	13	0.6	0.5	0.42
(1,1992)	1:126:A:HIS:HB3	1:126:A:HIS:HD2	13	0.59	0.02	0.59
(1,153)	1:103:A:GLU:HG3	1:104:A:LYS:H	13	0.59	0.32	0.58

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1878)	1:5:A:GLY:H	1:4:A:GLY:HA2	13	0.52	0.15	0.61
(1,573)	1:106:A:LEU:HD21	1:108:A:LEU:HA	13	0.51	0.26	0.48
(1,573)	1:106:A:LEU:HD22	1:108:A:LEU:HA	13	0.51	0.26	0.48
(1,573)	1:106:A:LEU:HD23	1:108:A:LEU:HA	13	0.51	0.26	0.48
(1,232)	1:91:A:LYS:H	1:91:A:LYS:HB3	13	0.42	0.16	0.39
(1,787)	1:75:A:ARG:HD3	1:75:A:ARG:HA	13	0.42	0.12	0.45
(1,18)	1:28:A:ARG:HA	1:28:A:ARG:HD2	13	0.4	0.1	0.42
(1,264)	1:85:A:LYS:HB3	1:86:A:ILE:H	13	0.38	0.13	0.35
(1,1058)	1:54:A:ARG:HA	1:54:A:ARG:HD3	13	0.38	0.12	0.41
(1,419)	1:6:A:ARG:HG3	1:6:A:ARG:H	13	0.37	0.2	0.35
(1,552)	1:31:A:ASN:HD21	1:33:A:SER:HB2	13	0.37	0.26	0.26
(1,1126)	1:104:A:LYS:HG3	1:104:A:LYS:HA	13	0.35	0.15	0.36
(1,700)	1:71:A:SER:HA	1:71:A:SER:HB2	13	0.3	0.01	0.3
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG21	13	0.29	0.03	0.3
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG22	13	0.29	0.03	0.3
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG23	13	0.29	0.03	0.3
(1,1385)	1:103:A:GLU:H	1:102:A:TYR:HA	13	0.24	0.05	0.24
(1,1387)	1:103:A:GLU:H	1:103:A:GLU:HB2	13	0.24	0.08	0.24
(1,1825)	1:45:A:CYS:HB3	1:45:A:CYS:H	13	0.21	0.01	0.21
(1,1887)	1:126:A:HIS:H	1:129:A:GLY:H	13	0.14	0.02	0.14
(1,1329)	1:121:A:LEU:H	1:118:A:VAL:H	13	0.13	0.02	0.13
(1,335)	1:39:A:LYS:HA	1:42:A:ILE:HG13	12	1.35	0.19	1.42
(1,696)	1:71:A:SER:HB3	1:75:A:ARG:HD2	12	1.15	0.78	0.79
(1,1810)	1:91:A:LYS:HB3	1:92:A:LYS:H	12	0.77	0.19	0.84
(1,2)	1:8:A:GLY:HA2	1:15:A:LYS:HD2	12	0.71	0.46	0.52
(1,2)	1:8:A:GLY:HA3	1:15:A:LYS:HD2	12	0.71	0.46	0.52
(1,209)	1:67:A:THR:HG21	1:68:A:LYS:HB3	12	0.7	0.35	0.64
(1,209)	1:67:A:THR:HG22	1:68:A:LYS:HB3	12	0.7	0.35	0.64
(1,209)	1:67:A:THR:HG23	1:68:A:LYS:HB3	12	0.7	0.35	0.64
(1,798)	1:138:A:LYS:HG3	1:138:A:LYS:HA	12	0.66	0.04	0.68
(1,441)	1:113:A:LEU:HD21	1:146:A:GLN:HG3	12	0.63	0.26	0.68
(1,441)	1:113:A:LEU:HD22	1:146:A:GLN:HG3	12	0.63	0.26	0.68
(1,441)	1:113:A:LEU:HD23	1:146:A:GLN:HG3	12	0.63	0.26	0.68
(1,1708)	1:115:A:LYS:H	1:115:A:LYS:HB2	12	0.57	0.06	0.57
(1,1580)	1:127:A:SER:H	1:126:A:HIS:HB2	12	0.56	0.03	0.57
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE1	12	0.55	0.33	0.42
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE2	12	0.55	0.33	0.42
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE3	12	0.55	0.33	0.42
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD1	12	0.52	0.29	0.44
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD2	12	0.52	0.29	0.44
(1,142)	1:88:A:GLU:HG3	1:89:A:LYS:H	12	0.51	0.2	0.54
(1,33)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	12	0.49	0.02	0.5

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1146)	1:115:A:LYS:HA	1:115:A:LYS:HG2	12	0.47	0.05	0.46
(1,1088)	1:81:A:MET:HE1	1:81:A:MET:HG2	12	0.28	0.02	0.29
(1,1088)	1:81:A:MET:HE2	1:81:A:MET:HG2	12	0.28	0.02	0.29
(1,1088)	1:81:A:MET:HE3	1:81:A:MET:HG2	12	0.28	0.02	0.29
(1,1725)	1:33:A:SER:H	1:33:A:SER:HB2	12	0.27	0.06	0.29
(1,163)	1:2:A:GLU:HA	1:2:A:GLU:HG2	12	0.26	0.13	0.21
(1,550)	1:36:A:THR:HB	1:33:A:SER:HB2	12	0.25	0.02	0.25
(1,251)	1:63:A:LYS:HB3	1:63:A:LYS:HE3	12	0.25	0.06	0.24
(1,1798)	1:42:A:ILE:HG13	1:43:A:SER:H	12	0.24	0.04	0.23
(1,952)	1:126:A:HIS:HB3	1:126:A:HIS:HA	12	0.21	0.01	0.21
(1,1101)	1:158:A:LYS:HA	1:158:A:LYS:HG3	12	0.2	0.16	0.16
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD11	12	0.2	0.01	0.2
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD12	12	0.2	0.01	0.2
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD13	12	0.2	0.01	0.2
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB1	12	0.19	0.06	0.18
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB2	12	0.19	0.06	0.18
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB3	12	0.19	0.06	0.18
(1,1802)	1:24:A:SER:H	1:25:A:LEU:HG	12	0.13	0.02	0.13
(1,244)	1:85:A:LYS:HB3	1:81:A:MET:HG2	11	1.19	1.43	0.8
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD11	11	1.02	0.38	1.24
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD12	11	1.02	0.38	1.24
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD13	11	1.02	0.38	1.24
(1,279)	1:67:A:THR:HB	1:69:A:ILE:HG13	11	0.96	0.33	0.96
(1,256)	1:86:A:ILE:H	1:81:A:MET:HG2	11	0.7	0.39	0.85
(1,418)	1:6:A:ARG:H	1:6:A:ARG:HG2	11	0.62	0.26	0.72
(1,1157)	1:101:A:LYS:HA	1:101:A:LYS:HD2	11	0.56	0.2	0.67
(1,1158)	1:101:A:LYS:HD3	1:101:A:LYS:HA	11	0.46	0.18	0.47
(1,869)	1:13:A:VAL:HG21	1:55:A:LEU:HB2	11	0.45	0.19	0.39
(1,869)	1:13:A:VAL:HG22	1:55:A:LEU:HB2	11	0.45	0.19	0.39
(1,869)	1:13:A:VAL:HG23	1:55:A:LEU:HB2	11	0.45	0.19	0.39
(1,786)	1:75:A:ARG:HA	1:75:A:ARG:HD2	11	0.44	0.28	0.45
(1,27)	1:117:A:ARG:HD3	1:117:A:ARG:HB3	11	0.42	0.14	0.34
(1,1879)	1:4:A:GLY:HA3	1:5:A:GLY:H	11	0.41	0.19	0.34
(1,1549)	1:130:A:GLU:H	1:130:A:GLU:HB2	11	0.39	0.04	0.37
(1,5)	1:9:A:ALA:HB1	1:8:A:GLY:HA2	11	0.36	0.13	0.34
(1,5)	1:9:A:ALA:HB2	1:8:A:GLY:HA2	11	0.36	0.13	0.34
(1,5)	1:9:A:ALA:HB3	1:8:A:GLY:HA2	11	0.36	0.13	0.34
(1,1386)	1:103:A:GLU:H	1:102:A:TYR:HB3	11	0.34	0.11	0.35
(1,1047)	1:77:A:MET:HE1	1:22:A:TYR:HB3	11	0.31	0.11	0.28
(1,1047)	1:77:A:MET:HE2	1:22:A:TYR:HB3	11	0.31	0.11	0.28
(1,1047)	1:77:A:MET:HE3	1:22:A:TYR:HB3	11	0.31	0.11	0.28
(1,154)	1:103:A:GLU:HB3	1:103:A:GLU:HG2	11	0.31	0.03	0.32

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,963)	1:110:A:SER:HB3	1:110:A:SER:HA	11	0.27	0.01	0.27
(1,545)	1:33:A:SER:HB3	1:34:A:LEU:H	11	0.26	0.02	0.27
(1,336)	1:42:A:ILE:H	1:42:A:ILE:HG13	11	0.23	0.06	0.22
(1,1527)	1:116:A:MET:H	1:115:A:LYS:HB2	11	0.19	0.08	0.19
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB1	11	0.16	0.05	0.13
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB2	11	0.16	0.05	0.13
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB3	11	0.16	0.05	0.13
(1,1614)	1:25:A:LEU:HD11	1:40:A:GLU:H	11	0.12	0.01	0.11
(1,1614)	1:25:A:LEU:HD12	1:40:A:GLU:H	11	0.12	0.01	0.11
(1,1614)	1:25:A:LEU:HD13	1:40:A:GLU:H	11	0.12	0.01	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG21	11	0.11	0.01	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG22	11	0.11	0.01	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG23	11	0.11	0.01	0.11
(1,1277)	1:128:A:TRP:HE1	1:127:A:SER:HB2	10	0.83	0.18	0.84
(1,254)	1:82:A:PRO:HD2	1:81:A:MET:HG2	10	0.8	0.44	1.03
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD1	10	0.76	0.5	0.72
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD2	10	0.76	0.5	0.72
(1,1969)	1:24:A:SER:HB3	1:44:A:PHE:HZ	10	0.65	0.25	0.62
(1,145)	1:85:A:LYS:HA	1:88:A:GLU:HG2	10	0.6	0.28	0.6
(1,152)	1:104:A:LYS:H	1:103:A:GLU:HG2	10	0.55	0.3	0.43
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE1	10	0.55	0.03	0.56
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE2	10	0.55	0.03	0.56
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE3	10	0.55	0.03	0.56
(1,26)	1:117:A:ARG:HB3	1:117:A:ARG:HD2	10	0.53	0.29	0.6
(1,531)	1:92:A:LYS:HD3	1:92:A:LYS:HB2	10	0.53	0.31	0.69
(1,1646)	1:88:A:GLU:HB3	1:87:A:CYS:H	10	0.53	0.12	0.47
(1,250)	1:63:A:LYS:HE3	1:63:A:LYS:HB2	10	0.49	0.33	0.32
(1,1104)	1:103:A:GLU:HG3	1:103:A:GLU:HA	10	0.47	0.18	0.57
(1,814)	1:38:A:GLU:HA	1:38:A:GLU:HG2	10	0.43	0.08	0.41
(1,582)	1:151:A:LYS:H	1:151:A:LYS:HG3	10	0.34	0.08	0.37
(1,755)	1:127:A:SER:HB3	1:127:A:SER:HA	10	0.29	0.0	0.29
(1,754)	1:127:A:SER:HA	1:127:A:SER:HB2	10	0.28	0.0	0.28
(1,1989)	1:156:A:HIS:HB3	1:156:A:HIS:HD2	10	0.27	0.03	0.26
(1,1548)	1:130:A:GLU:H	1:128:A:TRP:HB3	10	0.26	0.11	0.23
(1,86)	1:28:A:ARG:H	1:27:A:ASP:HB2	10	0.25	0.05	0.22
(1,312)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	10	0.21	0.05	0.2
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB2	10	0.17	0.04	0.17
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB3	10	0.17	0.04	0.17
(1,311)	1:91:A:LYS:HD3	1:95:A:SER:HA	9	1.06	0.46	1.26
(1,76)	1:140:A:ASP:HB2	1:135:A:CYS:HA	9	0.7	0.27	0.82
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD2	9	0.57	0.21	0.64
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD3	9	0.57	0.21	0.64

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,168)	1:17:A:PHE:H	1:16:A:GLU:HG2	9	0.53	0.2	0.64
(1,1871)	1:8:A:GLY:H	1:7:A:PRO:HG3	9	0.52	0.24	0.48
(1,568)	1:34:A:LEU:HD11	1:75:A:ARG:HD2	9	0.49	0.44	0.22
(1,568)	1:34:A:LEU:HD12	1:75:A:ARG:HD2	9	0.49	0.44	0.22
(1,568)	1:34:A:LEU:HD13	1:75:A:ARG:HD2	9	0.49	0.44	0.22
(1,21)	1:114:A:ARG:HD3	1:114:A:ARG:HB2	9	0.46	0.26	0.6
(1,19)	1:28:A:ARG:HD3	1:28:A:ARG:HA	9	0.45	0.36	0.25
(1,1363)	1:27:A:ASP:H	1:27:A:ASP:HB3	9	0.39	0.05	0.36
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE1	9	0.38	0.35	0.28
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE2	9	0.38	0.35	0.28
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE3	9	0.38	0.35	0.28
(1,1806)	1:24:A:SER:H	1:23:A:LYS:HB2	9	0.36	0.41	0.14
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD11	9	0.34	0.1	0.33
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD12	9	0.34	0.1	0.33
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD13	9	0.34	0.1	0.33
(1,1359)	1:63:A:LYS:HB3	1:65:A:ALA:H	9	0.33	0.37	0.19
(1,1666)	1:30:A:VAL:HB	1:28:A:ARG:HE	9	0.3	0.51	0.11
(1,1838)	1:114:A:ARG:HB3	1:114:A:ARG:H	9	0.3	0.23	0.21
(1,1756)	1:151:A:LYS:HB3	1:151:A:LYS:H	9	0.28	0.05	0.29
(1,1669)	1:93:A:LEU:HB3	1:94:A:ASP:H	9	0.26	0.11	0.2
(1,504)	1:54:A:ARG:H	1:54:A:ARG:HG3	9	0.24	0.02	0.24
(1,711)	1:139:A:THR:HG21	1:143:A:ASN:HB2	9	0.22	0.1	0.18
(1,711)	1:139:A:THR:HG22	1:143:A:ASN:HB2	9	0.22	0.1	0.18
(1,711)	1:139:A:THR:HG23	1:143:A:ASN:HB2	9	0.22	0.1	0.18
(1,1771)	1:35:A:ASP:H	1:34:A:LEU:HB3	9	0.2	0.05	0.22
(1,297)	1:99:A:GLU:HG3	1:99:A:GLU:HB2	9	0.2	0.02	0.2
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD2	9	0.16	0.03	0.17
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD3	9	0.16	0.03	0.17
(1,1964)	1:21:A:PHE:HD1	1:44:A:PHE:HZ	9	0.13	0.02	0.12
(1,1964)	1:21:A:PHE:HD2	1:44:A:PHE:HZ	9	0.13	0.02	0.12
(1,1718)	1:142:A:VAL:HG21	1:143:A:ASN:H	9	0.12	0.01	0.12
(1,1718)	1:142:A:VAL:HG22	1:143:A:ASN:H	9	0.12	0.01	0.12
(1,1718)	1:142:A:VAL:HG23	1:143:A:ASN:H	9	0.12	0.01	0.12
(1,1105)	1:103:A:GLU:HA	1:104:A:LYS:HG2	8	0.82	0.48	0.82
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD2	8	0.77	0.34	0.86
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD2	8	0.77	0.34	0.86
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD2	8	0.77	0.34	0.86
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD3	8	0.77	0.34	0.86
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD3	8	0.77	0.34	0.86
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD3	8	0.77	0.34	0.86
(1,1110)	1:116:A:MET:HA	1:117:A:ARG:HD2	8	0.63	0.37	0.48
(1,362)	1:75:A:ARG:HB2	1:75:A:ARG:HD2	8	0.57	0.1	0.54

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,532)	1:92:A:LYS:HB3	1:92:A:LYS:HD3	8	0.56	0.27	0.7
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB2	8	0.55	0.39	0.5
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB3	8	0.55	0.39	0.5
(1,48)	1:86:A:ILE:HG21	1:89:A:LYS:HE3	8	0.52	0.3	0.52
(1,48)	1:86:A:ILE:HG22	1:89:A:LYS:HE3	8	0.52	0.3	0.52
(1,48)	1:86:A:ILE:HG23	1:89:A:LYS:HE3	8	0.52	0.3	0.52
(1,687)	1:17:A:PHE:HA	1:20:A:ARG:HB2	8	0.5	0.2	0.52
(1,1318)	1:9:A:ALA:H	1:8:A:GLY:HA2	8	0.49	0.19	0.57
(1,437)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	8	0.49	0.02	0.49
(1,1008)	1:85:A:LYS:HA	1:88:A:GLU:HB3	8	0.48	0.06	0.48
(1,313)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	8	0.41	0.3	0.23
(1,438)	1:6:A:ARG:HG3	1:6:A:ARG:HB3	8	0.38	0.16	0.48
(1,1581)	1:126:A:HIS:HB3	1:127:A:SER:H	8	0.36	0.11	0.34
(1,557)	1:158:A:LYS:HE3	1:158:A:LYS:HG3	8	0.35	0.12	0.33
(1,557)	1:158:A:LYS:HE2	1:158:A:LYS:HG3	8	0.35	0.12	0.33
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD11	8	0.32	0.03	0.31
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD12	8	0.32	0.03	0.31
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD13	8	0.32	0.03	0.31
(1,1565)	1:117:A:ARG:H	1:116:A:MET:HB3	8	0.32	0.09	0.33
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD11	8	0.31	0.26	0.17
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD12	8	0.31	0.26	0.17
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD13	8	0.31	0.26	0.17
(1,583)	1:151:A:LYS:HG2	1:151:A:LYS:H	8	0.3	0.11	0.35
(1,1529)	1:131:A:GLU:H	1:131:A:GLU:HB2	8	0.28	0.09	0.3
(1,1291)	1:107:A:ASP:HB3	1:108:A:LEU:H	8	0.27	0.06	0.28
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE1	8	0.27	0.05	0.26
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE2	8	0.27	0.05	0.26
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE3	8	0.27	0.05	0.26
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE2	8	0.26	0.03	0.26
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE3	8	0.26	0.03	0.26
(1,1379)	1:158:A:LYS:H	1:157:A:PRO:HB3	8	0.24	0.11	0.26
(1,1703)	1:152:A:TYR:H	1:151:A:LYS:HB2	8	0.23	0.04	0.24
(1,1613)	1:40:A:GLU:H	1:39:A:LYS:HB3	8	0.19	0.05	0.19
(1,951)	1:126:A:HIS:HA	1:126:A:HIS:HB2	8	0.16	0.02	0.17
(1,220)	1:131:A:GLU:HG3	1:131:A:GLU:HB3	8	0.16	0.01	0.16
(1,1604)	1:54:A:ARG:HB3	1:54:A:ARG:H	8	0.13	0.02	0.13
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD2	8	0.13	0.01	0.13
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD3	8	0.13	0.01	0.13
(1,1471)	1:102:A:TYR:H	1:101:A:LYS:HA	8	0.12	0.01	0.13
(1,409)	1:161:A:LEU:H	1:161:A:LEU:HG	8	0.12	0.02	0.12
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE1	8	0.12	0.01	0.12
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE2	8	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)
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE3	8	0.12	0.01	0.12
(1,1049)	1:140:A:ASP:HB3	1:140:A:ASP:HA	8	0.11	0.01	0.11
(1,2012)	1:152:A:TYR:HE1	1:151:A:LYS:HE2	7	0.89	0.37	0.94
(1,2012)	1:152:A:TYR:HE2	1:151:A:LYS:HE2	7	0.89	0.37	0.94
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD11	7	0.72	0.31	0.71
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD12	7	0.72	0.31	0.71
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD13	7	0.72	0.31	0.71
(1,731)	1:148:A:LEU:HD21	1:151:A:LYS:HE2	7	0.62	0.55	0.32
(1,731)	1:148:A:LEU:HD22	1:151:A:LYS:HE2	7	0.62	0.55	0.32
(1,731)	1:148:A:LEU:HD23	1:151:A:LYS:HE2	7	0.62	0.55	0.32
(1,507)	1:92:A:LYS:HG3	1:93:A:LEU:H	7	0.58	0.14	0.59
(1,1055)	1:92:A:LYS:HG3	1:92:A:LYS:HA	7	0.56	0.08	0.59
(1,1991)	1:126:A:HIS:HD2	1:126:A:HIS:HB2	7	0.54	0.02	0.53
(1,584)	1:102:A:TYR:H	1:101:A:LYS:HG2	7	0.52	0.35	0.3
(1,1221)	1:65:A:ALA:HA	1:57:A:TYR:HD1	7	0.49	0.16	0.48
(1,1221)	1:65:A:ALA:HA	1:57:A:TYR:HD2	7	0.49	0.16	0.48
(1,1381)	1:158:A:LYS:H	1:158:A:LYS:HG3	7	0.46	0.2	0.39
(1,299)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	7	0.43	0.2	0.5
(1,112)	1:53:A:ASN:H	1:52:A:GLU:HG3	7	0.41	0.11	0.43
(1,165)	1:147:A:GLU:HG2	1:147:A:GLU:HA	7	0.4	0.08	0.44
(1,1316)	1:160:A:GLU:H	1:160:A:GLU:HB2	7	0.35	0.02	0.35
(1,1462)	1:107:A:ASP:HB3	1:109:A:ALA:H	7	0.35	0.12	0.38
(1,887)	1:65:A:ALA:HB1	1:57:A:TYR:HE1	7	0.32	0.11	0.33
(1,887)	1:65:A:ALA:HB1	1:57:A:TYR:HE2	7	0.32	0.11	0.33
(1,887)	1:65:A:ALA:HB2	1:57:A:TYR:HE1	7	0.32	0.11	0.33
(1,887)	1:65:A:ALA:HB2	1:57:A:TYR:HE2	7	0.32	0.11	0.33
(1,887)	1:65:A:ALA:HB3	1:57:A:TYR:HE1	7	0.32	0.11	0.33
(1,887)	1:65:A:ALA:HB3	1:57:A:TYR:HE2	7	0.32	0.11	0.33
(1,1836)	1:114:A:ARG:HD3	1:114:A:ARG:H	7	0.29	0.07	0.32
(1,1103)	1:103:A:GLU:HA	1:103:A:GLU:HG2	7	0.26	0.19	0.17
(1,28)	1:117:A:ARG:HG3	1:117:A:ARG:HD2	7	0.25	0.01	0.25
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG11	7	0.24	0.09	0.2
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG12	7	0.24	0.09	0.2
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG13	7	0.24	0.09	0.2
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG11	7	0.24	0.09	0.2
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG12	7	0.24	0.09	0.2
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG13	7	0.24	0.09	0.2
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG11	7	0.23	0.16	0.14
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG12	7	0.23	0.16	0.14
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG13	7	0.23	0.16	0.14
(1,1125)	1:104:A:LYS:HA	1:104:A:LYS:HG2	7	0.21	0.06	0.2
(1,17)	1:20:A:ARG:HB3	1:20:A:ARG:HD2	7	0.19	0.03	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1633)	1:87:A:CYS:H	1:87:A:CYS:HB3	7	0.14	0.01	0.14
(1,904)	1:83:A:ALA:HB1	1:19:A:ASN:HD22	7	0.13	0.02	0.13
(1,904)	1:83:A:ALA:HB2	1:19:A:ASN:HD22	7	0.13	0.02	0.13
(1,904)	1:83:A:ALA:HB3	1:19:A:ASN:HD22	7	0.13	0.02	0.13
(1,1988)	1:156:A:HIS:H	1:156:A:HIS:HD2	7	0.13	0.02	0.13
(1,390)	1:117:A:ARG:HG3	1:117:A:ARG:HA	7	0.12	0.02	0.12
(1,1818)	1:36:A:THR:HG21	1:31:A:ASN:HD22	7	0.12	0.01	0.12
(1,1818)	1:36:A:THR:HG22	1:31:A:ASN:HD22	7	0.12	0.01	0.12
(1,1818)	1:36:A:THR:HG23	1:31:A:ASN:HD22	7	0.12	0.01	0.12
(1,198)	1:112:A:ASP:H	1:111:A:VAL:HB	7	0.11	0.01	0.12
(1,245)	1:81:A:MET:HG3	1:85:A:LYS:HB3	6	1.4	1.45	1.03
(1,49)	1:159:A:THR:H	1:158:A:LYS:HE2	6	1.07	0.57	1.35
(1,1244)	1:7:A:PRO:HD2	1:6:A:ARG:HD2	6	0.87	0.23	0.9
(1,380)	1:81:A:MET:HG3	1:86:A:ILE:HG12	6	0.82	0.67	0.74
(1,1111)	1:117:A:ARG:HD3	1:116:A:MET:HA	6	0.79	0.56	0.73
(1,387)	1:86:A:ILE:HG21	1:76:A:PRO:HG3	6	0.68	1.05	0.24
(1,387)	1:86:A:ILE:HG22	1:76:A:PRO:HG3	6	0.68	1.05	0.24
(1,387)	1:86:A:ILE:HG23	1:76:A:PRO:HG3	6	0.68	1.05	0.24
(1,1245)	1:6:A:ARG:HD3	1:7:A:PRO:HD2	6	0.64	0.67	0.35
(1,1553)	1:93:A:LEU:H	1:92:A:LYS:HB2	6	0.51	0.3	0.56
(1,1054)	1:92:A:LYS:HA	1:92:A:LYS:HG2	6	0.5	0.05	0.5
(1,61)	1:122:A:LYS:HE3	1:141:A:TYR:HE1	6	0.49	0.35	0.38
(1,61)	1:122:A:LYS:HE3	1:141:A:TYR:HE2	6	0.49	0.35	0.38
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD21	6	0.46	0.38	0.38
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD22	6	0.46	0.38	0.38
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD23	6	0.46	0.38	0.38
(1,135)	1:74:A:THR:HG21	1:38:A:GLU:HG2	6	0.46	0.28	0.43
(1,135)	1:74:A:THR:HG22	1:38:A:GLU:HG2	6	0.46	0.28	0.43
(1,135)	1:74:A:THR:HG23	1:38:A:GLU:HG2	6	0.46	0.28	0.43
(1,1628)	1:148:A:LEU:H	1:147:A:GLU:HG2	6	0.44	0.07	0.45
(1,763)	1:155:A:THR:HG21	1:156:A:HIS:HB2	6	0.42	0.11	0.44
(1,763)	1:155:A:THR:HG22	1:156:A:HIS:HB2	6	0.42	0.11	0.44
(1,763)	1:155:A:THR:HG23	1:156:A:HIS:HB2	6	0.42	0.11	0.44
(1,353)	1:139:A:THR:HB	1:137:A:GLU:HG2	6	0.42	0.34	0.25
(1,2013)	1:151:A:LYS:HE3	1:152:A:TYR:HE1	6	0.42	0.38	0.26
(1,2013)	1:151:A:LYS:HE3	1:152:A:TYR:HE2	6	0.42	0.38	0.26
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD21	6	0.42	0.19	0.3
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD22	6	0.42	0.19	0.3
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD23	6	0.42	0.19	0.3
(1,585)	1:101:A:LYS:HG3	1:102:A:TYR:H	6	0.3	0.11	0.32
(1,122)	1:94:A:ASP:HB3	1:97:A:ILE:HB	6	0.29	0.22	0.18
(1,178)	1:136:A:ALA:HB1	1:137:A:GLU:HG2	6	0.27	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)
(1,178)	1:136:A:ALA:HB2	1:137:A:GLU:HG2	6	0.27	0.14	0.22
(1,178)	1:136:A:ALA:HB3	1:137:A:GLU:HG2	6	0.27	0.14	0.22
(1,921)	1:89:A:LYS:HA	1:89:A:LYS:HB2	6	0.25	0.01	0.26
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG21	6	0.23	0.06	0.26
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG22	6	0.23	0.06	0.26
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG23	6	0.23	0.06	0.26
(1,897)	1:52:A:GLU:HA	1:52:A:GLU:HG2	6	0.19	0.07	0.16
(1,105)	1:31:A:ASN:HB3	1:32:A:PHE:H	6	0.18	0.04	0.16
(1,566)	1:46:A:LEU:HD11	1:43:A:SER:HB3	6	0.17	0.05	0.16
(1,566)	1:46:A:LEU:HD12	1:43:A:SER:HB3	6	0.17	0.05	0.16
(1,566)	1:46:A:LEU:HD13	1:43:A:SER:HB3	6	0.17	0.05	0.16
(1,591)	1:49:A:LYS:HE2	1:49:A:LYS:HG2	6	0.17	0.08	0.15
(1,591)	1:49:A:LYS:HE3	1:49:A:LYS:HG2	6	0.17	0.08	0.15
(1,1901)	1:103:A:GLU:H	1:102:A:TYR:HD1	6	0.16	0.03	0.16
(1,1901)	1:103:A:GLU:H	1:102:A:TYR:HD2	6	0.16	0.03	0.16
(1,1311)	1:107:A:ASP:H	1:107:A:ASP:HB2	6	0.12	0.02	0.12
(1,1524)	1:117:A:ARG:H	1:116:A:MET:H	6	0.12	0.01	0.12
(1,1295)	1:108:A:LEU:H	1:107:A:ASP:H	6	0.11	0.01	0.11
(1,118)	1:19:A:ASN:HB3	1:16:A:GLU:HA	5	1.26	0.41	1.49
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB1	5	0.56	0.22	0.58
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB2	5	0.56	0.22	0.58
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB3	5	0.56	0.22	0.58
(1,435)	1:7:A:PRO:HD2	1:6:A:ARG:HG2	5	0.48	0.5	0.3
(1,1907)	1:64:A:ASP:HB3	1:57:A:TYR:HD1	5	0.45	0.34	0.25
(1,1907)	1:64:A:ASP:HB3	1:57:A:TYR:HD2	5	0.45	0.34	0.25
(1,363)	1:75:A:ARG:HD3	1:75:A:ARG:HB2	5	0.45	0.15	0.51
(1,936)	1:9:A:ALA:HB1	1:10:A:ASP:HB3	5	0.4	0.08	0.4
(1,936)	1:9:A:ALA:HB2	1:10:A:ASP:HB3	5	0.4	0.08	0.4
(1,936)	1:9:A:ALA:HB3	1:10:A:ASP:HB3	5	0.4	0.08	0.4
(1,116)	1:19:A:ASN:H	1:19:A:ASN:HB3	5	0.39	0.03	0.4
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD21	5	0.36	0.04	0.39
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD22	5	0.36	0.04	0.39
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD23	5	0.36	0.04	0.39
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD21	5	0.36	0.04	0.39
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD22	5	0.36	0.04	0.39
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD23	5	0.36	0.04	0.39
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD21	5	0.36	0.04	0.39
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD22	5	0.36	0.04	0.39
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD23	5	0.36	0.04	0.39
(1,815)	1:38:A:GLU:HG3	1:38:A:GLU:HA	5	0.36	0.07	0.36
(1,1206)	1:108:A:LEU:H	1:107:A:ASP:HA	5	0.32	0.04	0.34
(1,155)	1:103:A:GLU:HG3	1:103:A:GLU:HB3	5	0.31	0.01	0.31

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,719)	1:144:A:LEU:HB2	1:141:A:TYR:HA	5	0.29	0.19	0.15
(1,174)	1:137:A:GLU:H	1:137:A:GLU:HG2	5	0.28	0.05	0.27
(1,1275)	1:2:A:GLU:H	1:3:A:ALA:H	5	0.2	0.01	0.2
(1,1328)	1:2:A:GLU:HB2	1:2:A:GLU:H	5	0.2	0.08	0.17
(1,1876)	1:49:A:LYS:HB3	1:50:A:GLY:H	5	0.18	0.05	0.2
(1,300)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	5	0.18	0.04	0.19
(1,529)	1:92:A:LYS:H	1:92:A:LYS:HD2	5	0.16	0.05	0.17
(1,529)	1:92:A:LYS:H	1:92:A:LYS:HD3	5	0.16	0.05	0.17
(1,237)	1:148:A:LEU:HA	1:151:A:LYS:HB3	5	0.16	0.04	0.16
(1,30)	1:6:A:ARG:HA	1:6:A:ARG:HD2	5	0.16	0.06	0.13
(1,30)	1:6:A:ARG:HA	1:6:A:ARG:HD3	5	0.16	0.06	0.13
(1,765)	1:155:A:THR:H	1:155:A:THR:HG21	5	0.15	0.04	0.14
(1,765)	1:155:A:THR:H	1:155:A:THR:HG22	5	0.15	0.04	0.14
(1,765)	1:155:A:THR:H	1:155:A:THR:HG23	5	0.15	0.04	0.14
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE1	5	0.14	0.02	0.14
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE2	5	0.14	0.02	0.14
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE3	5	0.14	0.02	0.14
(1,979)	1:119:A:ALA:HB1	1:122:A:LYS:HD2	5	0.13	0.02	0.13
(1,979)	1:119:A:ALA:HB2	1:122:A:LYS:HD2	5	0.13	0.02	0.13
(1,979)	1:119:A:ALA:HB3	1:122:A:LYS:HD2	5	0.13	0.02	0.13
(1,1590)	1:55:A:LEU:H	1:100:A:LEU:HG	5	0.12	0.01	0.11
(1,1883)	1:49:A:LYS:H	1:48:A:THR:H	5	0.11	0.0	0.11
(1,1322)	1:46:A:LEU:H	1:43:A:SER:HB2	5	0.11	0.0	0.11
(1,1322)	1:46:A:LEU:H	1:43:A:SER:HB3	5	0.11	0.0	0.11
(1,577)	1:106:A:LEU:HD11	1:124:A:ILE:HG12	5	0.11	0.01	0.1
(1,577)	1:106:A:LEU:HD12	1:124:A:ILE:HG12	5	0.11	0.01	0.1
(1,577)	1:106:A:LEU:HD13	1:124:A:ILE:HG12	5	0.11	0.01	0.1
(1,577)	1:106:A:LEU:HD21	1:124:A:ILE:HG12	5	0.11	0.01	0.1
(1,577)	1:106:A:LEU:HD22	1:124:A:ILE:HG12	5	0.11	0.01	0.1
(1,577)	1:106:A:LEU:HD23	1:124:A:ILE:HG12	5	0.11	0.01	0.1
(1,69)	1:87:A:CYS:HA	1:90:A:LEU:HB3	4	1.37	0.54	1.52
(1,384)	1:96:A:GLN:HB3	1:58:A:TYR:HD1	4	1.33	0.8	1.06
(1,384)	1:96:A:GLN:HB3	1:58:A:TYR:HD2	4	1.33	0.8	1.06
(1,400)	1:59:A:LEU:HA	1:69:A:ILE:HG12	4	0.98	0.39	0.99
(1,535)	1:86:A:ILE:HA	1:89:A:LYS:HG2	4	0.87	0.54	0.8
(1,205)	1:158:A:LYS:HB2	1:158:A:LYS:HE2	4	0.76	0.29	0.88
(1,20)	1:114:A:ARG:HB2	1:114:A:ARG:HD2	4	0.73	0.03	0.74
(1,136)	1:38:A:GLU:HG3	1:74:A:THR:HG21	4	0.6	0.26	0.7
(1,136)	1:38:A:GLU:HG3	1:74:A:THR:HG22	4	0.6	0.26	0.7
(1,136)	1:38:A:GLU:HG3	1:74:A:THR:HG23	4	0.6	0.26	0.7
(1,1899)	1:69:A:ILE:HG12	1:60:A:GLY:H	4	0.6	0.44	0.5
(1,530)	1:92:A:LYS:HB3	1:92:A:LYS:HD2	4	0.51	0.13	0.44

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,530)	1:92:A:LYS:HB2	1:92:A:LYS:HD2	4	0.51	0.13	0.44
(1,1450)	1:96:A:GLN:H	1:94:A:ASP:HB2	4	0.48	0.28	0.38
(1,2008)	1:64:A:ASP:HB3	1:57:A:TYR:HE1	4	0.43	0.2	0.36
(1,2008)	1:64:A:ASP:HB3	1:57:A:TYR:HE2	4	0.43	0.2	0.36
(1,727)	1:62:A:THR:HG21	1:56:A:CYS:HB2	4	0.36	0.13	0.39
(1,727)	1:62:A:THR:HG22	1:56:A:CYS:HB2	4	0.36	0.13	0.39
(1,727)	1:62:A:THR:HG23	1:56:A:CYS:HB2	4	0.36	0.13	0.39
(1,1939)	1:55:A:LEU:HD21	1:17:A:PHE:HE1	4	0.36	0.2	0.32
(1,1939)	1:55:A:LEU:HD21	1:17:A:PHE:HE2	4	0.36	0.2	0.32
(1,1939)	1:55:A:LEU:HD22	1:17:A:PHE:HE1	4	0.36	0.2	0.32
(1,1939)	1:55:A:LEU:HD22	1:17:A:PHE:HE2	4	0.36	0.2	0.32
(1,1939)	1:55:A:LEU:HD23	1:17:A:PHE:HE1	4	0.36	0.2	0.32
(1,1939)	1:55:A:LEU:HD23	1:17:A:PHE:HE2	4	0.36	0.2	0.32
(1,1937)	1:58:A:TYR:HD1	1:97:A:ILE:HG13	4	0.33	0.21	0.3
(1,1937)	1:58:A:TYR:HD2	1:97:A:ILE:HG13	4	0.33	0.21	0.3
(1,959)	1:24:A:SER:HB3	1:21:A:PHE:HA	4	0.31	0.09	0.32
(1,439)	1:147:A:GLU:HG2	1:144:A:LEU:HG	4	0.29	0.16	0.24
(1,642)	1:54:A:ARG:HD3	1:100:A:LEU:HD21	4	0.28	0.09	0.32
(1,642)	1:54:A:ARG:HD3	1:100:A:LEU:HD22	4	0.28	0.09	0.32
(1,642)	1:54:A:ARG:HD3	1:100:A:LEU:HD23	4	0.28	0.09	0.32
(1,29)	1:117:A:ARG:HD3	1:117:A:ARG:HG3	4	0.25	0.01	0.25
(1,1677)	1:79:A:VAL:H	1:80:A:HIS:H	4	0.25	0.02	0.26
(1,906)	1:82:A:PRO:HB3	1:83:A:ALA:HB1	4	0.23	0.12	0.18
(1,906)	1:82:A:PRO:HB3	1:83:A:ALA:HB2	4	0.23	0.12	0.18
(1,906)	1:82:A:PRO:HB3	1:83:A:ALA:HB3	4	0.23	0.12	0.18
(1,1310)	1:107:A:ASP:HB3	1:107:A:ASP:H	4	0.2	0.07	0.2
(1,1972)	1:20:A:ARG:HB3	1:44:A:PHE:HZ	4	0.2	0.06	0.17
(1,298)	1:99:A:GLU:HB3	1:99:A:GLU:HG3	4	0.19	0.0	0.19
(1,1091)	1:14:A:CYS:HA	1:97:A:ILE:HG21	4	0.19	0.13	0.12
(1,1091)	1:14:A:CYS:HA	1:97:A:ILE:HG22	4	0.19	0.13	0.12
(1,1091)	1:14:A:CYS:HA	1:97:A:ILE:HG23	4	0.19	0.13	0.12
(1,942)	1:79:A:VAL:HG21	1:80:A:HIS:H	4	0.18	0.03	0.2
(1,942)	1:79:A:VAL:HG22	1:80:A:HIS:H	4	0.18	0.03	0.2
(1,942)	1:79:A:VAL:HG23	1:80:A:HIS:H	4	0.18	0.03	0.2
(1,219)	1:131:A:GLU:HB3	1:131:A:GLU:HG2	4	0.16	0.02	0.16
(1,1787)	1:73:A:VAL:H	1:71:A:SER:HA	4	0.16	0.01	0.16
(1,762)	1:105:A:THR:H	1:105:A:THR:HG21	4	0.15	0.04	0.14
(1,762)	1:105:A:THR:H	1:105:A:THR:HG22	4	0.15	0.04	0.14
(1,762)	1:105:A:THR:H	1:105:A:THR:HG23	4	0.15	0.04	0.14
(1,910)	1:108:A:LEU:H	1:153:A:ALA:HB1	4	0.15	0.03	0.14
(1,910)	1:108:A:LEU:H	1:153:A:ALA:HB2	4	0.15	0.03	0.14
(1,910)	1:108:A:LEU:H	1:153:A:ALA:HB3	4	0.15	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)
(1,262)	1:84:A:MET:H	1:85:A:LYS:HB2	4	0.14	0.05	0.12
(1,262)	1:84:A:MET:H	1:85:A:LYS:HB3	4	0.14	0.05	0.12
(1,415)	1:113:A:LEU:H	1:113:A:LEU:HG	4	0.14	0.02	0.14
(1,12)	1:28:A:ARG:H	1:28:A:ARG:HD2	4	0.13	0.01	0.13
(1,12)	1:28:A:ARG:H	1:28:A:ARG:HD3	4	0.13	0.01	0.13
(1,603)	1:111:A:VAL:H	1:110:A:SER:HB3	4	0.12	0.02	0.12
(1,1429)	1:155:A:THR:HB	1:156:A:HIS:H	4	0.12	0.01	0.12
(1,422)	1:106:A:LEU:HG	1:107:A:ASP:H	4	0.12	0.01	0.12
(1,1197)	1:156:A:HIS:HA	1:157:A:PRO:HD2	4	0.11	0.01	0.1
(1,445)	1:90:A:LEU:HD11	1:73:A:VAL:H	3	2.02	2.64	0.19
(1,445)	1:90:A:LEU:HD12	1:73:A:VAL:H	3	2.02	2.64	0.19
(1,445)	1:90:A:LEU:HD13	1:73:A:VAL:H	3	2.02	2.64	0.19
(1,361)	1:58:A:TYR:HE1	1:96:A:GLN:HB3	3	1.44	0.37	1.21
(1,361)	1:58:A:TYR:HE2	1:96:A:GLN:HB3	3	1.44	0.37	1.21
(1,1272)	1:106:A:LEU:HD21	1:128:A:TRP:HE1	3	0.91	0.14	0.98
(1,1272)	1:106:A:LEU:HD22	1:128:A:TRP:HE1	3	0.91	0.14	0.98
(1,1272)	1:106:A:LEU:HD23	1:128:A:TRP:HE1	3	0.91	0.14	0.98
(1,1915)	1:140:A:ASP:HB3	1:141:A:TYR:HD1	3	0.86	0.4	1.1
(1,1915)	1:140:A:ASP:HB3	1:141:A:TYR:HD2	3	0.86	0.4	1.1
(1,175)	1:137:A:GLU:HG3	1:137:A:GLU:H	3	0.77	0.21	0.87
(1,1716)	1:143:A:ASN:HB3	1:143:A:ASN:H	3	0.68	0.02	0.67
(1,436)	1:6:A:ARG:HG3	1:7:A:PRO:HD2	3	0.68	0.42	0.7
(1,93)	1:64:A:ASP:HB3	1:57:A:TYR:HD1	3	0.58	0.29	0.77
(1,93)	1:64:A:ASP:HB3	1:57:A:TYR:HD2	3	0.58	0.29	0.77
(1,1352)	1:25:A:LEU:HA	1:27:A:ASP:H	3	0.55	0.59	0.14
(1,1165)	1:117:A:ARG:HD3	1:117:A:ARG:HA	3	0.54	0.33	0.39
(1,32)	1:6:A:ARG:HG3	1:6:A:ARG:HD2	3	0.5	0.02	0.5
(1,43)	1:51:A:LYS:HE2	1:51:A:LYS:HG2	3	0.41	0.2	0.54
(1,204)	1:158:A:LYS:HE3	1:158:A:LYS:HB3	3	0.39	0.14	0.38
(1,176)	1:137:A:GLU:HB3	1:137:A:GLU:HG2	3	0.34	0.02	0.34
(1,1839)	1:114:A:ARG:H	1:114:A:ARG:HG3	3	0.34	0.27	0.17
(1,588)	1:63:A:LYS:HG3	1:63:A:LYS:HB2	3	0.33	0.01	0.33
(1,89)	1:47:A:ASP:H	1:47:A:ASP:HB2	3	0.31	0.01	0.3
(1,510)	1:115:A:LYS:H	1:115:A:LYS:HG3	3	0.27	0.04	0.24
(1,203)	1:158:A:LYS:HB3	1:158:A:LYS:HE2	3	0.26	0.12	0.26
(1,677)	1:59:A:LEU:HB3	1:56:A:CYS:HA	3	0.25	0.12	0.2
(1,2007)	1:57:A:TYR:HE1	1:64:A:ASP:HB2	3	0.23	0.14	0.18
(1,2007)	1:57:A:TYR:HE2	1:64:A:ASP:HB2	3	0.23	0.14	0.18
(1,1059)	1:54:A:ARG:HA	1:57:A:TYR:HB2	3	0.23	0.04	0.23
(1,169)	1:16:A:GLU:HA	1:16:A:GLU:HG2	3	0.22	0.15	0.13
(1,1142)	1:143:A:ASN:HA	1:143:A:ASN:HB2	3	0.22	0.01	0.22
(1,386)	1:77:A:MET:H	1:76:A:PRO:HG3	3	0.21	0.12	0.13

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,790)	1:95:A:SER:HA	1:91:A:LYS:HA	3	0.2	0.05	0.24
(1,1056)	1:116:A:MET:HG3	1:113:A:LEU:HA	3	0.19	0.04	0.17
(1,1308)	1:67:A:THR:HG21	1:66:A:ALA:H	3	0.19	0.06	0.16
(1,1308)	1:67:A:THR:HG22	1:66:A:ALA:H	3	0.19	0.06	0.16
(1,1308)	1:67:A:THR:HG23	1:66:A:ALA:H	3	0.19	0.06	0.16
(1,98)	1:121:A:LEU:HD11	1:141:A:TYR:HB2	3	0.16	0.01	0.16
(1,98)	1:121:A:LEU:HD12	1:141:A:TYR:HB2	3	0.16	0.01	0.16
(1,98)	1:121:A:LEU:HD13	1:141:A:TYR:HB2	3	0.16	0.01	0.16
(1,1473)	1:101:A:LYS:HB2	1:102:A:TYR:H	3	0.16	0.05	0.14
(1,514)	1:115:A:LYS:H	1:115:A:LYS:HG2	3	0.16	0.02	0.15
(1,322)	1:115:A:LYS:H	1:114:A:ARG:HB2	3	0.15	0.04	0.15
(1,964)	1:69:A:ILE:HA	1:70:A:LEU:HA	3	0.15	0.01	0.14
(1,213)	1:159:A:THR:H	1:158:A:LYS:HB2	3	0.14	0.02	0.15
(1,260)	1:86:A:ILE:HA	1:89:A:LYS:HB2	3	0.14	0.02	0.12
(1,260)	1:86:A:ILE:HA	1:89:A:LYS:HB3	3	0.14	0.02	0.12
(1,1446)	1:96:A:GLN:HG3	1:96:A:GLN:H	3	0.14	0.01	0.13
(1,1824)	1:31:A:ASN:HD21	1:32:A:PHE:HA	3	0.12	0.03	0.11
(1,1174)	1:49:A:LYS:HA	1:49:A:LYS:HG2	3	0.12	0.0	0.12
(1,1174)	1:49:A:LYS:HA	1:49:A:LYS:HG3	3	0.12	0.0	0.12
(1,931)	1:153:A:ALA:HB1	1:154:A:ALA:H	3	0.11	0.01	0.11
(1,931)	1:153:A:ALA:HB2	1:154:A:ALA:H	3	0.11	0.01	0.11
(1,931)	1:153:A:ALA:HB3	1:154:A:ALA:H	3	0.11	0.01	0.11
(1,1027)	1:124:A:ILE:HG21	1:116:A:MET:HE1	3	0.11	0.01	0.12
(1,1027)	1:124:A:ILE:HG21	1:116:A:MET:HE2	3	0.11	0.01	0.12
(1,1027)	1:124:A:ILE:HG21	1:116:A:MET:HE3	3	0.11	0.01	0.12
(1,1027)	1:124:A:ILE:HG22	1:116:A:MET:HE1	3	0.11	0.01	0.12
(1,1027)	1:124:A:ILE:HG22	1:116:A:MET:HE2	3	0.11	0.01	0.12
(1,1027)	1:124:A:ILE:HG22	1:116:A:MET:HE3	3	0.11	0.01	0.12
(1,1027)	1:124:A:ILE:HG23	1:116:A:MET:HE1	3	0.11	0.01	0.12
(1,1027)	1:124:A:ILE:HG23	1:116:A:MET:HE2	3	0.11	0.01	0.12
(1,1027)	1:124:A:ILE:HG23	1:116:A:MET:HE3	3	0.11	0.01	0.12
(1,1064)	1:77:A:MET:HE1	1:22:A:TYR:HA	3	0.11	0.01	0.11
(1,1064)	1:77:A:MET:HE2	1:22:A:TYR:HA	3	0.11	0.01	0.11
(1,1064)	1:77:A:MET:HE3	1:22:A:TYR:HA	3	0.11	0.01	0.11
(1,809)	1:27:A:ASP:HB2	1:24:A:SER:HA	2	2.92	1.76	2.92
(1,379)	1:86:A:ILE:HG12	1:81:A:MET:HG2	2	1.45	1.15	1.45
(1,170)	1:140:A:ASP:H	1:137:A:GLU:HG2	2	1.12	0.02	1.12
(1,1451)	1:94:A:ASP:HB3	1:96:A:GLN:H	2	1.04	0.03	1.04
(1,1667)	1:30:A:VAL:HG11	1:28:A:ARG:HE	2	0.8	0.68	0.8
(1,1667)	1:30:A:VAL:HG12	1:28:A:ARG:HE	2	0.8	0.68	0.8
(1,1667)	1:30:A:VAL:HG13	1:28:A:ARG:HE	2	0.8	0.68	0.8
(1,1648)	1:94:A:ASP:HB3	1:97:A:ILE:H	2	0.77	0.66	0.77

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,119)	1:58:A:TYR:HB2	1:97:A:ILE:HD11	2	0.76	0.34	0.76
(1,119)	1:58:A:TYR:HB2	1:97:A:ILE:HD12	2	0.76	0.34	0.76
(1,119)	1:58:A:TYR:HB2	1:97:A:ILE:HD13	2	0.76	0.34	0.76
(1,206)	1:158:A:LYS:HE3	1:158:A:LYS:HB2	2	0.55	0.21	0.55
(1,431)	1:141:A:TYR:HB3	1:121:A:LEU:HD21	2	0.55	0.22	0.55
(1,431)	1:141:A:TYR:HB3	1:121:A:LEU:HD22	2	0.55	0.22	0.55
(1,431)	1:141:A:TYR:HB3	1:121:A:LEU:HD23	2	0.55	0.22	0.55
(1,907)	1:18:A:LEU:HB3	1:83:A:ALA:HB1	2	0.53	0.31	0.53
(1,907)	1:18:A:LEU:HB3	1:83:A:ALA:HB2	2	0.53	0.31	0.53
(1,907)	1:18:A:LEU:HB3	1:83:A:ALA:HB3	2	0.53	0.31	0.53
(1,1412)	1:124:A:ILE:H	1:123:A:GLN:HB2	2	0.53	0.16	0.53
(1,1987)	1:157:A:PRO:HD2	1:156:A:HIS:HD2	2	0.5	0.25	0.5
(1,261)	1:28:A:ARG:HB3	1:29:A:GLY:H	2	0.48	0.12	0.48
(1,84)	1:47:A:ASP:HB3	1:48:A:THR:HG21	2	0.45	0.16	0.45
(1,84)	1:47:A:ASP:HB3	1:48:A:THR:HG22	2	0.45	0.16	0.45
(1,84)	1:47:A:ASP:HB3	1:48:A:THR:HG23	2	0.45	0.16	0.45
(1,1427)	1:63:A:LYS:HB3	1:63:A:LYS:H	2	0.45	0.02	0.45
(1,826)	1:111:A:VAL:HG11	1:116:A:MET:HE1	2	0.43	0.03	0.43
(1,826)	1:111:A:VAL:HG11	1:116:A:MET:HE2	2	0.43	0.03	0.43
(1,826)	1:111:A:VAL:HG11	1:116:A:MET:HE3	2	0.43	0.03	0.43
(1,826)	1:111:A:VAL:HG12	1:116:A:MET:HE1	2	0.43	0.03	0.43
(1,826)	1:111:A:VAL:HG12	1:116:A:MET:HE2	2	0.43	0.03	0.43
(1,826)	1:111:A:VAL:HG12	1:116:A:MET:HE3	2	0.43	0.03	0.43
(1,826)	1:111:A:VAL:HG13	1:116:A:MET:HE1	2	0.43	0.03	0.43
(1,826)	1:111:A:VAL:HG13	1:116:A:MET:HE2	2	0.43	0.03	0.43
(1,826)	1:111:A:VAL:HG13	1:116:A:MET:HE3	2	0.43	0.03	0.43
(1,890)	1:65:A:ALA:HB1	1:64:A:ASP:HB2	2	0.4	0.08	0.4
(1,890)	1:65:A:ALA:HB2	1:64:A:ASP:HB2	2	0.4	0.08	0.4
(1,890)	1:65:A:ALA:HB3	1:64:A:ASP:HB2	2	0.4	0.08	0.4
(1,855)	1:61:A:ALA:HB1	1:45:A:CYS:HB3	2	0.39	0.0	0.39
(1,855)	1:61:A:ALA:HB2	1:45:A:CYS:HB3	2	0.39	0.0	0.39
(1,855)	1:61:A:ALA:HB3	1:45:A:CYS:HB3	2	0.39	0.0	0.39
(1,1777)	1:28:A:ARG:H	1:28:A:ARG:HB2	2	0.36	0.01	0.36
(1,1602)	1:54:A:ARG:HD2	1:54:A:ARG:H	2	0.34	0.18	0.34
(1,671)	1:113:A:LEU:HB3	1:142:A:VAL:HG11	2	0.34	0.0	0.34
(1,671)	1:113:A:LEU:HB3	1:142:A:VAL:HG12	2	0.34	0.0	0.34
(1,671)	1:113:A:LEU:HB3	1:142:A:VAL:HG13	2	0.34	0.0	0.34
(1,1223)	1:10:A:ASP:H	1:9:A:ALA:HA	2	0.34	0.01	0.34
(1,92)	1:64:A:ASP:HB3	1:57:A:TYR:HE1	2	0.33	0.16	0.33
(1,92)	1:64:A:ASP:HB3	1:57:A:TYR:HE2	2	0.33	0.16	0.33
(1,41)	1:51:A:LYS:HE3	1:51:A:LYS:HG2	2	0.32	0.22	0.32
(1,151)	1:103:A:GLU:H	1:103:A:GLU:HG2	2	0.32	0.05	0.32

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,151)	1:103:A:GLU:H	1:103:A:GLU:HG3	2	0.32	0.05	0.32
(1,701)	1:71:A:SER:HB3	1:71:A:SER:HA	2	0.32	0.02	0.32
(1,1358)	1:65:A:ALA:H	1:63:A:LYS:HB2	2	0.3	0.16	0.3
(1,1870)	1:29:A:GLY:H	1:26:A:ILE:HG21	2	0.26	0.1	0.26
(1,1870)	1:29:A:GLY:H	1:26:A:ILE:HG22	2	0.26	0.1	0.26
(1,1870)	1:29:A:GLY:H	1:26:A:ILE:HG23	2	0.26	0.1	0.26
(1,54)	1:151:A:LYS:HE2	1:151:A:LYS:HG3	2	0.25	0.01	0.25
(1,54)	1:151:A:LYS:HE3	1:151:A:LYS:HG3	2	0.25	0.01	0.25
(1,1951)	1:44:A:PHE:HE1	1:24:A:SER:HB3	2	0.25	0.03	0.25
(1,1951)	1:44:A:PHE:HE2	1:24:A:SER:HB3	2	0.25	0.03	0.25
(1,280)	1:104:A:LYS:H	1:103:A:GLU:HB3	2	0.24	0.04	0.24
(1,171)	1:137:A:GLU:HG3	1:140:A:ASP:H	2	0.24	0.02	0.24
(1,655)	1:161:A:LEU:HA	1:161:A:LEU:HD11	2	0.24	0.05	0.24
(1,655)	1:161:A:LEU:HA	1:161:A:LEU:HD12	2	0.24	0.05	0.24
(1,655)	1:161:A:LEU:HA	1:161:A:LEU:HD13	2	0.24	0.05	0.24
(1,1038)	1:121:A:LEU:HD11	1:121:A:LEU:HA	2	0.23	0.09	0.23
(1,1038)	1:121:A:LEU:HD12	1:121:A:LEU:HA	2	0.23	0.09	0.23
(1,1038)	1:121:A:LEU:HD13	1:121:A:LEU:HA	2	0.23	0.09	0.23
(1,274)	1:73:A:VAL:HA	1:76:A:PRO:HB2	2	0.22	0.04	0.22
(1,602)	1:55:A:LEU:HD11	1:100:A:LEU:HG	2	0.2	0.06	0.2
(1,602)	1:55:A:LEU:HD12	1:100:A:LEU:HG	2	0.2	0.06	0.2
(1,602)	1:55:A:LEU:HD13	1:100:A:LEU:HG	2	0.2	0.06	0.2
(1,497)	1:93:A:LEU:HD11	1:90:A:LEU:HA	2	0.2	0.08	0.2
(1,497)	1:93:A:LEU:HD12	1:90:A:LEU:HA	2	0.2	0.08	0.2
(1,497)	1:93:A:LEU:HD13	1:90:A:LEU:HA	2	0.2	0.08	0.2
(1,252)	1:151:A:LYS:HB3	1:152:A:TYR:HD1	2	0.2	0.05	0.2
(1,252)	1:151:A:LYS:HB3	1:152:A:TYR:HD2	2	0.2	0.05	0.2
(1,1499)	1:90:A:LEU:H	1:86:A:ILE:HA	2	0.2	0.01	0.2
(1,1278)	1:127:A:SER:HB3	1:128:A:TRP:HE1	2	0.19	0.06	0.19
(1,929)	1:23:A:LYS:HB3	1:23:A:LYS:HA	2	0.18	0.01	0.18
(1,993)	1:63:A:LYS:HA	1:63:A:LYS:HB2	2	0.18	0.02	0.18
(1,1235)	1:61:A:ALA:HA	1:42:A:ILE:HG13	2	0.18	0.04	0.18
(1,1326)	1:1:A:GLN:HA	1:2:A:GLU:H	2	0.18	0.02	0.18
(1,782)	1:155:A:THR:HA	1:156:A:HIS:H	2	0.17	0.01	0.17
(1,1128)	1:103:A:GLU:HB3	1:103:A:GLU:HA	2	0.16	0.01	0.16
(1,537)	1:70:A:LEU:HD21	1:68:A:LYS:HG2	2	0.16	0.06	0.16
(1,537)	1:70:A:LEU:HD22	1:68:A:LYS:HG2	2	0.16	0.06	0.16
(1,537)	1:70:A:LEU:HD23	1:68:A:LYS:HG2	2	0.16	0.06	0.16
(1,537)	1:70:A:LEU:HD21	1:68:A:LYS:HG3	2	0.16	0.06	0.16
(1,537)	1:70:A:LEU:HD22	1:68:A:LYS:HG3	2	0.16	0.06	0.16
(1,537)	1:70:A:LEU:HD23	1:68:A:LYS:HG3	2	0.16	0.06	0.16
(1,1815)	1:33:A:SER:HB2	1:31:A:ASN:HD22	2	0.16	0.05	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,188)	1:96:A:GLN:HA	1:96:A:GLN:HG2	2	0.15	0.01	0.15
(1,856)	1:59:A:LEU:HB3	1:61:A:ALA:HB1	2	0.15	0.0	0.15
(1,856)	1:59:A:LEU:HB3	1:61:A:ALA:HB2	2	0.15	0.0	0.15
(1,856)	1:59:A:LEU:HB3	1:61:A:ALA:HB3	2	0.15	0.0	0.15
(1,161)	1:3:A:ALA:HB1	1:2:A:GLU:HG2	2	0.15	0.03	0.15
(1,161)	1:3:A:ALA:HB2	1:2:A:GLU:HG2	2	0.15	0.03	0.15
(1,161)	1:3:A:ALA:HB3	1:2:A:GLU:HG2	2	0.15	0.03	0.15
(1,161)	1:3:A:ALA:HB1	1:2:A:GLU:HG3	2	0.15	0.03	0.15
(1,161)	1:3:A:ALA:HB2	1:2:A:GLU:HG3	2	0.15	0.03	0.15
(1,161)	1:3:A:ALA:HB3	1:2:A:GLU:HG3	2	0.15	0.03	0.15
(1,1368)	1:113:A:LEU:H	1:112:A:ASP:H	2	0.15	0.02	0.15
(1,1472)	1:102:A:TYR:HB2	1:102:A:TYR:H	2	0.14	0.03	0.14
(1,513)	1:121:A:LEU:HD21	1:138:A:LYS:HG2	2	0.14	0.01	0.14
(1,513)	1:121:A:LEU:HD22	1:138:A:LYS:HG2	2	0.14	0.01	0.14
(1,513)	1:121:A:LEU:HD23	1:138:A:LYS:HG2	2	0.14	0.01	0.14
(1,513)	1:121:A:LEU:HD21	1:138:A:LYS:HG3	2	0.14	0.01	0.14
(1,513)	1:121:A:LEU:HD22	1:138:A:LYS:HG3	2	0.14	0.01	0.14
(1,513)	1:121:A:LEU:HD23	1:138:A:LYS:HG3	2	0.14	0.01	0.14
(1,16)	1:20:A:ARG:HD2	1:20:A:ARG:HB2	2	0.12	0.02	0.12
(1,999)	1:114:A:ARG:HA	1:114:A:ARG:HB2	2	0.12	0.01	0.12
(1,1202)	1:59:A:LEU:HA	1:69:A:ILE:HD11	2	0.12	0.02	0.12
(1,1202)	1:59:A:LEU:HA	1:69:A:ILE:HD12	2	0.12	0.02	0.12
(1,1202)	1:59:A:LEU:HA	1:69:A:ILE:HD13	2	0.12	0.02	0.12
(1,522)	1:13:A:VAL:HA	1:55:A:LEU:HD11	2	0.12	0.01	0.12
(1,522)	1:13:A:VAL:HA	1:55:A:LEU:HD12	2	0.12	0.01	0.12
(1,522)	1:13:A:VAL:HA	1:55:A:LEU:HD13	2	0.12	0.01	0.12
(1,884)	1:61:A:ALA:HB1	1:56:A:CYS:HB2	2	0.12	0.01	0.12
(1,884)	1:61:A:ALA:HB2	1:56:A:CYS:HB2	2	0.12	0.01	0.12
(1,884)	1:61:A:ALA:HB3	1:56:A:CYS:HB2	2	0.12	0.01	0.12
(1,1750)	1:18:A:LEU:HB3	1:18:A:LEU:H	2	0.12	0.0	0.12
(1,340)	1:36:A:THR:HA	1:39:A:LYS:HD2	2	0.12	0.02	0.12
(1,340)	1:36:A:THR:HA	1:39:A:LYS:HD3	2	0.12	0.02	0.12
(1,1218)	1:67:A:THR:H	1:66:A:ALA:HA	2	0.12	0.0	0.12
(1,292)	1:105:A:THR:HB	1:105:A:THR:HA	2	0.11	0.01	0.11
(1,302)	1:155:A:THR:HB	1:155:A:THR:HA	2	0.11	0.0	0.11
(1,512)	1:115:A:LYS:HG2	1:115:A:LYS:HE2	2	0.11	0.0	0.11
(1,512)	1:115:A:LYS:HG2	1:115:A:LYS:HE3	2	0.11	0.0	0.11
(1,1003)	1:124:A:ILE:HB	1:125:A:LEU:HA	2	0.11	0.0	0.11
(1,1113)	1:111:A:VAL:HB	1:108:A:LEU:HA	2	0.11	0.0	0.11
(1,1461)	1:107:A:ASP:HA	1:109:A:ALA:H	2	0.11	0.0	0.11
(1,1930)	1:25:A:LEU:HD21	1:22:A:TYR:HD1	2	0.11	0.0	0.11
(1,1930)	1:25:A:LEU:HD21	1:22:A:TYR:HD2	2	0.11	0.0	0.11

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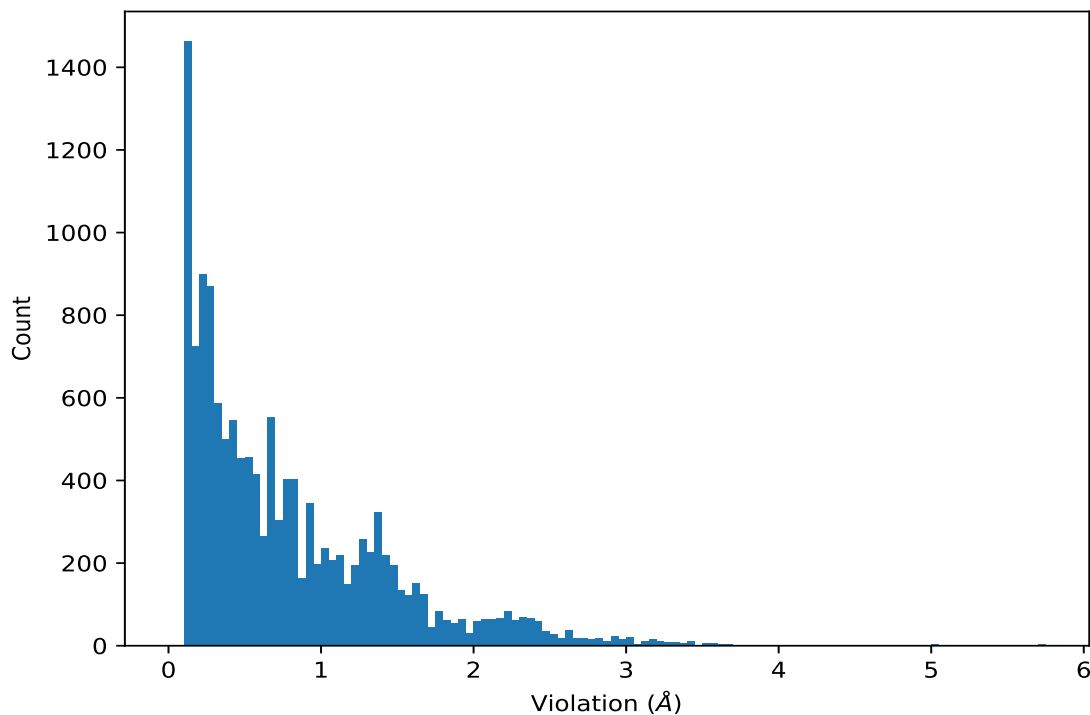
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1930)	1:25:A:LEU:HD22	1:22:A:TYR:HD1	2	0.11	0.0	0.11
(1,1930)	1:25:A:LEU:HD22	1:22:A:TYR:HD2	2	0.11	0.0	0.11
(1,1930)	1:25:A:LEU:HD23	1:22:A:TYR:HD1	2	0.11	0.0	0.11
(1,1930)	1:25:A:LEU:HD23	1:22:A:TYR:HD2	2	0.11	0.0	0.11

<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)
(1,445)	1:90:A:LEU:HD11	1:73:A:VAL:H	3	5.75
(1,445)	1:90:A:LEU:HD12	1:73:A:VAL:H	3	5.75
(1,445)	1:90:A:LEU:HD13	1:73:A:VAL:H	3	5.75
(1,244)	1:85:A:LYS:HB3	1:81:A:MET:HG2	3	5.31
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	5	5.04
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	5	5.04
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	5	5.04
(1,809)	1:27:A:ASP:HB2	1:24:A:SER:HA	4	4.67
(1,245)	1:81:A:MET:HG3	1:85:A:LYS:HB3	3	4.56
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	14	3.67
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	14	3.67
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	14	3.67
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	20	3.63
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	20	3.63
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	20	3.63
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	10	3.56
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	10	3.56
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	10	3.56
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	13	3.56
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	13	3.56
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	13	3.56
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	13	3.52
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	13	3.52
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	13	3.52
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	5	3.51
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	5	3.51
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	5	3.51
(1,1147)	1:83:A:ALA:HA	1:86:A:ILE:HG12	3	3.5
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	3	3.44
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	3	3.44
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	3	3.44
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	4	3.44
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	4	3.44
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	4	3.44
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	10	3.42
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	10	3.42
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	10	3.42
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	17	3.42
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	17	3.42
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	17	3.42
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	14	3.39
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	14	3.39
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	14	3.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1966)	1:25:A:LEU:HB2	1:32:A:PHE:HZ	4	3.35
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	19	3.35
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	19	3.35
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	19	3.35
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	7	3.33
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	7	3.33
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	7	3.33
(1,243)	1:81:A:MET:HG3	1:85:A:LYS:HB2	3	3.33
(1,243)	1:81:A:MET:HG2	1:85:A:LYS:HB2	3	3.33
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	13	3.32
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	13	3.32
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	13	3.32
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	9	3.28
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	9	3.28
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	9	3.28
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	10	3.28
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	10	3.28
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	10	3.28
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	9	3.25
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	9	3.25
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	9	3.25
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	19	3.24
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	19	3.24
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	19	3.24
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	2	3.23
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	2	3.23
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	2	3.23
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	2	3.2
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	2	3.2
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	2	3.2
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	8	3.2
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	8	3.2
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	8	3.2
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	9	3.18
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	9	3.18
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	9	3.18
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	12	3.18
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	12	3.18
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	12	3.18
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	1	3.18
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	1	3.18
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	1	3.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	16	3.17
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	16	3.17
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	16	3.17
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	14	3.16
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	14	3.16
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	14	3.16
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	12	3.15
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	12	3.15
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	12	3.15
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	16	3.14
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	16	3.14
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	16	3.14
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	1	3.12
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	1	3.12
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	1	3.12
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	15	3.11
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	15	3.11
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	15	3.11
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	11	3.09
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	11	3.09
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	11	3.09
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	6	3.05
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	6	3.05
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	6	3.05
(1,717)	1:37:A:ILE:HD11	1:78:A:SER:HA	3	3.05
(1,717)	1:37:A:ILE:HD12	1:78:A:SER:HA	3	3.05
(1,717)	1:37:A:ILE:HD13	1:78:A:SER:HA	3	3.05
(1,1135)	1:83:A:ALA:HA	1:86:A:ILE:HD11	3	3.04
(1,1135)	1:83:A:ALA:HA	1:86:A:ILE:HD12	3	3.04
(1,1135)	1:83:A:ALA:HA	1:86:A:ILE:HD13	3	3.04
(1,387)	1:86:A:ILE:HG21	1:76:A:PRO:HG3	3	3.03
(1,387)	1:86:A:ILE:HG22	1:76:A:PRO:HG3	3	3.03
(1,387)	1:86:A:ILE:HG23	1:76:A:PRO:HG3	3	3.03
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	1	3.03
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	1	3.03
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	1	3.03
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	4	3.02
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	4	3.02
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	4	3.02
(1,11)	1:8:A:GLY:HA3	1:15:A:LYS:HE3	7	3.01
(1,11)	1:8:A:GLY:HA3	1:15:A:LYS:HE3	18	3.0
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	13	2.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	13	2.98
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	13	2.98
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	18	2.97
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	18	2.97
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	18	2.97
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	18	2.96
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	18	2.96
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	18	2.96
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	10	2.96
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	10	2.96
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	10	2.96
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	15	2.95
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	15	2.95
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	15	2.95
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	10	2.94
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	10	2.94
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	10	2.94
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	14	2.93
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	14	2.93
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	14	2.93
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	20	2.93
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	20	2.93
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	20	2.93
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	16	2.92
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	16	2.92
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	16	2.92
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	3	2.91
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	3	2.91
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	3	2.91
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	7	2.91
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	7	2.91
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	7	2.91
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	4	2.91
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	4	2.91
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	4	2.91
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	19	2.91
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	19	2.91
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	19	2.91
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	14	2.89
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	14	2.89
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	14	2.89
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	13	2.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	13	2.88
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	13	2.88
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	1	2.87
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	1	2.87
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	1	2.87
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	2	2.86
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	20	2.83
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	20	2.83
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	20	2.83
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	4	2.82
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	4	2.82
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	4	2.82
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	8	2.81
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	8	2.81
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	8	2.81
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	14	2.81
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	14	2.81
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	14	2.81
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	4	2.81
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	4	2.81
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	4	2.81
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	11	2.81
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	7	2.81
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	7	2.81
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	7	2.81
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	15	2.8
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	15	2.8
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	15	2.8
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	19	2.8
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	19	2.8
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	19	2.8
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	17	2.8
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	17	2.8
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	17	2.8
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	1	2.79
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	1	2.79
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	1	2.79
(1,11)	1:8:A:GLY:HA3	1:15:A:LYS:HE3	1	2.77
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	1	2.75
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	1	2.75
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	1	2.75
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	15	2.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	15	2.73
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	15	2.73
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	5	2.73
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	5	2.73
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	5	2.73
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	11	2.72
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	11	2.72
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	11	2.72
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	6	2.71
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	6	2.71
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	6	2.71
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	10	2.7
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	10	2.7
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	10	2.7
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	7	2.7
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	7	2.7
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	7	2.7
(1,11)	1:8:A:GLY:HA3	1:15:A:LYS:HE3	14	2.68
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	8	2.67
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	8	2.67
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	8	2.67
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	17	2.67
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	17	2.67
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	17	2.67
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	3	2.67
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	3	2.67
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	3	2.67
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	3	2.66
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	3	2.66
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	3	2.66
(1,384)	1:96:A:GLN:HB3	1:58:A:TYR:HD1	5	2.66
(1,384)	1:96:A:GLN:HB3	1:58:A:TYR:HD2	5	2.66
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	14	2.66
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	14	2.66
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	14	2.66
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	14	2.65
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	14	2.65
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	14	2.65
(1,696)	1:71:A:SER:HB3	1:75:A:ARG:HD2	13	2.64
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	10	2.63
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	10	2.63
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	10	2.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	19	2.63
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	19	2.63
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	19	2.63
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	6	2.63
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	6	2.63
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	6	2.63
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	11	2.62
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	11	2.62
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	11	2.62
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	20	2.61
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	20	2.61
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	20	2.61
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	20	2.61
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	20	2.61
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	20	2.61
(1,379)	1:86:A:ILE:HG12	1:81:A:MET:HG2	3	2.61
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	5	2.61
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	5	2.61
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	5	2.61
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	3	2.6
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	3	2.6
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	3	2.6
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	16	2.6
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	16	2.6
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	16	2.6
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	17	2.6
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	17	2.6
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	17	2.6
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	20	2.6
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	20	2.6
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	20	2.6
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	9	2.59
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	9	2.59
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	9	2.59
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	7	2.59
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	7	2.59
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	7	2.59
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	20	2.59
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	20	2.59
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	20	2.59
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG11	4	2.58
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG12	4	2.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,851)	1:122:A:LYS:HD3	1:118:A:VAL:HG13	4	2.58
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	9	2.58
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	9	2.58
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	9	2.58
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	11	2.57
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	1	2.56
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	1	2.56
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	1	2.56
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	2	2.55
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	2	2.55
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	2	2.55
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	2	2.55
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	2	2.55
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	2	2.55
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	2	2.53
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	2	2.53
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	2	2.53
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	17	2.53
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	15	2.52
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	15	2.52
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	15	2.52
(1,132)	1:83:A:ALA:HA	1:86:A:ILE:HB	3	2.52
(1,11)	1:8:A:GLY:HA3	1:15:A:LYS:HE3	4	2.52
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	14	2.51
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	14	2.51
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	14	2.51
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	10	2.5
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	10	2.5
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	10	2.5
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	11	2.5
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	11	2.5
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	11	2.5
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	18	2.5
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	18	2.5
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	18	2.5
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	10	2.49
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	10	2.49
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	10	2.49
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	5	2.49
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	5	2.49
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	5	2.49
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	16	2.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	16	2.49
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	16	2.49
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	16	2.49
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	16	2.49
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	16	2.49
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	16	2.49
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	16	2.49
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	16	2.49
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	19	2.49
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	19	2.49
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	19	2.49
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	12	2.46
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	12	2.46
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	12	2.46
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	18	2.46
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	18	2.46
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	18	2.46
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	19	2.46
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	19	2.46
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	19	2.46
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	2	2.46
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	3	2.46
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	3	2.46
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	3	2.46
(1,11)	1:8:A:GLY:HA3	1:15:A:LYS:HE3	3	2.46
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	9	2.45
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	9	2.45
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	9	2.45
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	4	2.44
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	4	2.44
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	4	2.44
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	5	2.44
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	5	2.44
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	5	2.44
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	12	2.44
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	12	2.44
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	12	2.44
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	8	2.44
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	8	2.44
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	8	2.44
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	20	2.44
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	6	2.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	6	2.43
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	6	2.43
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	7	2.43
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	7	2.43
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	7	2.43
(1,389)	1:86:A:ILE:HG21	1:76:A:PRO:HG2	3	2.43
(1,389)	1:86:A:ILE:HG22	1:76:A:PRO:HG2	3	2.43
(1,389)	1:86:A:ILE:HG23	1:76:A:PRO:HG2	3	2.43
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	8	2.43
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	8	2.43
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	8	2.43
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	11	2.42
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	11	2.42
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	11	2.42
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	8	2.42
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	8	2.42
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	8	2.42
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	1	2.42
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	18	2.42
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	18	2.42
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	18	2.42
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	6	2.41
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	6	2.41
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	6	2.41
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	11	2.41
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	11	2.41
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	11	2.41
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	19	2.41
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	19	2.41
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	19	2.41
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	13	2.41
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	13	2.41
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	13	2.41
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	17	2.41
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	17	2.41
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	17	2.41
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	14	2.41
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	14	2.41
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	14	2.41
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	5	2.41
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	5	2.41
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	5	2.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	5	2.41
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	5	2.41
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	5	2.41
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	15	2.4
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	15	2.4
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	15	2.4
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	16	2.4
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	16	2.4
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	16	2.4
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	12	2.4
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	7	2.4
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	18	2.39
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	18	2.39
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	18	2.39
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	17	2.39
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	17	2.39
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	17	2.39
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	3	2.38
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	3	2.38
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	3	2.38
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	2	2.38
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	2	2.38
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	2	2.38
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	2	2.38
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	2	2.38
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	2	2.38
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	7	2.38
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	11	2.38
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	11	2.38
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	11	2.38
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	15	2.37
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	15	2.37
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	15	2.37
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	4	2.37
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	11	2.36
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	11	2.36
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	11	2.36
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	4	2.36
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	4	2.36
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	4	2.36
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	7	2.36
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	7	2.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	7	2.36
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	13	2.36
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	13	2.36
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	13	2.36
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	15	2.36
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	15	2.36
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	15	2.36
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	18	2.36
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	18	2.36
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	18	2.36
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	11	2.36
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	11	2.36
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	11	2.36
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	11	2.36
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	11	2.36
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	11	2.36
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	18	2.36
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	18	2.36
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	18	2.36
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	20	2.35
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	20	2.35
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	20	2.35
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	6	2.35
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	6	2.35
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	6	2.35
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	12	2.35
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	12	2.35
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	12	2.35
(1,1178)	1:77:A:MET:HG3	1:86:A:ILE:HD11	3	2.34
(1,1178)	1:77:A:MET:HG3	1:86:A:ILE:HD12	3	2.34
(1,1178)	1:77:A:MET:HG3	1:86:A:ILE:HD13	3	2.34
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	1	2.34
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	1	2.34
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	1	2.34
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	7	2.34
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	7	2.34
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	7	2.34
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	8	2.34
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	8	2.34
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	8	2.34
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	4	2.34
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	4	2.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	4	2.34
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	19	2.33
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	19	2.33
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	19	2.33
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	10	2.33
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	10	2.33
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	10	2.33
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	12	2.33
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	12	2.33
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	12	2.33
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	16	2.33
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	16	2.33
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	16	2.33
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	7	2.33
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	7	2.33
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	7	2.33
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	9	2.33
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	9	2.33
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	9	2.33
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	20	2.33
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	20	2.33
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	20	2.33
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	8	2.33
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	8	2.33
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	8	2.33
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	3	2.32
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	3	2.32
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	3	2.32
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	13	2.32
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	13	2.32
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	13	2.32
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	9	2.32
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	9	2.32
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	9	2.32
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	14	2.32
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	14	2.32
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	14	2.32
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	12	2.32
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	12	2.32
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	12	2.32
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	12	2.32
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	12	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	12	2.32
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	4	2.32
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	4	2.32
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	4	2.32
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	4	2.32
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	4	2.32
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	4	2.32
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	6	2.32
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	6	2.32
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	6	2.32
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	17	2.31
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	17	2.31
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	17	2.31
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	18	2.3
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	18	2.3
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	18	2.3
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	2	2.3
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	2	2.3
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	2	2.3
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	9	2.3
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	9	2.3
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	9	2.3
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	14	2.3
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	14	2.3
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	14	2.3
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	13	2.3
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	16	2.3
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	16	2.3
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	16	2.3
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	1	2.29
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	1	2.29
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	1	2.29
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	9	2.28
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	9	2.28
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	9	2.28
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	6	2.28
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	13	2.27
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	13	2.27
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	13	2.27
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	4	2.27
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	4	2.27
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	4	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	20	2.27
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	20	2.27
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	20	2.27
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	20	2.27
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	20	2.27
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	20	2.27
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	9	2.27
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	9	2.27
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	9	2.27
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	12	2.26
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	12	2.26
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	12	2.26
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	9	2.26
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	9	2.26
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	9	2.26
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	6	2.26
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	6	2.26
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	6	2.26
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	7	2.26
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	7	2.26
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	7	2.26
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	5	2.26
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	5	2.26
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	5	2.26
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	5	2.26
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	7	2.25
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	7	2.25
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	7	2.25
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	14	2.25
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	6	2.25
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	6	2.25
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	6	2.25
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	1	2.24
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	1	2.24
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	1	2.24
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	2	2.24
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	2	2.24
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	2	2.24
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	2	2.24
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	2	2.24
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	2	2.24
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	5	2.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	5	2.24
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	5	2.24
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	5	2.24
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	5	2.24
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	5	2.24
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	11	2.23
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	11	2.23
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	11	2.23
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	4	2.23
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	4	2.23
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	4	2.23
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	4	2.23
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	4	2.23
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	4	2.23
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	2	2.23
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	2	2.23
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	2	2.23
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	14	2.23
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	14	2.23
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	14	2.23
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	3	2.22
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	3	2.22
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	3	2.22
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	16	2.22
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	16	2.22
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	16	2.22
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	14	2.22
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	14	2.22
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	14	2.22
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	5	2.22
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	5	2.22
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	5	2.22
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	10	2.22
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	10	2.22
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	10	2.22
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	10	2.22
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	10	2.22
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	10	2.22
(1,244)	1:85:A:LYS:HB3	1:81:A:MET:HG2	5	2.22
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	12	2.21
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	12	2.21
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	12	2.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	8	2.21
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	8	2.21
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	8	2.21
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	9	2.21
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	9	2.21
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	9	2.21
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	9	2.21
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	9	2.21
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	9	2.21
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	13	2.21
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	13	2.21
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	13	2.21
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	1	2.2
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	1	2.2
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	1	2.2
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	19	2.2
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	19	2.2
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	19	2.2
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	5	2.2
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	5	2.2
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	5	2.2
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	8	2.2
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	8	2.2
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	8	2.2
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	12	2.2
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	12	2.2
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	12	2.2
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	2	2.2
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	2	2.2
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	2	2.2
(1,380)	1:81:A:MET:HG3	1:86:A:ILE:HG12	3	2.2
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	10	2.19
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	10	2.19
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	10	2.19
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	2	2.19
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	2	2.19
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	2	2.19
(1,696)	1:71:A:SER:HB3	1:75:A:ARG:HD2	20	2.19
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	5	2.19
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	5	2.19
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	5	2.19
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	12	2.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	12	2.18
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	12	2.18
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	15	2.18
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	15	2.18
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	15	2.18
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	2	2.18
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	2	2.18
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	2	2.18
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	13	2.18
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	13	2.18
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	13	2.18
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	13	2.18
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	13	2.18
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	13	2.18
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	15	2.18
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	15	2.18
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	15	2.18
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	14	2.17
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	14	2.17
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	14	2.17
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	14	2.17
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	14	2.17
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	14	2.17
(1,634)	1:32:A:PHE:HE1	1:26:A:ILE:HA	4	2.17
(1,634)	1:32:A:PHE:HE2	1:26:A:ILE:HA	4	2.17
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	20	2.17
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	20	2.17
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	20	2.17
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	20	2.17
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	12	2.17
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	5	2.16
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	5	2.16
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	5	2.16
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	19	2.16
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	19	2.16
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	19	2.16
(1,3)	1:15:A:LYS:HD3	1:8:A:GLY:HA2	9	2.16
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	10	2.15
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	10	2.15
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	10	2.15
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	11	2.15
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	11	2.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	11	2.15
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	18	2.15
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	18	2.15
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	18	2.15
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	16	2.15
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	16	2.15
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	16	2.15
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	13	2.15
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	13	2.15
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	13	2.15
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	17	2.15
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	17	2.15
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	17	2.15
(1,1245)	1:6:A:ARG:HD3	1:7:A:PRO:HD2	7	2.14
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	1	2.14
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	1	2.14
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	1	2.14
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	11	2.14
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	11	2.14
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	11	2.14
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	13	2.14
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	13	2.14
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	13	2.14
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	13	2.14
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	13	2.14
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	13	2.14
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	7	2.14
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	12	2.13
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	12	2.13
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	12	2.13
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	20	2.13
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	20	2.13
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	20	2.13
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	19	2.13
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	19	2.13
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	19	2.13
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	19	2.13
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	19	2.13
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	19	2.13
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	13	2.12
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	13	2.12
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	13	2.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	9	2.11
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	9	2.11
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	9	2.11
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	15	2.11
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	15	2.11
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	15	2.11
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	19	2.11
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	19	2.11
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	19	2.11
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	17	2.11
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	17	2.11
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	17	2.11
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	18	2.11
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	18	2.11
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	18	2.11
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	14	2.11
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	14	2.11
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	14	2.11
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	14	2.11
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	14	2.11
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	14	2.11
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	3	2.1
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	3	2.1
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	3	2.1
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	2	2.1
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	2	2.1
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	2	2.1
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	16	2.1
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	16	2.1
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	16	2.1
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	5	2.1
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	1	2.1
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	1	2.1
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	1	2.1
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	12	2.09
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	12	2.09
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	12	2.09
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	19	2.09
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	19	2.09
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	19	2.09
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	1	2.09
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	1	2.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	1	2.09
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	20	2.09
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	20	2.09
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	20	2.09
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	18	2.09
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	18	2.09
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	18	2.09
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	18	2.09
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	18	2.09
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	18	2.09
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	14	2.09
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	14	2.09
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	14	2.09
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	14	2.09
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	14	2.09
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	14	2.09
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	18	2.09
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	18	2.09
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	18	2.09
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	5	2.08
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	5	2.08
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	5	2.08
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	15	2.08
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	15	2.08
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	15	2.08
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	9	2.08
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	9	2.08
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	9	2.08
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	1	2.08
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	1	2.08
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	1	2.08
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	1	2.08
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	1	2.08
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	1	2.08
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	3	2.08
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	3	2.08
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	3	2.08
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	3	2.08
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	3	2.08
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	3	2.08
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	11	2.07
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	11	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	11	2.07
(1,696)	1:71:A:SER:HB3	1:75:A:ARG:HD2	9	2.07
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	3	2.06
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	3	2.06
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	3	2.06
(1,1210)	1:37:A:ILE:HD11	1:78:A:SER:H	3	2.06
(1,1210)	1:37:A:ILE:HD12	1:78:A:SER:H	3	2.06
(1,1210)	1:37:A:ILE:HD13	1:78:A:SER:H	3	2.06
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	7	2.06
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	7	2.06
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	7	2.06
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	10	2.06
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	10	2.06
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	10	2.06
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	7	2.05
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	7	2.05
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	7	2.05
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	16	2.05
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	16	2.05
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	16	2.05
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	3	2.05
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	3	2.05
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	3	2.05
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	7	2.05
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	7	2.05
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	7	2.05
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	3	2.04
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	3	2.04
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	3	2.04
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	1	2.04
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	1	2.04
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	1	2.04
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD1	5	2.03
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD2	5	2.03
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	1	2.03
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	1	2.03
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	1	2.03
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	10	2.03
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	10	2.03
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	10	2.03
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	10	2.03
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	10	2.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	10	2.03
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	8	2.03
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	8	2.03
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	8	2.03
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	18	2.03
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	18	2.03
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	18	2.03
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	13	2.03
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	13	2.03
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	13	2.03
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	2	2.02
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	2	2.02
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	2	2.02
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	2	2.02
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	2	2.02
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	2	2.02
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	14	2.02
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	5	2.01
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	5	2.01
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	5	2.01
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	13	2.01
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	13	2.01
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	13	2.01
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	10	2.01
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	10	2.01
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	10	2.01
(1,845)	1:118:A:VAL:HG11	1:122:A:LYS:HG2	15	2.0
(1,845)	1:118:A:VAL:HG12	1:122:A:LYS:HG2	15	2.0
(1,845)	1:118:A:VAL:HG13	1:122:A:LYS:HG2	15	2.0
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	8	2.0
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	8	2.0
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	8	2.0
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	16	1.99
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	16	1.99
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	16	1.99
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	12	1.98
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	12	1.98
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	12	1.98
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	19	1.98
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	19	1.98
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	19	1.98
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	11	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,396)	1:122:A:LYS:HG3	1:118:A:VAL:HA	14	1.98
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	2	1.98
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	2	1.98
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	2	1.98
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	5	1.97
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	5	1.97
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	5	1.97
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	3	1.97
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	3	1.97
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	3	1.97
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	1	1.97
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	1	1.97
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	1	1.97
(1,361)	1:58:A:TYR:HE1	1:96:A:GLN:HB3	5	1.97
(1,361)	1:58:A:TYR:HE2	1:96:A:GLN:HB3	5	1.97
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	1	1.96
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	1	1.96
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	1	1.96
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	7	1.96
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	7	1.96
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	7	1.96
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	16	1.95
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	16	1.95
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	16	1.95
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	7	1.95
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	7	1.95
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	7	1.95
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	7	1.95
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	7	1.95
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	7	1.95
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	16	1.95
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	16	1.95
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	16	1.95
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	16	1.95
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	16	1.95
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	16	1.95
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	17	1.95
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	17	1.95
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	17	1.95
(1,69)	1:87:A:CYS:HA	1:90:A:LEU:HB3	4	1.95
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	8	1.94
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	8	1.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	8	1.94
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	11	1.94
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	11	1.94
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	11	1.94
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	3	1.94
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	3	1.94
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	3	1.94
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	18	1.94
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	18	1.94
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	18	1.94
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	15	1.94
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	20	1.94
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	4	1.94
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	4	1.94
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	4	1.94
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	15	1.93
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	15	1.93
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	15	1.93
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	5	1.93
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	5	1.93
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	5	1.93
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	12	1.93
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	12	1.93
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	12	1.93
(1,696)	1:71:A:SER:HB3	1:75:A:ARG:HD2	6	1.93
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD11	12	1.93
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD12	12	1.93
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD13	12	1.93
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	3	1.93
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	19	1.92
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	18	1.92
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	18	1.92
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	18	1.92
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	11	1.92
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	11	1.92
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	11	1.92
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	14	1.92
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	14	1.92
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	14	1.92
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	5	1.92
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD11	10	1.91
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD12	10	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD13	10	1.91
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	11	1.9
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	2	1.89
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	2	1.89
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	2	1.89
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	13	1.89
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	13	1.89
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	13	1.89
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	5	1.89
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	2	1.88
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	5	1.88
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	5	1.88
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	5	1.88
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	17	1.88
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	17	1.88
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	17	1.88
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	6	1.88
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	6	1.88
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	6	1.88
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	19	1.88
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	19	1.88
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	19	1.88
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	14	1.88
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	16	1.88
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	17	1.88
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	15	1.87
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	15	1.87
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	15	1.87
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	2	1.87
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	2	1.87
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	2	1.87
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	5	1.87
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	7	1.86
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	10	1.86
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	13	1.86
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	17	1.86
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	20	1.86
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	16	1.86
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	16	1.86
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	16	1.86
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	2	1.86
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	3	1.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	18	1.86
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	5	1.85
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	15	1.85
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	15	1.85
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	15	1.85
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	17	1.85
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	17	1.85
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	17	1.85
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	8	1.85
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	9	1.85
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	10	1.85
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	6	1.85
(1,3)	1:15:A:LYS:HD3	1:8:A:GLY:HA2	13	1.85
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	15	1.84
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	20	1.84
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	20	1.84
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	20	1.84
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	12	1.83
(1,1111)	1:117:A:ARG:HD3	1:116:A:MET:HA	15	1.83
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	13	1.83
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	13	1.83
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	13	1.83
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	8	1.83
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	8	1.83
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	8	1.83
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	10	1.83
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	10	1.83
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	10	1.83
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	13	1.83
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	13	1.83
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	13	1.83
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	9	1.83
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	9	1.83
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	9	1.83
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	16	1.83
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	1	1.82
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	4	1.82
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	4	1.82
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	4	1.82
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	16	1.82
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	16	1.82
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	16	1.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	5	1.82
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG21	6	1.82
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG22	6	1.82
(1,75)	1:107:A:ASP:HB3	1:111:A:VAL:HG23	6	1.82
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	17	1.81
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	17	1.81
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	5	1.81
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	5	1.81
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	5	1.81
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	3	1.81
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	3	1.81
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	3	1.81
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG11	4	1.81
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG12	4	1.81
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG13	4	1.81
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG11	13	1.81
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG12	13	1.81
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG13	13	1.81
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	10	1.81
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	10	1.81
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	10	1.81
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	18	1.8
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	10	1.8
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	10	1.8
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	3	1.8
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	3	1.8
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	3	1.8
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	4	1.8
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	4	1.8
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	4	1.8
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	3	1.8
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	3	1.8
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	3	1.8
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	3	1.79
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	8	1.79
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	1	1.79
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	1	1.79
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	20	1.79
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	20	1.79
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	20	1.79
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	19	1.79
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	6	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	6	1.79
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	6	1.79
(1,1905)	1:58:A:TYR:HD1	1:57:A:TYR:HD1	5	1.78
(1,1905)	1:58:A:TYR:HD1	1:57:A:TYR:HD2	5	1.78
(1,1905)	1:58:A:TYR:HD2	1:57:A:TYR:HD1	5	1.78
(1,1905)	1:58:A:TYR:HD2	1:57:A:TYR:HD2	5	1.78
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	5	1.78
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	11	1.78
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	16	1.78
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	3	1.78
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	3	1.78
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	3	1.78
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	11	1.78
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	11	1.78
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	11	1.78
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG11	19	1.78
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG12	19	1.78
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG13	19	1.78
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	13	1.78
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	13	1.78
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	13	1.78
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	5	1.78
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	5	1.78
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	5	1.78
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	12	1.78
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	12	1.77
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	12	1.77
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	12	1.77
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	15	1.76
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	15	1.76
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	15	1.76
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	10	1.76
(1,1666)	1:30:A:VAL:HB	1:28:A:ARG:HE	4	1.76
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB1	3	1.76
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB2	3	1.76
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB3	3	1.76
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	9	1.76
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	9	1.76
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	9	1.76
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	15	1.76
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	15	1.76
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	15	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	8	1.76
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	8	1.76
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	8	1.76
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	6	1.76
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	6	1.76
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	6	1.76
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	4	1.76
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	14	1.76
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	16	1.75
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	16	1.75
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	16	1.75
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	12	1.75
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	12	1.75
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	12	1.75
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	11	1.75
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	11	1.75
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	11	1.75
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	5	1.75
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	5	1.75
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	5	1.75
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	8	1.75
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	8	1.75
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	8	1.75
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	11	1.75
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	11	1.75
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	11	1.75
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	16	1.75
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	16	1.75
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	16	1.75
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	18	1.75
(1,3)	1:15:A:LYS:HD3	1:8:A:GLY:HA2	12	1.75
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	18	1.75
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	3	1.74
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	3	1.74
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	3	1.74
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	9	1.74
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	9	1.74
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	9	1.74
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	7	1.74
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	7	1.74
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	7	1.74
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	12	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	12	1.74
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	12	1.74
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	10	1.74
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	10	1.74
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	10	1.74
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	10	1.74
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	10	1.74
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	10	1.74
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	13	1.74
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	16	1.73
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	16	1.73
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	16	1.73
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	18	1.73
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	18	1.73
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	18	1.73
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	16	1.72
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	16	1.72
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	16	1.72
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	18	1.72
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	18	1.72
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	18	1.72
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	5	1.72
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	5	1.72
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	5	1.72
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE1	5	1.71
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE2	5	1.71
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE3	5	1.71
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	19	1.71
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	19	1.71
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	19	1.71
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	18	1.71
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	18	1.71
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	18	1.71
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	14	1.71
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	9	1.71
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	1	1.7
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	1	1.7
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	1	1.7
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	4	1.7
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	14	1.7
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	14	1.7
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	16	1.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	16	1.7
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	7	1.7
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	7	1.7
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	7	1.7
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	1	1.7
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	1	1.7
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	1	1.7
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	10	1.7
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	10	1.7
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	10	1.7
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	19	1.7
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	19	1.7
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	19	1.7
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	13	1.7
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	13	1.7
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	13	1.7
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	1	1.7
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	1	1.7
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	1	1.7
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	19	1.7
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	19	1.7
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	19	1.7
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	19	1.7
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	19	1.7
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	19	1.7
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	11	1.69
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	11	1.69
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	11	1.69
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	14	1.69
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	14	1.69
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	14	1.69
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	1	1.69
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	1	1.69
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	1	1.69
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	12	1.69
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	12	1.69
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	3	1.69
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	3	1.69
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	3	1.69
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	2	1.69
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	2	1.69
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	2	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	8	1.69
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	8	1.69
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	8	1.69
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	3	1.69
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	3	1.69
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	3	1.69
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	10	1.69
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	10	1.68
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	10	1.68
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	10	1.68
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	11	1.68
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	11	1.68
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	4	1.68
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	4	1.68
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	4	1.68
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	11	1.68
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	11	1.68
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	11	1.68
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	4	1.68
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	4	1.68
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	4	1.68
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	1	1.68
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	1	1.68
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	1	1.68
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	20	1.68
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	20	1.68
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	20	1.68
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	11	1.68
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	2	1.68
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	2	1.68
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	2	1.68
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	17	1.68
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	17	1.68
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	17	1.68
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	3	1.68
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	4	1.68
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	16	1.67
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	4	1.67
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	4	1.67
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	6	1.67
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	6	1.67
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	6	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG11	9	1.67
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG12	9	1.67
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG13	9	1.67
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	4	1.67
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	4	1.67
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	4	1.67
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	16	1.67
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	5	1.67
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	10	1.67
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	10	1.67
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	10	1.67
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	13	1.67
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	18	1.66
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	18	1.66
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	18	1.66
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	11	1.66
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	8	1.66
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	8	1.66
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	18	1.66
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	18	1.66
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	7	1.66
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	7	1.66
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	7	1.66
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	17	1.66
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	17	1.66
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	17	1.66
(1,535)	1:86:A:ILE:HA	1:89:A:LYS:HG2	8	1.66
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	2	1.66
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	2	1.66
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	2	1.66
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	2	1.66
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	2	1.66
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	2	1.66
(1,118)	1:19:A:ASN:HB3	1:16:A:GLU:HA	10	1.66
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	7	1.65
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	7	1.65
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	7	1.65
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	15	1.65
(1,1105)	1:103:A:GLU:HA	1:104:A:LYS:HG2	12	1.65
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	11	1.65
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	11	1.65
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	11	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	5	1.65
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	5	1.65
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	5	1.65
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	17	1.65
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	17	1.65
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	17	1.65
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	20	1.65
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	20	1.65
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	20	1.65
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	5	1.65
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	5	1.65
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	5	1.65
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	18	1.65
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	18	1.65
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	18	1.65
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	9	1.65
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	9	1.65
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	9	1.65
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	17	1.65
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	5	1.64
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	5	1.64
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	5	1.64
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	19	1.64
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	19	1.64
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	19	1.64
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	19	1.64
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	19	1.64
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	8	1.64
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	8	1.64
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	8	1.64
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	20	1.64
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	20	1.64
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	20	1.64
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	9	1.64
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	9	1.64
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	9	1.64
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	11	1.64
(1,69)	1:87:A:CYS:HA	1:90:A:LEU:HB3	2	1.64
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	3	1.64
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	2	1.63
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	2	1.63
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	2	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	20	1.63
(1,1106)	1:104:A:LYS:HG3	1:103:A:GLU:HA	10	1.63
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	1	1.63
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	1	1.63
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	1	1.63
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	10	1.63
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	10	1.63
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	10	1.63
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	16	1.63
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	16	1.63
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	16	1.63
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	18	1.63
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	8	1.63
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	8	1.63
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	8	1.63
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	10	1.63
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	2	1.63
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	2	1.63
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	2	1.63
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	12	1.63
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	12	1.63
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	12	1.63
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	9	1.63
(1,9)	1:8:A:GLY:HA2	1:15:A:LYS:HE2	19	1.63
(1,9)	1:8:A:GLY:HA3	1:15:A:LYS:HE2	19	1.63
(1,2)	1:8:A:GLY:HA2	1:15:A:LYS:HD2	17	1.63
(1,2)	1:8:A:GLY:HA3	1:15:A:LYS:HD2	17	1.63
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	3	1.62
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	6	1.62
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	6	1.62
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	6	1.62
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	9	1.62
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	9	1.62
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	9	1.62
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	18	1.62
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	18	1.62
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	18	1.62
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	2	1.62
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	2	1.62
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	2	1.62
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	4	1.62
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	4	1.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	4	1.62
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	17	1.62
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	17	1.62
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	17	1.62
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	8	1.62
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	20	1.62
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	20	1.62
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	20	1.62
(1,3)	1:15:A:LYS:HD3	1:8:A:GLY:HA2	8	1.62
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	7	1.62
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	6	1.61
(1,911)	1:9:A:ALA:HB1	1:15:A:LYS:HD2	16	1.61
(1,911)	1:9:A:ALA:HB2	1:15:A:LYS:HD2	16	1.61
(1,911)	1:9:A:ALA:HB3	1:15:A:LYS:HD2	16	1.61
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	18	1.61
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	18	1.61
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	18	1.61
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	1	1.61
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	1	1.61
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	1	1.61
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	19	1.61
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	19	1.61
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	19	1.61
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	14	1.61
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	14	1.61
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	14	1.61
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	2	1.61
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	2	1.61
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	2	1.61
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	15	1.61
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	15	1.61
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	15	1.61
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	17	1.61
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	18	1.61
(1,207)	1:81:A:MET:HB2	1:86:A:ILE:HD11	3	1.61
(1,207)	1:81:A:MET:HB2	1:86:A:ILE:HD12	3	1.61
(1,207)	1:81:A:MET:HB2	1:86:A:ILE:HD13	3	1.61
(1,49)	1:159:A:THR:H	1:158:A:LYS:HE2	19	1.61
(1,3)	1:15:A:LYS:HD3	1:8:A:GLY:HA2	17	1.61
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	20	1.6
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	20	1.6
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	17	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	17	1.6
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	17	1.6
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	20	1.6
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	20	1.6
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	20	1.6
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	20	1.6
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	20	1.6
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	20	1.6
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	13	1.6
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	18	1.6
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	18	1.6
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	18	1.6
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	3	1.6
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	3	1.6
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	3	1.6
(1,11)	1:8:A:GLY:HA3	1:15:A:LYS:HE3	11	1.6
(1,3)	1:15:A:LYS:HD3	1:8:A:GLY:HA2	19	1.6
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	19	1.59
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	1	1.59
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	1	1.59
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	1	1.59
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	6	1.59
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	6	1.59
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	6	1.59
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	13	1.59
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	13	1.59
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	13	1.59
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	19	1.59
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	19	1.59
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	19	1.59
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	11	1.59
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	11	1.59
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	11	1.59
(1,311)	1:91:A:LYS:HD3	1:95:A:SER:HA	9	1.59
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	5	1.59
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	5	1.59
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	5	1.59
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	8	1.59
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	8	1.59
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	8	1.59
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	19	1.59
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	19	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	19	1.59
(1,118)	1:19:A:ASN:HB3	1:16:A:GLU:HA	16	1.59
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	13	1.58
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	13	1.58
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	12	1.58
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	12	1.58
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	12	1.58
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	5	1.58
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	5	1.58
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	5	1.58
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	6	1.58
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	6	1.58
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	6	1.58
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	7	1.58
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	7	1.58
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	7	1.58
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	12	1.58
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	12	1.58
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	12	1.58
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	18	1.58
(1,335)	1:39:A:LYS:HA	1:42:A:ILE:HG13	4	1.58
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	14	1.58
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	14	1.58
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	14	1.58
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	3	1.58
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	19	1.58
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	3	1.58
(1,1586)	1:143:A:ASN:HB3	1:142:A:VAL:H	15	1.57
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	6	1.57
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	6	1.57
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	6	1.57
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	10	1.57
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	10	1.57
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	10	1.57
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	15	1.57
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	15	1.57
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	15	1.57
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	15	1.57
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	15	1.57
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	15	1.57
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	16	1.57
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	17	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	6	1.56
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	6	1.56
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	6	1.56
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	8	1.56
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	8	1.56
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	8	1.56
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	14	1.56
(1,1147)	1:83:A:ALA:HA	1:86:A:ILE:HG12	7	1.56
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	1	1.56
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	2	1.56
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	13	1.56
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	13	1.56
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	13	1.56
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	12	1.56
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	12	1.56
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	12	1.56
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	3	1.56
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	3	1.56
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	3	1.56
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	8	1.56
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	8	1.56
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	8	1.56
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	18	1.56
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	18	1.56
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	18	1.56
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	4	1.56
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	4	1.56
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	4	1.56
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	19	1.56
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	19	1.56
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	19	1.56
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	1	1.56
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	1	1.56
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	1	1.56
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	1	1.56
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	1	1.56
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	1	1.56
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	19	1.56
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	19	1.56
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	19	1.56
(1,49)	1:159:A:THR:H	1:158:A:LYS:HE2	8	1.56
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	6	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	7	1.55
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	7	1.55
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	14	1.55
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	14	1.55
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	14	1.55
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	10	1.55
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	10	1.55
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	10	1.55
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	5	1.55
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	5	1.55
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	5	1.55
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	20	1.55
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	12	1.55
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	14	1.55
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	18	1.54
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	18	1.54
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	18	1.54
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	10	1.54
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	6	1.54
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	6	1.54
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	13	1.54
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	13	1.54
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	13	1.54
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	17	1.54
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	17	1.54
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	17	1.54
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	1	1.54
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	1	1.54
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	1	1.54
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	11	1.54
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	11	1.54
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	11	1.54
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	12	1.54
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	12	1.54
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	12	1.54
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	11	1.54
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	20	1.53
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	20	1.53
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	20	1.53
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	1	1.53
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	7	1.53
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	9	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1106)	1:104:A:LYS:HG3	1:103:A:GLU:HA	5	1.53
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	2	1.53
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	2	1.53
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	20	1.53
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	20	1.53
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	20	1.53
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	8	1.53
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	8	1.53
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	8	1.53
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	15	1.53
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	7	1.53
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	7	1.53
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	7	1.53
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	9	1.53
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	9	1.53
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	9	1.53
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	16	1.53
(1,1545)	1:119:A:ALA:H	1:122:A:LYS:HG2	9	1.52
(1,1019)	1:84:A:MET:HE1	1:15:A:LYS:HD2	8	1.52
(1,1019)	1:84:A:MET:HE2	1:15:A:LYS:HD2	8	1.52
(1,1019)	1:84:A:MET:HE3	1:15:A:LYS:HD2	8	1.52
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	2	1.52
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	2	1.52
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	2	1.52
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	19	1.52
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	19	1.52
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	19	1.52
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	18	1.52
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	18	1.52
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	18	1.52
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	11	1.52
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	11	1.52
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	11	1.52
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	15	1.52
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	15	1.52
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	15	1.52
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	1	1.52
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	8	1.52
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	8	1.52
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	8	1.52
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	17	1.52
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	10	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	17	1.52
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	4	1.52
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	4	1.52
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	4	1.52
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	6	1.52
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	20	1.52
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	9	1.52
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	14	1.51
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	14	1.51
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	14	1.51
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	5	1.51
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	9	1.51
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	4	1.51
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	4	1.51
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	4	1.51
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	4	1.51
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	4	1.51
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	4	1.51
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	7	1.51
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	7	1.51
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	7	1.51
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	3	1.51
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	3	1.51
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	3	1.51
(1,335)	1:39:A:LYS:HA	1:42:A:ILE:HG13	6	1.51
(1,243)	1:81:A:MET:HG3	1:85:A:LYS:HB2	12	1.51
(1,243)	1:81:A:MET:HG2	1:85:A:LYS:HB2	12	1.51
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	15	1.51
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	20	1.5
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	4	1.5
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	14	1.5
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	14	1.5
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	14	1.5
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	14	1.5
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	13	1.5
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	13	1.5
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	13	1.5
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	3	1.5
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	3	1.5
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	3	1.5
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	13	1.5
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	13	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	13	1.5
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	1	1.5
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	1	1.5
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	1	1.5
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	20	1.5
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	20	1.5
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	20	1.5
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	12	1.5
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	12	1.5
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	12	1.5
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	12	1.5
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	12	1.5
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	12	1.5
(1,335)	1:39:A:LYS:HA	1:42:A:ILE:HG13	13	1.5
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	7	1.5
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	6	1.5
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	6	1.5
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	6	1.5
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	15	1.5
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	16	1.5
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	16	1.5
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	16	1.5
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	2	1.5
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	7	1.49
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	7	1.49
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	7	1.49
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	11	1.49
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	11	1.49
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	11	1.49
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	7	1.49
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	7	1.49
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	7	1.49
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	9	1.49
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	9	1.49
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	9	1.49
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	14	1.49
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	14	1.49
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	14	1.49
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	19	1.49
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	19	1.49
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	19	1.49
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	14	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	14	1.49
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	14	1.49
(1,731)	1:148:A:LEU:HD21	1:151:A:LYS:HE2	19	1.49
(1,731)	1:148:A:LEU:HD22	1:151:A:LYS:HE2	19	1.49
(1,731)	1:148:A:LEU:HD23	1:151:A:LYS:HE2	19	1.49
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG21	5	1.49
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG22	5	1.49
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG23	5	1.49
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG21	5	1.49
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG22	5	1.49
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG23	5	1.49
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG21	5	1.49
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG22	5	1.49
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG23	5	1.49
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG21	5	1.49
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG22	5	1.49
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG23	5	1.49
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG21	5	1.49
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG22	5	1.49
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG23	5	1.49
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG21	5	1.49
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG22	5	1.49
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG23	5	1.49
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	13	1.49
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	18	1.49
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	18	1.49
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	18	1.49
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	18	1.49
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	18	1.49
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	18	1.49
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	13	1.49
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	4	1.49
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	20	1.49
(1,118)	1:19:A:ASN:HB3	1:16:A:GLU:HA	3	1.49
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	12	1.49
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	12	1.49
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	12	1.49
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	1	1.49
(1,1667)	1:30:A:VAL:HG11	1:28:A:ARG:HE	4	1.48
(1,1667)	1:30:A:VAL:HG12	1:28:A:ARG:HE	4	1.48
(1,1667)	1:30:A:VAL:HG13	1:28:A:ARG:HE	4	1.48
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD11	15	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD12	15	1.48
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD13	15	1.48
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	8	1.48
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	8	1.48
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	8	1.48
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	16	1.48
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	16	1.48
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	16	1.48
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	16	1.48
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	16	1.48
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	16	1.48
(1,946)	1:79:A:VAL:HG21	1:76:A:PRO:HA	17	1.48
(1,946)	1:79:A:VAL:HG22	1:76:A:PRO:HA	17	1.48
(1,946)	1:79:A:VAL:HG23	1:76:A:PRO:HA	17	1.48
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	16	1.48
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	16	1.48
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	16	1.48
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	8	1.48
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	8	1.48
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	8	1.48
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	17	1.48
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	17	1.48
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	17	1.48
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	2	1.48
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	2	1.48
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	2	1.48
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	7	1.48
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	7	1.48
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	7	1.48
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	8	1.48
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	20	1.48
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	20	1.48
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	20	1.48
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	17	1.48
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	17	1.48
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	17	1.48
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	10	1.48
(1,335)	1:39:A:LYS:HA	1:42:A:ILE:HG13	20	1.48
(1,311)	1:91:A:LYS:HD3	1:95:A:SER:HA	20	1.48
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	9	1.48
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	11	1.48
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	11	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	11	1.48
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	19	1.48
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE1	2	1.47
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE2	2	1.47
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE3	2	1.47
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	1	1.47
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	1	1.47
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	1	1.47
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	2	1.47
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	2	1.47
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	2	1.47
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	15	1.47
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	15	1.47
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	15	1.47
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	5	1.47
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	5	1.47
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	5	1.47
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	7	1.47
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	7	1.47
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	7	1.47
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	4	1.47
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	4	1.47
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	4	1.47
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	15	1.47
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	15	1.47
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	15	1.47
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	10	1.47
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	10	1.47
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	10	1.47
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	11	1.47
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	11	1.47
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	11	1.47
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	17	1.47
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	17	1.47
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	17	1.47
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD11	15	1.47
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD12	15	1.47
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD13	15	1.47
(1,435)	1:7:A:PRO:HD2	1:6:A:ARG:HG2	18	1.47
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	4	1.47
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	18	1.47
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	9	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	9	1.47
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	9	1.47
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	14	1.46
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	14	1.46
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	14	1.46
(1,1586)	1:143:A:ASN:HB3	1:142:A:VAL:H	7	1.46
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	15	1.46
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	15	1.46
(1,1019)	1:84:A:MET:HE1	1:15:A:LYS:HD2	4	1.46
(1,1019)	1:84:A:MET:HE2	1:15:A:LYS:HD2	4	1.46
(1,1019)	1:84:A:MET:HE3	1:15:A:LYS:HD2	4	1.46
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	8	1.46
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	8	1.46
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	8	1.46
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	18	1.46
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	18	1.46
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	18	1.46
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	9	1.46
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	9	1.46
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	9	1.46
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	16	1.46
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	16	1.46
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	16	1.46
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	1	1.46
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	1	1.46
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	1	1.46
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	15	1.46
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	15	1.46
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	15	1.46
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	9	1.46
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	9	1.46
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	9	1.46
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	9	1.46
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	9	1.46
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	9	1.46
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	9	1.46
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	9	1.46
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	9	1.46
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	6	1.46
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	6	1.46
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	6	1.46
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	7	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	7	1.46
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	7	1.46
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	10	1.46
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	8	1.46
(1,138)	1:42:A:ILE:HD11	1:38:A:GLU:HG2	19	1.46
(1,138)	1:42:A:ILE:HD12	1:38:A:GLU:HG2	19	1.46
(1,138)	1:42:A:ILE:HD13	1:38:A:GLU:HG2	19	1.46
(1,3)	1:15:A:LYS:HD3	1:8:A:GLY:HA2	5	1.46
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	2	1.45
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	2	1.45
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	2	1.45
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	12	1.45
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	12	1.45
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	12	1.45
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	12	1.45
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	6	1.45
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	2	1.45
(1,863)	1:111:A:VAL:HG21	1:108:A:LEU:HG	4	1.45
(1,863)	1:111:A:VAL:HG22	1:108:A:LEU:HG	4	1.45
(1,863)	1:111:A:VAL:HG23	1:108:A:LEU:HG	4	1.45
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	20	1.45
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	20	1.45
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	20	1.45
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	8	1.45
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	8	1.45
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	8	1.45
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	15	1.45
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	15	1.45
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	15	1.45
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	9	1.45
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	9	1.45
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	9	1.45
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	9	1.45
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	9	1.45
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	9	1.45
(1,335)	1:39:A:LYS:HA	1:42:A:ILE:HG13	7	1.45
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	16	1.45
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	2	1.45
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	16	1.45
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	16	1.45
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	16	1.45
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	19	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	12	1.45
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	12	1.45
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	12	1.45
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	18	1.45
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	18	1.45
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	18	1.45
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	4	1.45
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	4	1.45
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	4	1.45
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	1	1.44
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	1	1.44
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	1	1.44
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	1	1.44
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	1	1.44
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	1	1.44
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	18	1.44
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	8	1.44
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	8	1.44
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	8	1.44
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	6	1.44
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	6	1.44
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	6	1.44
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	5	1.44
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	5	1.44
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	5	1.44
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	17	1.44
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	17	1.44
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	17	1.44
(1,911)	1:9:A:ALA:HB1	1:15:A:LYS:HD2	15	1.44
(1,911)	1:9:A:ALA:HB2	1:15:A:LYS:HD2	15	1.44
(1,911)	1:9:A:ALA:HB3	1:15:A:LYS:HD2	15	1.44
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	6	1.44
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	6	1.44
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	6	1.44
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	14	1.44
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	14	1.44
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	14	1.44
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	18	1.44
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	18	1.44
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	18	1.44
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	13	1.44
(1,731)	1:148:A:LEU:HD21	1:151:A:LYS:HE2	10	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,731)	1:148:A:LEU:HD22	1:151:A:LYS:HE2	10	1.44
(1,731)	1:148:A:LEU:HD23	1:151:A:LYS:HE2	10	1.44
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	8	1.44
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	17	1.43
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	17	1.43
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	17	1.43
(1,1648)	1:94:A:ASP:HB3	1:97:A:ILE:H	2	1.43
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	16	1.43
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	16	1.43
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	16	1.43
(1,1085)	1:56:A:CYS:HB3	1:53:A:ASN:HA	5	1.43
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	9	1.43
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	9	1.43
(1,1019)	1:84:A:MET:HE1	1:15:A:LYS:HD2	1	1.43
(1,1019)	1:84:A:MET:HE2	1:15:A:LYS:HD2	1	1.43
(1,1019)	1:84:A:MET:HE3	1:15:A:LYS:HD2	1	1.43
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	2	1.43
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	2	1.43
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	2	1.43
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	4	1.43
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	4	1.43
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	4	1.43
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG11	14	1.43
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG12	14	1.43
(1,842)	1:119:A:ALA:HA	1:118:A:VAL:HG13	14	1.43
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	9	1.43
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	9	1.43
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	9	1.43
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	9	1.43
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	9	1.43
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	9	1.43
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	12	1.43
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	12	1.43
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	12	1.43
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	6	1.43
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	6	1.43
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	6	1.43
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	6	1.43
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	6	1.43
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	6	1.43
(1,335)	1:39:A:LYS:HA	1:42:A:ILE:HG13	15	1.43
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	9	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	9	1.43
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	9	1.43
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	17	1.43
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	17	1.43
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	17	1.43
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	15	1.42
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	15	1.42
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	15	1.42
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	16	1.42
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	16	1.42
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	16	1.42
(1,1586)	1:143:A:ASN:HB3	1:142:A:VAL:H	14	1.42
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	20	1.42
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	13	1.42
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	13	1.42
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	13	1.42
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	12	1.42
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	3	1.42
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	3	1.42
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	3	1.42
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	7	1.42
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	7	1.42
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	7	1.42
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	2	1.42
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	2	1.42
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	2	1.42
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	9	1.42
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	3	1.42
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	3	1.42
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	3	1.42
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	8	1.42
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	8	1.42
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	8	1.42
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	14	1.42
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	14	1.42
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	14	1.42
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	15	1.42
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	15	1.42
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	15	1.42
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	20	1.42
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	20	1.42
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	20	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	20	1.42
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	20	1.42
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	20	1.42
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	13	1.42
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	13	1.42
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	13	1.42
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	13	1.42
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	13	1.42
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	13	1.42
(1,400)	1:59:A:LEU:HA	1:69:A:ILE:HG12	5	1.42
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	1	1.42
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	1	1.42
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	1	1.42
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	1	1.42
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	1	1.42
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	1	1.42
(1,335)	1:39:A:LYS:HA	1:42:A:ILE:HG13	16	1.42
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	1	1.42
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	1	1.42
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	1	1.42
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	11	1.42
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	7	1.42
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	3	1.42
(1,2012)	1:152:A:TYR:HE1	1:151:A:LYS:HE2	2	1.41
(1,2012)	1:152:A:TYR:HE2	1:151:A:LYS:HE2	2	1.41
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	19	1.41
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	19	1.41
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	19	1.41
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	14	1.41
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	4	1.41
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	4	1.41
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	4	1.41
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	10	1.41
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	10	1.41
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	10	1.41
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	1	1.41
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	1	1.41
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	1	1.41
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	19	1.41
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	19	1.41
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	19	1.41
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	14	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	14	1.41
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	14	1.41
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	1	1.41
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	1	1.41
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	1	1.41
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	2	1.41
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	2	1.41
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	2	1.41
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	17	1.41
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	17	1.41
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	17	1.41
(1,311)	1:91:A:LYS:HD3	1:95:A:SER:HA	14	1.41
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	6	1.41
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	17	1.41
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	19	1.41
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	19	1.41
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	19	1.41
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	9	1.4
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	9	1.4
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	9	1.4
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	19	1.4
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	17	1.4
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	17	1.4
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	17	1.4
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	2	1.4
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	2	1.4
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	2	1.4
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	16	1.4
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	16	1.4
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	16	1.4
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	4	1.4
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	8	1.4
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	8	1.4
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	8	1.4
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	10	1.4
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	10	1.4
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	10	1.4
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	10	1.4
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	10	1.4
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	10	1.4
(1,335)	1:39:A:LYS:HA	1:42:A:ILE:HG13	3	1.4
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	12	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	14	1.4
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	14	1.4
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	14	1.4
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	19	1.4
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	19	1.4
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	19	1.4
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG21	5	1.4
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG22	5	1.4
(1,53)	1:138:A:LYS:HE3	1:118:A:VAL:HG23	5	1.4
(1,1993)	1:130:A:GLU:HB2	1:128:A:TRP:HE3	10	1.39
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	2	1.39
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	2	1.39
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	2	1.39
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	14	1.39
(1,1352)	1:25:A:LEU:HA	1:27:A:ASP:H	4	1.39
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	4	1.39
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	1	1.39
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	1	1.39
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	1	1.39
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	18	1.39
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	18	1.39
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	18	1.39
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	3	1.39
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	3	1.39
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	3	1.39
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	15	1.39
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	15	1.39
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	15	1.39
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	19	1.39
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	19	1.39
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	19	1.39
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	18	1.39
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	18	1.39
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	18	1.39
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	19	1.39
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	19	1.39
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	19	1.39
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	19	1.39
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	19	1.39
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	19	1.39
(1,279)	1:67:A:THR:HB	1:69:A:ILE:HG13	9	1.39
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	8	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	5	1.39
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	5	1.39
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	5	1.39
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	20	1.39
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	20	1.39
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	20	1.39
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	6	1.39
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	3	1.39
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	3	1.39
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	3	1.39
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	13	1.39
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	13	1.39
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	13	1.39
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	14	1.39
(1,69)	1:87:A:CYS:HA	1:90:A:LEU:HB3	3	1.39
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	2	1.39
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	2	1.39
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	2	1.39
(1,3)	1:15:A:LYS:HD3	1:8:A:GLY:HA2	16	1.39
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	10	1.39
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	11	1.38
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	15	1.38
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	2	1.38
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	2	1.38
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	2	1.38
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	11	1.38
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	11	1.38
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	11	1.38
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	12	1.38
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	12	1.38
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	12	1.38
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	19	1.38
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	19	1.38
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	19	1.38
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	20	1.38
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	20	1.38
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	20	1.38
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	7	1.38
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	7	1.38
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	7	1.38
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	8	1.38
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	8	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	8	1.38
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	14	1.38
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	14	1.38
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	14	1.38
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	19	1.38
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	19	1.38
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	19	1.38
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	5	1.38
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	5	1.38
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	5	1.38
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	12	1.38
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	12	1.38
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	12	1.38
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	18	1.38
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	18	1.38
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	18	1.38
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	8	1.38
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	8	1.38
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	8	1.38
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	12	1.38
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	12	1.38
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	12	1.38
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	4	1.38
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	4	1.38
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	4	1.38
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	16	1.38
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	16	1.38
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	16	1.38
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	10	1.38
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	10	1.38
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	10	1.38
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	10	1.38
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	10	1.38
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	10	1.38
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	15	1.38
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	10	1.38
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	10	1.38
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	10	1.38
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	14	1.37
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	14	1.37
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	14	1.37
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	17	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	17	1.37
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	17	1.37
(1,1359)	1:63:A:LYS:HB3	1:65:A:ALA:H	5	1.37
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	4	1.37
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	4	1.37
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	4	1.37
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	9	1.37
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	9	1.37
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	9	1.37
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	13	1.37
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	13	1.37
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	13	1.37
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	17	1.37
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	17	1.37
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	17	1.37
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE1	16	1.37
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE2	16	1.37
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE3	16	1.37
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	11	1.37
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	11	1.37
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	11	1.37
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	15	1.37
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	15	1.37
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	15	1.37
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	5	1.37
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	5	1.37
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	5	1.37
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	18	1.37
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	18	1.37
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	18	1.37
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	10	1.37
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	10	1.37
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	10	1.37
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	13	1.37
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	13	1.37
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	13	1.37
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	9	1.37
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	6	1.37
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	6	1.37
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	6	1.37
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	6	1.37
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	6	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	6	1.37
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	17	1.37
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG21	4	1.37
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG22	4	1.37
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG23	4	1.37
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	20	1.37
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	20	1.37
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	20	1.37
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	18	1.37
(1,9)	1:8:A:GLY:HA2	1:15:A:LYS:HE2	2	1.37
(1,9)	1:8:A:GLY:HA3	1:15:A:LYS:HE2	2	1.37
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	10	1.36
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	10	1.36
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	10	1.36
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	12	1.36
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	12	1.36
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	12	1.36
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	11	1.36
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	11	1.36
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	11	1.36
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	13	1.36
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	13	1.36
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	13	1.36
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	13	1.36
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	13	1.36
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	13	1.36
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	3	1.36
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	3	1.36
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	3	1.36
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	11	1.36
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	11	1.36
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	11	1.36
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG21	8	1.36
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG22	8	1.36
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG23	8	1.36
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG21	8	1.36
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG22	8	1.36
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG23	8	1.36
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG21	8	1.36
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG22	8	1.36
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG23	8	1.36
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG21	8	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG22	8	1.36
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG23	8	1.36
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG21	8	1.36
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG22	8	1.36
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG23	8	1.36
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG21	8	1.36
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG22	8	1.36
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG23	8	1.36
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	13	1.36
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	13	1.36
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	13	1.36
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	5	1.36
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	5	1.36
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	5	1.36
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	20	1.36
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	20	1.36
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	20	1.36
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	20	1.36
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	20	1.36
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	20	1.36
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	2	1.36
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	3	1.36
(1,311)	1:91:A:LYS:HD3	1:95:A:SER:HA	3	1.36
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	18	1.36
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	13	1.36
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	13	1.36
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	13	1.36
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	17	1.36
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	17	1.36
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	17	1.36
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	17	1.36
(1,49)	1:159:A:THR:H	1:158:A:LYS:HE2	13	1.36
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	20	1.36
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	1	1.35
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	1	1.35
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	1	1.35
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	6	1.35
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	6	1.35
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	6	1.35
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	18	1.35
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	18	1.35
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	18	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:111:A:VAL:HG21	1:108:A:LEU:HA	14	1.35
(1,862)	1:111:A:VAL:HG22	1:108:A:LEU:HA	14	1.35
(1,862)	1:111:A:VAL:HG23	1:108:A:LEU:HA	14	1.35
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	16	1.35
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	16	1.35
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	16	1.35
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	4	1.35
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	4	1.35
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	4	1.35
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	4	1.35
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	4	1.35
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	4	1.35
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	4	1.35
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	4	1.35
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	4	1.35
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	12	1.35
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	12	1.35
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	12	1.35
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	3	1.35
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	3	1.35
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	3	1.35
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	3	1.35
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	3	1.35
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	3	1.35
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	16	1.35
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	16	1.35
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	16	1.35
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	16	1.35
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	16	1.35
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	16	1.35
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	1	1.35
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	16	1.35
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	16	1.35
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	16	1.35
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD11	9	1.35
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD12	9	1.35
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD13	9	1.35
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	1	1.35
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	1	1.35
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	1	1.35
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	11	1.35
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	11	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	11	1.35
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	14	1.35
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	14	1.35
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	14	1.35
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	4	1.34
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	16	1.34
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	16	1.34
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	16	1.34
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	8	1.34
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	8	1.34
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	8	1.34
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	3	1.34
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	3	1.34
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	3	1.34
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	5	1.34
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	5	1.34
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	5	1.34
(1,911)	1:9:A:ALA:HB1	1:15:A:LYS:HD2	6	1.34
(1,911)	1:9:A:ALA:HB2	1:15:A:LYS:HD2	6	1.34
(1,911)	1:9:A:ALA:HB3	1:15:A:LYS:HD2	6	1.34
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	9	1.34
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	9	1.34
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	9	1.34
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	8	1.34
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	8	1.34
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	8	1.34
(1,648)	1:118:A:VAL:HG21	1:138:A:LYS:HA	4	1.34
(1,648)	1:118:A:VAL:HG22	1:138:A:LYS:HA	4	1.34
(1,648)	1:118:A:VAL:HG23	1:138:A:LYS:HA	4	1.34
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD11	1	1.34
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD12	1	1.34
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD13	1	1.34
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD11	18	1.34
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD12	18	1.34
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD13	18	1.34
(1,568)	1:34:A:LEU:HD11	1:75:A:ARG:HD2	9	1.34
(1,568)	1:34:A:LEU:HD12	1:75:A:ARG:HD2	9	1.34
(1,568)	1:34:A:LEU:HD13	1:75:A:ARG:HD2	9	1.34
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	13	1.34
(1,183)	1:101:A:LYS:HB2	1:102:A:TYR:HA	2	1.34
(1,183)	1:101:A:LYS:HB2	1:102:A:TYR:HA	9	1.34
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	5	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	5	1.34
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	5	1.34
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	19	1.34
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	19	1.34
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	19	1.34
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	13	1.34
(1,49)	1:159:A:THR:H	1:158:A:LYS:HE2	11	1.34
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	20	1.33
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	10	1.33
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	10	1.33
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	10	1.33
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	13	1.33
(1,1105)	1:103:A:GLU:HA	1:104:A:LYS:HG2	9	1.33
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB1	20	1.33
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB2	20	1.33
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB3	20	1.33
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	13	1.33
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	13	1.33
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	13	1.33
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	6	1.33
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	6	1.33
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	6	1.33
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	6	1.33
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	6	1.33
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	6	1.33
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	17	1.33
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	17	1.33
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	17	1.33
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	19	1.33
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	19	1.33
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	19	1.33
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	1	1.33
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	1	1.33
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	1	1.33
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	11	1.33
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	11	1.33
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	11	1.33
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	6	1.33
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	6	1.33
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	6	1.33
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	4	1.33
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	4	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	4	1.33
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	14	1.33
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	14	1.33
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	14	1.33
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	14	1.33
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	14	1.33
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	14	1.33
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	18	1.33
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	18	1.33
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	18	1.33
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	12	1.33
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	19	1.33
(1,244)	1:85:A:LYS:HB3	1:81:A:MET:HG2	12	1.33
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	8	1.33
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	8	1.33
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	8	1.33
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	9	1.32
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	9	1.32
(1,1933)	1:55:A:LEU:HA	1:58:A:TYR:HD1	5	1.32
(1,1933)	1:55:A:LEU:HA	1:58:A:TYR:HD2	5	1.32
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	6	1.32
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	6	1.32
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	6	1.32
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	8	1.32
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	8	1.32
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	8	1.32
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	9	1.32
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	9	1.32
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	9	1.32
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	5	1.32
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	5	1.32
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	5	1.32
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	16	1.32
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	16	1.32
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	16	1.32
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	16	1.32
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	16	1.32
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	16	1.32
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	16	1.32
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	16	1.32
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	16	1.32
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	6	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	6	1.32
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	6	1.32
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	18	1.32
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	18	1.32
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	18	1.32
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	19	1.32
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	19	1.32
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	19	1.32
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	12	1.32
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	10	1.32
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	10	1.32
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	10	1.32
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	12	1.32
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	12	1.32
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	12	1.32
(1,1993)	1:130:A:GLU:HB2	1:128:A:TRP:HE3	5	1.31
(1,1993)	1:130:A:GLU:HB2	1:128:A:TRP:HE3	18	1.31
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	5	1.31
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	5	1.31
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	5	1.31
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	9	1.31
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	9	1.31
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	9	1.31
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	18	1.31
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	18	1.31
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	18	1.31
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	7	1.31
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	7	1.31
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	7	1.31
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	14	1.31
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	14	1.31
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	14	1.31
(1,1145)	1:142:A:VAL:HG21	1:143:A:ASN:HA	15	1.31
(1,1145)	1:142:A:VAL:HG22	1:143:A:ASN:HA	15	1.31
(1,1145)	1:142:A:VAL:HG23	1:143:A:ASN:HA	15	1.31
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	17	1.31
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	8	1.31
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	8	1.31
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	8	1.31
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	20	1.31
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	20	1.31
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	20	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	12	1.31
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	12	1.31
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	12	1.31
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	8	1.31
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	8	1.31
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	8	1.31
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	13	1.31
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	13	1.31
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	13	1.31
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	4	1.31
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	4	1.31
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	4	1.31
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	4	1.31
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	4	1.31
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	4	1.31
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	3	1.31
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	3	1.31
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	3	1.31
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	19	1.31
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	19	1.31
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	19	1.31
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	10	1.31
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	10	1.31
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	10	1.31
(1,611)	1:111:A:VAL:HA	1:110:A:SER:HB2	17	1.31
(1,400)	1:59:A:LEU:HA	1:69:A:ILE:HG12	17	1.31
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	7	1.31
(1,335)	1:39:A:LYS:HA	1:42:A:ILE:HG13	19	1.31
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	7	1.31
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	7	1.31
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	7	1.31
(1,183)	1:101:A:LYS:HB2	1:102:A:TYR:HA	1	1.31
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	20	1.31
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	20	1.31
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	20	1.31
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	6	1.31
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	6	1.31
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	6	1.31
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	13	1.3
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	13	1.3
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	13	1.3
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG11	9	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG12	9	1.3
(1,1776)	1:28:A:ARG:H	1:30:A:VAL:HG13	9	1.3
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE1	3	1.3
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE2	3	1.3
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE3	3	1.3
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	16	1.3
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	16	1.3
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	16	1.3
(1,611)	1:111:A:VAL:HA	1:110:A:SER:HB2	20	1.3
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	4	1.3
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	4	1.3
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	4	1.3
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	4	1.3
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	4	1.3
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	4	1.3
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	5	1.3
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	5	1.3
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	5	1.3
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	7	1.3
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	7	1.3
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	7	1.3
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	14	1.29
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	14	1.29
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	14	1.29
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	11	1.29
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	11	1.29
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	11	1.29
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	16	1.29
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	16	1.29
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	16	1.29
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	19	1.29
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	19	1.29
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	19	1.29
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	4	1.29
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	4	1.29
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	4	1.29
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	13	1.29
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	13	1.29
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	13	1.29
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	20	1.29
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	20	1.29
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	20	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	4	1.29
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	4	1.29
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	4	1.29
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	6	1.29
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	6	1.29
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	6	1.29
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	9	1.29
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	9	1.29
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	9	1.29
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	13	1.29
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	5	1.29
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	5	1.29
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	5	1.29
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	6	1.29
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	6	1.29
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	6	1.29
(1,611)	1:111:A:VAL:HA	1:110:A:SER:HB2	10	1.29
(1,611)	1:111:A:VAL:HA	1:110:A:SER:HB2	13	1.29
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD11	18	1.29
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD12	18	1.29
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD13	18	1.29
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	13	1.29
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	4	1.29
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	10	1.29
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	2	1.29
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	2	1.29
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	2	1.29
(1,9)	1:8:A:GLY:HA2	1:15:A:LYS:HE2	10	1.29
(1,9)	1:8:A:GLY:HA3	1:15:A:LYS:HE2	10	1.29
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	18	1.29
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	18	1.29
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	18	1.29
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	13	1.29
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	6	1.29
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	13	1.28
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	9	1.28
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	9	1.28
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	9	1.28
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	12	1.28
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	12	1.28
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	12	1.28
(1,1147)	1:83:A:ALA:HA	1:86:A:ILE:HG12	6	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1019)	1:84:A:MET:HE1	1:15:A:LYS:HD2	9	1.28
(1,1019)	1:84:A:MET:HE2	1:15:A:LYS:HD2	9	1.28
(1,1019)	1:84:A:MET:HE3	1:15:A:LYS:HD2	9	1.28
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	2	1.28
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	2	1.28
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	2	1.28
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	4	1.28
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	4	1.28
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	4	1.28
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	10	1.28
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	10	1.28
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	10	1.28
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	13	1.28
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	13	1.28
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	13	1.28
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	19	1.28
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	19	1.28
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	19	1.28
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	5	1.28
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	5	1.28
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	5	1.28
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	4	1.28
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	4	1.28
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	4	1.28
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	16	1.28
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	16	1.28
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	16	1.28
(1,611)	1:111:A:VAL:HA	1:110:A:SER:HB2	14	1.28
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	11	1.28
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	11	1.28
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	11	1.28
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	11	1.28
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	11	1.28
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	11	1.28
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD11	1	1.28
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD12	1	1.28
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD13	1	1.28
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	5	1.28
(1,2)	1:8:A:GLY:HA2	1:15:A:LYS:HD2	10	1.28
(1,2)	1:8:A:GLY:HA3	1:15:A:LYS:HD2	10	1.28
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	15	1.27
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	15	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	15	1.27
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG11	6	1.27
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG12	6	1.27
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG13	6	1.27
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	14	1.27
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	14	1.27
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	14	1.27
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	5	1.27
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	5	1.27
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	5	1.27
(1,611)	1:111:A:VAL:HA	1:110:A:SER:HB2	4	1.27
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD11	14	1.27
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD12	14	1.27
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD13	14	1.27
(1,559)	1:158:A:LYS:HE3	1:158:A:LYS:HG2	4	1.27
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	18	1.27
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	18	1.27
(1,279)	1:67:A:THR:HB	1:69:A:ILE:HG13	10	1.27
(1,256)	1:86:A:ILE:H	1:81:A:MET:HG2	3	1.27
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	1	1.27
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	1	1.27
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	1	1.27
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	4	1.27
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	4	1.27
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	4	1.27
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	6	1.27
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	6	1.27
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	6	1.27
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	11	1.27
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	11	1.27
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	11	1.27
(1,2)	1:8:A:GLY:HA2	1:15:A:LYS:HD2	16	1.27
(1,2)	1:8:A:GLY:HA3	1:15:A:LYS:HD2	16	1.27
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	1	1.26
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	1	1.26
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	1	1.26
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	4	1.26
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	4	1.26
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	4	1.26
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	9	1.26
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	9	1.26
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	9	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	2	1.26
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	2	1.26
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	2	1.26
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	6	1.26
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	6	1.26
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	6	1.26
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	14	1.26
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	14	1.26
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	14	1.26
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	12	1.26
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	12	1.26
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	12	1.26
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	6	1.26
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	6	1.26
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	6	1.26
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	10	1.26
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	10	1.26
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	10	1.26
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	18	1.26
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	18	1.26
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	18	1.26
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	2	1.26
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	2	1.26
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	2	1.26
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	11	1.26
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	11	1.26
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	11	1.26
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD2	13	1.26
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD2	13	1.26
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD2	13	1.26
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD3	13	1.26
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD3	13	1.26
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD3	13	1.26
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	3	1.26
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	3	1.26
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	3	1.26
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	18	1.26
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	18	1.26
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	18	1.26
(1,611)	1:111:A:VAL:HA	1:110:A:SER:HB2	2	1.26
(1,611)	1:111:A:VAL:HA	1:110:A:SER:HB2	6	1.26
(1,559)	1:158:A:LYS:HE3	1:158:A:LYS:HG2	1	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,558)	1:158:A:LYS:HG2	1:158:A:LYS:HE2	17	1.26
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	1	1.26
(1,311)	1:91:A:LYS:HD3	1:95:A:SER:HA	16	1.26
(1,279)	1:67:A:THR:HB	1:69:A:ILE:HG13	5	1.26
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	20	1.26
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	20	1.26
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	20	1.26
(1,9)	1:8:A:GLY:HA2	1:15:A:LYS:HE2	13	1.26
(1,9)	1:8:A:GLY:HA3	1:15:A:LYS:HE2	13	1.26
(1,1993)	1:130:A:GLU:HB2	1:128:A:TRP:HE3	12	1.25
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD1	4	1.25
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD2	4	1.25
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	18	1.25
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	18	1.25
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	18	1.25
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	19	1.25
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	19	1.25
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	19	1.25
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	3	1.25
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	3	1.25
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	3	1.25
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	19	1.25
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	19	1.25
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	19	1.25
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	5	1.25
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	5	1.25
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	12	1.25
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	12	1.25
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	12	1.25
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	3	1.25
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	3	1.25
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	3	1.25
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	12	1.25
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	12	1.25
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	12	1.25
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	15	1.25
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	15	1.25
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	15	1.25
(1,611)	1:111:A:VAL:HA	1:110:A:SER:HB2	18	1.25
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	17	1.25
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	17	1.25
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	17	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	17	1.25
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	17	1.25
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	17	1.25
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD11	7	1.25
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD12	7	1.25
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD13	7	1.25
(1,559)	1:158:A:LYS:HE3	1:158:A:LYS:HG2	6	1.25
(1,559)	1:158:A:LYS:HE3	1:158:A:LYS:HG2	9	1.25
(1,559)	1:158:A:LYS:HE3	1:158:A:LYS:HG2	14	1.25
(1,559)	1:158:A:LYS:HE3	1:158:A:LYS:HG2	16	1.25
(1,559)	1:158:A:LYS:HE3	1:158:A:LYS:HG2	20	1.25
(1,558)	1:158:A:LYS:HG2	1:158:A:LYS:HE2	15	1.25
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	9	1.25
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	16	1.25
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB2	2	1.25
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB3	2	1.25
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	18	1.25
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	1	1.25
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	7	1.25
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	7	1.25
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	7	1.25
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	3	1.25
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	3	1.25
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	3	1.25
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	16	1.25
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	16	1.25
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	16	1.25
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	4	1.24
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	4	1.24
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	4	1.24
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	13	1.24
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	13	1.24
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	13	1.24
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	16	1.24
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	16	1.24
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	16	1.24
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	3	1.24
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	5	1.24
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	10	1.24
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	10	1.24
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	10	1.24
(1,1110)	1:116:A:MET:HA	1:117:A:ARG:HD2	19	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	20	1.24
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	20	1.24
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	20	1.24
(1,911)	1:9:A:ALA:HB1	1:15:A:LYS:HD2	18	1.24
(1,911)	1:9:A:ALA:HB2	1:15:A:LYS:HD2	18	1.24
(1,911)	1:9:A:ALA:HB3	1:15:A:LYS:HD2	18	1.24
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	5	1.24
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	5	1.24
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	2	1.24
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	2	1.24
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	2	1.24
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	2	1.24
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	2	1.24
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	2	1.24
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	2	1.24
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	2	1.24
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	2	1.24
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD11	2	1.24
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD12	2	1.24
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD13	2	1.24
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	1	1.24
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	11	1.24
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	9	1.24
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	9	1.24
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	9	1.24
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	13	1.24
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	13	1.24
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	13	1.24
(1,2013)	1:151:A:LYS:HE3	1:152:A:TYR:HE1	1	1.23
(1,2013)	1:151:A:LYS:HE3	1:152:A:TYR:HE2	1	1.23
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	15	1.23
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	15	1.23
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	11	1.23
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	2	1.23
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	5	1.23
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	3	1.23
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	3	1.23
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	3	1.23
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	18	1.23
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	18	1.23
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	18	1.23
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG21	12	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG22	12	1.23
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG23	12	1.23
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG21	12	1.23
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG22	12	1.23
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG23	12	1.23
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG21	12	1.23
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG22	12	1.23
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG23	12	1.23
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG21	12	1.23
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG22	12	1.23
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG23	12	1.23
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG21	12	1.23
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG22	12	1.23
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG23	12	1.23
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG21	12	1.23
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG22	12	1.23
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG23	12	1.23
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB2	11	1.23
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB3	11	1.23
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	18	1.23
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	18	1.23
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	18	1.23
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	18	1.23
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	18	1.23
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	18	1.23
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	18	1.23
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	18	1.23
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	18	1.23
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	16	1.23
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	16	1.23
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	16	1.23
(1,611)	1:111:A:VAL:HA	1:110:A:SER:HB2	5	1.23
(1,611)	1:111:A:VAL:HA	1:110:A:SER:HB2	8	1.23
(1,559)	1:158:A:LYS:HE3	1:158:A:LYS:HG2	10	1.23
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	13	1.23
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	7	1.23
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	7	1.23
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	7	1.23
(1,1946)	1:25:A:LEU:HB2	1:32:A:PHE:HE1	4	1.22
(1,1946)	1:25:A:LEU:HB2	1:32:A:PHE:HE2	4	1.22
(1,1899)	1:69:A:ILE:HG12	1:60:A:GLY:H	5	1.22
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	3	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	3	1.22
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	3	1.22
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	8	1.22
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	8	1.22
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	8	1.22
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	9	1.22
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	16	1.22
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	20	1.22
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	20	1.22
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	20	1.22
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE1	15	1.22
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE2	15	1.22
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE3	15	1.22
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	9	1.22
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	9	1.22
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	9	1.22
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB1	4	1.22
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB2	4	1.22
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB3	4	1.22
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	1	1.22
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	1	1.22
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	1	1.22
(1,860)	1:111:A:VAL:HG21	1:110:A:SER:H	12	1.22
(1,860)	1:111:A:VAL:HG22	1:110:A:SER:H	12	1.22
(1,860)	1:111:A:VAL:HG23	1:110:A:SER:H	12	1.22
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	16	1.22
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	16	1.22
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	16	1.22
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	18	1.22
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	18	1.22
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	18	1.22
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	14	1.22
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	14	1.22
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	14	1.22
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	17	1.22
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	17	1.22
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	17	1.22
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	2	1.22
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	2	1.22
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	2	1.22
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	6	1.22
(1,254)	1:82:A:PRO:HD2	1:81:A:MET:HG2	16	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	7	1.22
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	19	1.22
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	8	1.22
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	8	1.22
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	8	1.22
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	15	1.22
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	15	1.22
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	15	1.22
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	2	1.22
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	19	1.22
(1,1993)	1:130:A:GLU:HB2	1:128:A:TRP:HE3	4	1.21
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	8	1.21
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	1	1.21
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	1	1.21
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	1	1.21
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	5	1.21
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	5	1.21
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	5	1.21
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	17	1.21
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	17	1.21
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	17	1.21
(1,850)	1:118:A:VAL:HG11	1:122:A:LYS:HD2	4	1.21
(1,850)	1:118:A:VAL:HG12	1:122:A:LYS:HD2	4	1.21
(1,850)	1:118:A:VAL:HG13	1:122:A:LYS:HD2	4	1.21
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	11	1.21
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	11	1.21
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	11	1.21
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG21	16	1.21
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG22	16	1.21
(1,821)	1:143:A:ASN:HB3	1:142:A:VAL:HG23	16	1.21
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	20	1.21
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	20	1.21
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	20	1.21
(1,773)	1:30:A:VAL:HG21	1:40:A:GLU:HG3	4	1.21
(1,773)	1:30:A:VAL:HG22	1:40:A:GLU:HG3	4	1.21
(1,773)	1:30:A:VAL:HG23	1:40:A:GLU:HG3	4	1.21
(1,773)	1:30:A:VAL:HG21	1:40:A:GLU:HG2	4	1.21
(1,773)	1:30:A:VAL:HG22	1:40:A:GLU:HG2	4	1.21
(1,773)	1:30:A:VAL:HG23	1:40:A:GLU:HG2	4	1.21
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	9	1.21
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	9	1.21
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	9	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	15	1.21
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	15	1.21
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	15	1.21
(1,361)	1:58:A:TYR:HE1	1:96:A:GLN:HB3	10	1.21
(1,361)	1:58:A:TYR:HE2	1:96:A:GLN:HB3	10	1.21
(1,279)	1:67:A:THR:HB	1:69:A:ILE:HG13	7	1.21
(1,138)	1:42:A:ILE:HD11	1:38:A:GLU:HG2	16	1.21
(1,138)	1:42:A:ILE:HD12	1:38:A:GLU:HG2	16	1.21
(1,138)	1:42:A:ILE:HD13	1:38:A:GLU:HG2	16	1.21
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	16	1.21
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	16	1.21
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	16	1.21
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	5	1.2
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	5	1.2
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	5	1.2
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	12	1.2
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB1	9	1.2
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB2	9	1.2
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB3	9	1.2
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	9	1.2
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	9	1.2
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	9	1.2
(1,568)	1:34:A:LEU:HD11	1:75:A:ARG:HD2	3	1.2
(1,568)	1:34:A:LEU:HD12	1:75:A:ARG:HD2	3	1.2
(1,568)	1:34:A:LEU:HD13	1:75:A:ARG:HD2	3	1.2
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	11	1.2
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	4	1.2
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	13	1.2
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	1	1.2
(1,209)	1:67:A:THR:HG21	1:68:A:LYS:HB3	8	1.2
(1,209)	1:67:A:THR:HG22	1:68:A:LYS:HB3	8	1.2
(1,209)	1:67:A:THR:HG23	1:68:A:LYS:HB3	8	1.2
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	9	1.2
(1,1915)	1:140:A:ASP:HB3	1:141:A:TYR:HD1	14	1.19
(1,1915)	1:140:A:ASP:HB3	1:141:A:TYR:HD2	14	1.19
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	3	1.19
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	3	1.19
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	3	1.19
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	10	1.19
(1,1147)	1:83:A:ALA:HA	1:86:A:ILE:HG12	14	1.19
(1,1147)	1:83:A:ALA:HA	1:86:A:ILE:HG12	18	1.19
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	9	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	9	1.19
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	9	1.19
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	1	1.19
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	1	1.19
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	1	1.19
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	11	1.19
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	11	1.19
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	11	1.19
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	5	1.19
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	5	1.19
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	5	1.19
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	5	1.19
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	5	1.19
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	5	1.19
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	19	1.19
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	19	1.19
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	19	1.19
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	19	1.19
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	19	1.19
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	19	1.19
(1,183)	1:101:A:LYS:HB2	1:102:A:TYR:HA	14	1.19
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	1	1.19
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	18	1.18
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	18	1.18
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	18	1.18
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	20	1.18
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	14	1.18
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	14	1.18
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	14	1.18
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	7	1.18
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	7	1.18
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	7	1.18
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	18	1.18
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	18	1.18
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	18	1.18
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	10	1.18
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	10	1.18
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	10	1.18
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	5	1.18
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	5	1.18
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	5	1.18
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	15	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,436)	1:6:A:ARG:HG3	1:7:A:PRO:HD2	7	1.18
(1,335)	1:39:A:LYS:HA	1:42:A:ILE:HG13	17	1.18
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	11	1.17
(1,1806)	1:24:A:SER:H	1:23:A:LYS:HB2	1	1.17
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	8	1.17
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	18	1.17
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	3	1.17
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	14	1.17
(1,1082)	1:14:A:CYS:HB2	1:97:A:ILE:HG21	5	1.17
(1,1082)	1:14:A:CYS:HB2	1:97:A:ILE:HG22	5	1.17
(1,1082)	1:14:A:CYS:HB2	1:97:A:ILE:HG23	5	1.17
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	3	1.17
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	3	1.17
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	3	1.17
(1,770)	1:30:A:VAL:HG21	1:36:A:THR:HB	6	1.17
(1,770)	1:30:A:VAL:HG22	1:36:A:THR:HB	6	1.17
(1,770)	1:30:A:VAL:HG23	1:36:A:THR:HB	6	1.17
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD21	17	1.17
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD22	17	1.17
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD23	17	1.17
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	16	1.17
(1,279)	1:67:A:THR:HB	1:69:A:ILE:HG13	1	1.17
(1,254)	1:82:A:PRO:HD2	1:81:A:MET:HG2	12	1.17
(1,243)	1:81:A:MET:HG3	1:85:A:LYS:HB2	13	1.17
(1,243)	1:81:A:MET:HG2	1:85:A:LYS:HB2	13	1.17
(1,19)	1:28:A:ARG:HD3	1:28:A:ARG:HA	15	1.17
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	17	1.16
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	8	1.16
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	8	1.16
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	8	1.16
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	11	1.16
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	11	1.16
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	11	1.16
(1,1277)	1:128:A:TRP:HE1	1:127:A:SER:HB2	11	1.16
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	16	1.16
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	17	1.16
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	10	1.16
(1,1110)	1:116:A:MET:HA	1:117:A:ARG:HD2	1	1.16
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	3	1.16
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	3	1.16
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	3	1.16
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	11	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	11	1.16
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	11	1.16
(1,809)	1:27:A:ASP:HB2	1:24:A:SER:HA	3	1.16
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	8	1.16
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	8	1.16
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	8	1.16
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	8	1.16
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	8	1.16
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	8	1.16
(1,558)	1:158:A:LYS:HG2	1:158:A:LYS:HE2	8	1.16
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	7	1.16
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	12	1.16
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	12	1.16
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	12	1.16
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	12	1.16
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	12	1.16
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	12	1.16
(1,324)	1:142:A:VAL:HG21	1:114:A:ARG:HB2	1	1.16
(1,324)	1:142:A:VAL:HG22	1:114:A:ARG:HB2	1	1.16
(1,324)	1:142:A:VAL:HG23	1:114:A:ARG:HB2	1	1.16
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	15	1.16
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	15	1.16
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	15	1.16
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	18	1.16
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	18	1.16
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	18	1.16
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	18	1.16
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	18	1.16
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	18	1.16
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	8	1.16
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	8	1.16
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	8	1.16
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	10	1.16
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	10	1.16
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	10	1.16
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	4	1.15
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	6	1.15
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	6	1.15
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	6	1.15
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	5	1.15
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	15	1.15
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	15	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	15	1.15
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	6	1.15
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	6	1.15
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	6	1.15
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	5	1.15
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	9	1.15
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	9	1.15
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	9	1.15
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	6	1.15
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	6	1.15
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	6	1.15
(1,820)	1:142:A:VAL:HG21	1:143:A:ASN:HB2	6	1.15
(1,820)	1:142:A:VAL:HG22	1:143:A:ASN:HB2	6	1.15
(1,820)	1:142:A:VAL:HG23	1:143:A:ASN:HB2	6	1.15
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	19	1.15
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	19	1.15
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	19	1.15
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	5	1.15
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	5	1.15
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	5	1.15
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	5	1.15
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	5	1.15
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	5	1.15
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	5	1.15
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	5	1.15
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	5	1.15
(1,361)	1:58:A:TYR:HE1	1:96:A:GLN:HB3	1	1.15
(1,361)	1:58:A:TYR:HE2	1:96:A:GLN:HB3	1	1.15
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	12	1.15
(1,138)	1:42:A:ILE:HD11	1:38:A:GLU:HG2	15	1.15
(1,138)	1:42:A:ILE:HD12	1:38:A:GLU:HG2	15	1.15
(1,138)	1:42:A:ILE:HD13	1:38:A:GLU:HG2	15	1.15
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	12	1.15
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG11	9	1.15
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG12	9	1.15
(1,97)	1:141:A:TYR:HB3	1:142:A:VAL:HG13	9	1.15
(1,2012)	1:152:A:TYR:HE1	1:151:A:LYS:HE2	20	1.14
(1,2012)	1:152:A:TYR:HE2	1:151:A:LYS:HE2	20	1.14
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	19	1.14
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	1	1.14
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	3	1.14
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	4	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	4	1.14
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	4	1.14
(1,1244)	1:7:A:PRO:HD2	1:6:A:ARG:HD2	20	1.14
(1,1147)	1:83:A:ALA:HA	1:86:A:ILE:HG12	20	1.14
(1,1106)	1:104:A:LYS:HG3	1:103:A:GLU:HA	1	1.14
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE1	3	1.14
(1,1060)	1:54:A:ARG:HA	1:57:A:TYR:HE2	3	1.14
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	17	1.14
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	17	1.14
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	17	1.14
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	14	1.14
(1,245)	1:81:A:MET:HG3	1:85:A:LYS:HB3	5	1.14
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	2	1.14
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	14	1.14
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	14	1.14
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	14	1.14
(1,170)	1:140:A:ASP:H	1:137:A:GLU:HG2	18	1.14
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	7	1.14
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	17	1.14
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	17	1.14
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	17	1.14
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	10	1.13
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	10	1.13
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG11	20	1.13
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG12	20	1.13
(1,1869)	1:29:A:GLY:H	1:30:A:VAL:HG13	20	1.13
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	12	1.13
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	9	1.13
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	9	1.13
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	9	1.13
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	19	1.13
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	19	1.13
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	19	1.13
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	4	1.13
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	4	1.13
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	4	1.13
(1,1244)	1:7:A:PRO:HD2	1:6:A:ARG:HD2	18	1.13
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	6	1.13
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG21	5	1.13
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG22	5	1.13
(1,1153)	1:121:A:LEU:HB2	1:124:A:ILE:HG23	5	1.13
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE1	18	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE2	18	1.13
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE3	18	1.13
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE1	13	1.13
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE2	13	1.13
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE3	13	1.13
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	8	1.13
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	8	1.13
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	8	1.13
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	2	1.13
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	13	1.13
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	13	1.13
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	13	1.13
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	2	1.13
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	2	1.13
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	2	1.13
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	2	1.13
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	2	1.13
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	2	1.13
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	8	1.13
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	15	1.13
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	2	1.13
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	13	1.13
(1,245)	1:81:A:MET:HG3	1:85:A:LYS:HB3	7	1.13
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	15	1.13
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	15	1.13
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	15	1.13
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	15	1.13
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	15	1.13
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	15	1.13
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	7	1.13
(1,1993)	1:130:A:GLU:HB2	1:128:A:TRP:HE3	1	1.12
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	2	1.12
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	6	1.12
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	8	1.12
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	5	1.12
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	5	1.12
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	5	1.12
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	10	1.12
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	3	1.12
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	3	1.12
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	3	1.12
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	16	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	16	1.12
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	16	1.12
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	4	1.12
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	4	1.12
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	4	1.12
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	4	1.12
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	4	1.12
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	4	1.12
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	4	1.12
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	4	1.12
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	4	1.12
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	5	1.12
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	5	1.12
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	5	1.12
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	20	1.12
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	5	1.12
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB2	4	1.12
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB3	4	1.12
(1,145)	1:85:A:LYS:HA	1:88:A:GLU:HG2	1	1.12
(1,11)	1:8:A:GLY:HA3	1:15:A:LYS:HE3	20	1.12
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	14	1.12
(1,3)	1:15:A:LYS:HD3	1:8:A:GLY:HA2	11	1.12
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	13	1.11
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	2	1.11
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	13	1.11
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	6	1.11
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	6	1.11
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	6	1.11
(1,947)	1:79:A:VAL:HG21	1:76:A:PRO:HB3	3	1.11
(1,947)	1:79:A:VAL:HG22	1:76:A:PRO:HB3	3	1.11
(1,947)	1:79:A:VAL:HG23	1:76:A:PRO:HB3	3	1.11
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	11	1.11
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	11	1.11
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	11	1.11
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	7	1.11
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	7	1.11
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	7	1.11
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	7	1.11
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	7	1.11
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	7	1.11
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	9	1.11
(1,311)	1:91:A:LYS:HD3	1:95:A:SER:HA	19	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	11	1.11
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	14	1.11
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	14	1.11
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	14	1.11
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	1	1.11
(1,1915)	1:140:A:ASP:HB3	1:141:A:TYR:HD1	5	1.1
(1,1915)	1:140:A:ASP:HB3	1:141:A:TYR:HD2	5	1.1
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	10	1.1
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	15	1.1
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	15	1.1
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	15	1.1
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	9	1.1
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	13	1.1
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	13	1.1
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	13	1.1
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	18	1.1
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	18	1.1
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	18	1.1
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	8	1.1
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	2	1.1
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	2	1.1
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	2	1.1
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	19	1.1
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	19	1.1
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	19	1.1
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	13	1.1
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	13	1.1
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	13	1.1
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	13	1.1
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	13	1.1
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	13	1.1
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	13	1.1
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	13	1.1
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	13	1.1
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD11	15	1.1
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD12	15	1.1
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD13	15	1.1
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD21	15	1.1
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD22	15	1.1
(1,578)	1:124:A:ILE:HG13	1:106:A:LEU:HD23	15	1.1
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	8	1.1
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	15	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	9	1.1
(1,152)	1:104:A:LYS:H	1:103:A:GLU:HG2	19	1.1
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	18	1.1
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	1	1.09
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	3	1.09
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	2	1.09
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	2	1.09
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	2	1.09
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	16	1.09
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	3	1.09
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	5	1.09
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	5	1.09
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	5	1.09
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	2	1.09
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	2	1.09
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	2	1.09
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	7	1.09
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	7	1.09
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	7	1.09
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	20	1.09
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	20	1.09
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	20	1.09
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	11	1.09
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	4	1.09
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	4	1.09
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	4	1.09
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	15	1.09
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	16	1.09
(1,209)	1:67:A:THR:HG21	1:68:A:LYS:HB3	16	1.09
(1,209)	1:67:A:THR:HG22	1:68:A:LYS:HB3	16	1.09
(1,209)	1:67:A:THR:HG23	1:68:A:LYS:HB3	16	1.09
(1,170)	1:140:A:ASP:H	1:137:A:GLU:HG2	5	1.09
(1,153)	1:103:A:GLU:HG3	1:104:A:LYS:H	9	1.09
(1,119)	1:58:A:TYR:HB2	1:97:A:ILE:HD11	5	1.09
(1,119)	1:58:A:TYR:HB2	1:97:A:ILE:HD12	5	1.09
(1,119)	1:58:A:TYR:HB2	1:97:A:ILE:HD13	5	1.09
(1,2012)	1:152:A:TYR:HE1	1:151:A:LYS:HE2	15	1.08
(1,2012)	1:152:A:TYR:HE2	1:151:A:LYS:HE2	15	1.08
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	15	1.08
(1,1806)	1:24:A:SER:H	1:23:A:LYS:HB2	8	1.08
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	16	1.08
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	16	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	16	1.08
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	16	1.08
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	16	1.08
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	16	1.08
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	16	1.08
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	16	1.08
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	16	1.08
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	16	1.08
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	5	1.08
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	5	1.08
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	5	1.08
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	8	1.08
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	8	1.08
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	8	1.08
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	15	1.08
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	15	1.08
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	15	1.08
(1,384)	1:96:A:GLN:HB3	1:58:A:TYR:HD1	10	1.08
(1,384)	1:96:A:GLN:HB3	1:58:A:TYR:HD2	10	1.08
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	4	1.08
(1,254)	1:82:A:PRO:HD2	1:81:A:MET:HG2	2	1.08
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	8	1.08
(1,138)	1:42:A:ILE:HD11	1:38:A:GLU:HG2	7	1.08
(1,138)	1:42:A:ILE:HD12	1:38:A:GLU:HG2	7	1.08
(1,138)	1:42:A:ILE:HD13	1:38:A:GLU:HG2	7	1.08
(1,61)	1:122:A:LYS:HE3	1:141:A:TYR:HE1	9	1.08
(1,61)	1:122:A:LYS:HE3	1:141:A:TYR:HE2	9	1.08
(1,1451)	1:94:A:ASP:HB3	1:96:A:GLN:H	4	1.07
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD11	14	1.07
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD12	14	1.07
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD13	14	1.07
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	7	1.07
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE1	13	1.07
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE2	13	1.07
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE3	13	1.07
(1,1017)	1:84:A:MET:HE1	1:15:A:LYS:HE2	1	1.07
(1,1017)	1:84:A:MET:HE2	1:15:A:LYS:HE2	1	1.07
(1,1017)	1:84:A:MET:HE3	1:15:A:LYS:HE2	1	1.07
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	3	1.07
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	3	1.07
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	3	1.07
(1,584)	1:102:A:TYR:H	1:101:A:LYS:HG2	1	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	14	1.07
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	17	1.07
(1,256)	1:86:A:ILE:H	1:81:A:MET:HG2	5	1.07
(1,244)	1:85:A:LYS:HB3	1:81:A:MET:HG2	7	1.07
(1,209)	1:67:A:THR:HG21	1:68:A:LYS:HB3	1	1.07
(1,209)	1:67:A:THR:HG22	1:68:A:LYS:HB3	1	1.07
(1,209)	1:67:A:THR:HG23	1:68:A:LYS:HB3	1	1.07
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	4	1.07
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	4	1.07
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	4	1.07
(1,183)	1:101:A:LYS:HB2	1:102:A:TYR:HA	11	1.07
(1,1993)	1:130:A:GLU:HB2	1:128:A:TRP:HE3	11	1.06
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	14	1.06
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD11	7	1.06
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD12	7	1.06
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD13	7	1.06
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	18	1.06
(1,1144)	1:146:A:GLN:HB3	1:143:A:ASN:HA	18	1.06
(1,1106)	1:104:A:LYS:HG3	1:103:A:GLU:HA	2	1.06
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE1	11	1.06
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE2	11	1.06
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE3	11	1.06
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	11	1.06
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	11	1.06
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	11	1.06
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD2	7	1.06
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD2	7	1.06
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD2	7	1.06
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD3	7	1.06
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD3	7	1.06
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD3	7	1.06
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	14	1.06
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	14	1.06
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	14	1.06
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG21	10	1.06
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG22	10	1.06
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG23	10	1.06
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG21	10	1.06
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG22	10	1.06
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG23	10	1.06
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG21	10	1.06
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG22	10	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG23	10	1.06
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG21	10	1.06
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG22	10	1.06
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG23	10	1.06
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG21	10	1.06
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG22	10	1.06
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG23	10	1.06
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG21	10	1.06
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG22	10	1.06
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG23	10	1.06
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	15	1.06
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	15	1.06
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	15	1.06
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	13	1.06
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	8	1.06
(1,324)	1:142:A:VAL:HG21	1:114:A:ARG:HB2	7	1.06
(1,324)	1:142:A:VAL:HG22	1:114:A:ARG:HB2	7	1.06
(1,324)	1:142:A:VAL:HG23	1:114:A:ARG:HB2	7	1.06
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB2	3	1.06
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB3	3	1.06
(1,254)	1:82:A:PRO:HD2	1:81:A:MET:HG2	5	1.06
(1,209)	1:67:A:THR:HG21	1:68:A:LYS:HB3	6	1.06
(1,209)	1:67:A:THR:HG22	1:68:A:LYS:HB3	6	1.06
(1,209)	1:67:A:THR:HG23	1:68:A:LYS:HB3	6	1.06
(1,138)	1:42:A:ILE:HD11	1:38:A:GLU:HG2	13	1.06
(1,138)	1:42:A:ILE:HD12	1:38:A:GLU:HG2	13	1.06
(1,138)	1:42:A:ILE:HD13	1:38:A:GLU:HG2	13	1.06
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	13	1.06
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	15	1.06
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	15	1.06
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	15	1.06
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	18	1.06
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	16	1.06
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	2	1.05
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	2	1.05
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	2	1.05
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	12	1.05
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	12	1.05
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	12	1.05
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	1	1.05
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	4	1.05
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	19	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	6	1.05
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	6	1.05
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	6	1.05
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	17	1.05
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	17	1.05
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	17	1.05
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	9	1.05
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	9	1.05
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	9	1.05
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	4	1.05
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	4	1.05
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	4	1.05
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	1	1.05
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	1	1.05
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	1	1.05
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	1	1.05
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	1	1.05
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	1	1.05
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	1	1.05
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	1	1.05
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	1	1.05
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	12	1.05
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	12	1.05
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	12	1.05
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	12	1.05
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	12	1.05
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	12	1.05
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	12	1.05
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	12	1.05
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	12	1.05
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	7	1.05
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	7	1.05
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	7	1.05
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	3	1.05
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	3	1.05
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	3	1.05
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	4	1.05
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	4	1.05
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	4	1.05
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	6	1.05
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	10	1.05
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	19	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	8	1.05
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	13	1.04
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	2	1.04
(1,1019)	1:84:A:MET:HE1	1:15:A:LYS:HD2	7	1.04
(1,1019)	1:84:A:MET:HE2	1:15:A:LYS:HD2	7	1.04
(1,1019)	1:84:A:MET:HE3	1:15:A:LYS:HD2	7	1.04
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	4	1.04
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	4	1.04
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	4	1.04
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG21	11	1.04
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG22	11	1.04
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG23	11	1.04
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG21	11	1.04
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG22	11	1.04
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG23	11	1.04
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG21	11	1.04
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG22	11	1.04
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG23	11	1.04
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG21	11	1.04
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG22	11	1.04
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG23	11	1.04
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG21	11	1.04
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG22	11	1.04
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG23	11	1.04
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG21	11	1.04
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG22	11	1.04
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG23	11	1.04
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	9	1.04
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	9	1.04
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	9	1.04
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD11	16	1.04
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD12	16	1.04
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD13	16	1.04
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	12	1.04
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	12	1.04
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	12	1.04
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	2	1.04
(1,384)	1:96:A:GLN:HB3	1:58:A:TYR:HD1	1	1.04
(1,384)	1:96:A:GLN:HB3	1:58:A:TYR:HD2	1	1.04
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	1	1.04
(1,353)	1:139:A:THR:HB	1:137:A:GLU:HG2	5	1.04
(1,324)	1:142:A:VAL:HG21	1:114:A:ARG:HB2	8	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,324)	1:142:A:VAL:HG22	1:114:A:ARG:HB2	8	1.04
(1,324)	1:142:A:VAL:HG23	1:114:A:ARG:HB2	8	1.04
(1,254)	1:82:A:PRO:HD2	1:81:A:MET:HG2	9	1.04
(1,138)	1:42:A:ILE:HD11	1:38:A:GLU:HG2	18	1.04
(1,138)	1:42:A:ILE:HD12	1:38:A:GLU:HG2	18	1.04
(1,138)	1:42:A:ILE:HD13	1:38:A:GLU:HG2	18	1.04
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG21	9	1.04
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG22	9	1.04
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG23	9	1.04
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	14	1.04
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	2	1.03
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	5	1.03
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	14	1.03
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	14	1.03
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	10	1.03
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	10	1.03
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	10	1.03
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	12	1.03
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	12	1.03
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	12	1.03
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	15	1.03
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	15	1.03
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	15	1.03
(1,1272)	1:106:A:LEU:HD21	1:128:A:TRP:HE1	6	1.03
(1,1272)	1:106:A:LEU:HD22	1:128:A:TRP:HE1	6	1.03
(1,1272)	1:106:A:LEU:HD23	1:128:A:TRP:HE1	6	1.03
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	16	1.03
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	13	1.03
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	17	1.03
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	17	1.03
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	17	1.03
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	2	1.03
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	2	1.03
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	15	1.03
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	17	1.03
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	17	1.03
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	17	1.03
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	17	1.03
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	17	1.03
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	17	1.03
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	17	1.03
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	17	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	17	1.03
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	12	1.03
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	12	1.03
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	12	1.03
(1,584)	1:102:A:TYR:H	1:101:A:LYS:HG2	5	1.03
(1,335)	1:39:A:LYS:HA	1:42:A:ILE:HG13	5	1.03
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB2	14	1.03
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB3	14	1.03
(1,230)	1:36:A:THR:HA	1:39:A:LYS:HB3	6	1.03
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	5	1.03
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	5	1.03
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	5	1.03
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	18	1.02
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	18	1.02
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	18	1.02
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	8	1.02
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	12	1.02
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	18	1.02
(1,1085)	1:56:A:CYS:HB3	1:53:A:ASN:HA	3	1.02
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	9	1.02
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	9	1.02
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	9	1.02
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	13	1.02
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	13	1.02
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	13	1.02
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	11	1.02
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	11	1.02
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	11	1.02
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	16	1.02
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	16	1.02
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	7	1.02
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	7	1.02
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	7	1.02
(1,652)	1:142:A:VAL:HG11	1:141:A:TYR:HB2	10	1.02
(1,652)	1:142:A:VAL:HG12	1:141:A:TYR:HB2	10	1.02
(1,652)	1:142:A:VAL:HG13	1:141:A:TYR:HB2	10	1.02
(1,535)	1:86:A:ILE:HA	1:89:A:LYS:HG2	17	1.02
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	3	1.02
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	18	1.02
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	19	1.02
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	5	1.02
(1,254)	1:82:A:PRO:HD2	1:81:A:MET:HG2	10	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,254)	1:82:A:PRO:HD2	1:81:A:MET:HG2	14	1.02
(1,243)	1:81:A:MET:HG3	1:85:A:LYS:HB2	14	1.02
(1,243)	1:81:A:MET:HG2	1:85:A:LYS:HB2	14	1.02
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	19	1.02
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	3	1.02
(1,2)	1:8:A:GLY:HA2	1:15:A:LYS:HD2	18	1.02
(1,2)	1:8:A:GLY:HA3	1:15:A:LYS:HD2	18	1.02
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	7	1.01
(1,1969)	1:24:A:SER:HB3	1:44:A:PHE:HZ	13	1.01
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	3	1.01
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	3	1.01
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	9	1.01
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	11	1.01
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	14	1.01
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	20	1.01
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	20	1.01
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	20	1.01
(1,1553)	1:93:A:LEU:H	1:92:A:LYS:HB2	2	1.01
(1,1451)	1:94:A:ASP:HB3	1:96:A:GLN:H	2	1.01
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	19	1.01
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	19	1.01
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	19	1.01
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG11	16	1.01
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG12	16	1.01
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG13	16	1.01
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	15	1.01
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	15	1.01
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	15	1.01
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	10	1.01
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	10	1.01
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	10	1.01
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	10	1.01
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	10	1.01
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	10	1.01
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	10	1.01
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	10	1.01
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	10	1.01
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	1	1.01
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	1	1.01
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	1	1.01
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	1	1.01
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	16	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	4	1.01
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	13	1.01
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	13	1.01
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	13	1.01
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	6	1.01
(1,205)	1:158:A:LYS:HB2	1:158:A:LYS:HE2	19	1.01
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	10	1.01
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	10	1.01
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	10	1.01
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	12	1.01
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	12	1.01
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	12	1.01
(1,1993)	1:130:A:GLU:HB2	1:128:A:TRP:HE3	2	1.0
(1,1993)	1:130:A:GLU:HB2	1:128:A:TRP:HE3	19	1.0
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	17	1.0
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	1	1.0
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	20	1.0
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	12	1.0
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	15	1.0
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	15	1.0
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	15	1.0
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	15	1.0
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	15	1.0
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	15	1.0
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	15	1.0
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	15	1.0
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	15	1.0
(1,1111)	1:117:A:ARG:HD3	1:116:A:MET:HA	20	1.0
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	12	1.0
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	12	1.0
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	12	1.0
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	14	1.0
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	14	1.0
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	14	1.0
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	2	1.0
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	2	1.0
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	2	1.0
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG11	18	1.0
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG12	18	1.0
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG13	18	1.0
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	1	1.0
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	1	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	1	1.0
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	3	1.0
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	11	1.0
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	6	1.0
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	6	1.0
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	6	1.0
(1,696)	1:71:A:SER:HB3	1:75:A:ARG:HD2	14	1.0
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	11	1.0
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	11	1.0
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	11	1.0
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	11	1.0
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	11	1.0
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	11	1.0
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	11	1.0
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	11	1.0
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	11	1.0
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	3	1.0
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	3	1.0
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	3	1.0
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	3	1.0
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	3	1.0
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	3	1.0
(1,418)	1:6:A:ARG:H	1:6:A:ARG:HG2	12	1.0
(1,256)	1:86:A:ILE:H	1:81:A:MET:HG2	12	1.0
(1,153)	1:103:A:GLU:HG3	1:104:A:LYS:H	15	1.0
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	8	1.0
(1,76)	1:140:A:ASP:HB2	1:135:A:CYS:HA	13	1.0
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	15	0.99
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	7	0.99
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	7	0.99
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	7	0.99
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	14	0.99
(1,1810)	1:91:A:LYS:HB3	1:92:A:LYS:H	20	0.99
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	3	0.99
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	5	0.99
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	8	0.99
(1,1476)	1:111:A:VAL:HG21	1:109:A:ALA:H	20	0.99
(1,1476)	1:111:A:VAL:HG22	1:109:A:ALA:H	20	0.99
(1,1476)	1:111:A:VAL:HG23	1:109:A:ALA:H	20	0.99
(1,1277)	1:128:A:TRP:HE1	1:127:A:SER:HB2	9	0.99
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	7	0.99
(1,1165)	1:117:A:ARG:HD3	1:117:A:ARG:HA	15	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	11	0.99
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	11	0.99
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	11	0.99
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	13	0.99
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	13	0.99
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	13	0.99
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	10	0.99
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	10	0.99
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	7	0.99
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	7	0.99
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	7	0.99
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	7	0.99
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	7	0.99
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	7	0.99
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	7	0.99
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	7	0.99
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	7	0.99
(1,552)	1:31:A:ASN:HD21	1:33:A:SER:HB2	2	0.99
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	12	0.99
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	8	0.99
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB2	12	0.99
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB3	12	0.99
(1,250)	1:63:A:LYS:HE3	1:63:A:LYS:HB2	9	0.99
(1,250)	1:63:A:LYS:HE3	1:63:A:LYS:HB2	12	0.99
(1,250)	1:63:A:LYS:HE3	1:63:A:LYS:HB2	14	0.99
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	5	0.99
(1,135)	1:74:A:THR:HG21	1:38:A:GLU:HG2	8	0.99
(1,135)	1:74:A:THR:HG22	1:38:A:GLU:HG2	8	0.99
(1,135)	1:74:A:THR:HG23	1:38:A:GLU:HG2	8	0.99
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	7	0.98
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	7	0.98
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	2	0.98
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	2	0.98
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	2	0.98
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	4	0.98
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	10	0.98
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	9	0.98
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	9	0.98
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	9	0.98
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	9	0.98
(1,1272)	1:106:A:LEU:HD21	1:128:A:TRP:HE1	11	0.98
(1,1272)	1:106:A:LEU:HD22	1:128:A:TRP:HE1	11	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1272)	1:106:A:LEU:HD23	1:128:A:TRP:HE1	11	0.98
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD11	20	0.98
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD12	20	0.98
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD13	20	0.98
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	2	0.98
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	2	0.98
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	2	0.98
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	2	0.98
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	2	0.98
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	2	0.98
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	9	0.98
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	9	0.98
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	9	0.98
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	3	0.98
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	3	0.98
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	3	0.98
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	10	0.98
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	10	0.98
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	10	0.98
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	19	0.98
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	19	0.98
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	19	0.98
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	17	0.98
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	17	0.98
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	17	0.98
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	2	0.98
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	2	0.98
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	2	0.98
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG21	2	0.98
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG22	2	0.98
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG23	2	0.98
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG21	2	0.98
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG22	2	0.98
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG23	2	0.98
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG21	2	0.98
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG22	2	0.98
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG23	2	0.98
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG21	2	0.98
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG22	2	0.98
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG23	2	0.98
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG21	2	0.98
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG22	2	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG23	2	0.98
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG21	2	0.98
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG22	2	0.98
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG23	2	0.98
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB2	10	0.98
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB3	10	0.98
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	15	0.98
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	15	0.98
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	15	0.98
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	6	0.98
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	7	0.98
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	3	0.98
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	11	0.98
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	13	0.98
(1,324)	1:142:A:VAL:HG21	1:114:A:ARG:HB2	14	0.98
(1,324)	1:142:A:VAL:HG22	1:114:A:ARG:HB2	14	0.98
(1,324)	1:142:A:VAL:HG23	1:114:A:ARG:HB2	14	0.98
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	14	0.98
(1,145)	1:85:A:LYS:HA	1:88:A:GLU:HG2	8	0.98
(1,19)	1:28:A:ARG:HD3	1:28:A:ARG:HA	4	0.98
(1,11)	1:8:A:GLY:HA3	1:15:A:LYS:HE3	10	0.98
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	4	0.98
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	1	0.97
(1,1277)	1:128:A:TRP:HE1	1:127:A:SER:HB2	6	0.97
(1,1106)	1:104:A:LYS:HG3	1:103:A:GLU:HA	13	0.97
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB1	5	0.97
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB2	5	0.97
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB3	5	0.97
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	18	0.97
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	18	0.97
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	18	0.97
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	20	0.97
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	20	0.97
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	20	0.97
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	6	0.97
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	6	0.97
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	13	0.97
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	13	0.97
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	3	0.97
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	3	0.97
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	3	0.97
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	3	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	3	0.97
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	3	0.97
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD11	6	0.97
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD12	6	0.97
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD13	6	0.97
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	1	0.97
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	1	0.97
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	1	0.97
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	6	0.97
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	6	0.97
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	6	0.97
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	20	0.97
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	20	0.97
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	20	0.97
(1,335)	1:39:A:LYS:HA	1:42:A:ILE:HG13	9	0.97
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	1	0.97
(1,175)	1:137:A:GLU:HG3	1:137:A:GLU:H	18	0.97
(1,153)	1:103:A:GLU:HG3	1:104:A:LYS:H	14	0.97
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	9	0.97
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	9	0.97
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	9	0.97
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD1	1	0.96
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD2	1	0.96
(1,1810)	1:91:A:LYS:HB3	1:92:A:LYS:H	9	0.96
(1,1810)	1:91:A:LYS:HB3	1:92:A:LYS:H	16	0.96
(1,1764)	1:120:A:GLU:H	1:117:A:ARG:HB2	15	0.96
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	6	0.96
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	14	0.96
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	14	0.96
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	14	0.96
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	3	0.96
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	15	0.96
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	17	0.96
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	18	0.96
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	19	0.96
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	20	0.96
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	9	0.96
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	4	0.96
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	4	0.96
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	4	0.96
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	20	0.96
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	20	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	20	0.96
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	9	0.96
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	9	0.96
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	9	0.96
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG11	15	0.96
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG12	15	0.96
(1,846)	1:122:A:LYS:HG3	1:118:A:VAL:HG13	15	0.96
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	15	0.96
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	15	0.96
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	8	0.96
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	8	0.96
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	8	0.96
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	10	0.96
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	3	0.96
(1,279)	1:67:A:THR:HB	1:69:A:ILE:HG13	20	0.96
(1,1969)	1:24:A:SER:HB3	1:44:A:PHE:HZ	12	0.95
(1,1810)	1:91:A:LYS:HB3	1:92:A:LYS:H	14	0.95
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	16	0.95
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	7	0.95
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	7	0.95
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	7	0.95
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	10	0.95
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	10	0.95
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	10	0.95
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	13	0.95
(1,1450)	1:96:A:GLN:H	1:94:A:ASP:HB2	5	0.95
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	7	0.95
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	17	0.95
(1,1019)	1:84:A:MET:HE1	1:15:A:LYS:HD2	3	0.95
(1,1019)	1:84:A:MET:HE2	1:15:A:LYS:HD2	3	0.95
(1,1019)	1:84:A:MET:HE3	1:15:A:LYS:HD2	3	0.95
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	10	0.95
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	10	0.95
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	10	0.95
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	12	0.95
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	12	0.95
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	12	0.95
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	2	0.95
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	2	0.95
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	2	0.95
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	12	0.95
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	12	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	12	0.95
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	7	0.95
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	7	0.95
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	7	0.95
(1,573)	1:106:A:LEU:HD21	1:108:A:LEU:HA	2	0.95
(1,573)	1:106:A:LEU:HD22	1:108:A:LEU:HA	2	0.95
(1,573)	1:106:A:LEU:HD23	1:108:A:LEU:HA	2	0.95
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	4	0.95
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	4	0.95
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	4	0.95
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	8	0.95
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	8	0.95
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	8	0.95
(1,232)	1:91:A:LYS:H	1:91:A:LYS:HB3	2	0.95
(1,183)	1:101:A:LYS:HB2	1:102:A:TYR:HA	16	0.95
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	20	0.95
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	20	0.95
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	20	0.95
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	4	0.95
(1,3)	1:15:A:LYS:HD3	1:8:A:GLY:HA2	2	0.95
(1,2012)	1:152:A:TYR:HE1	1:151:A:LYS:HE2	19	0.94
(1,2012)	1:152:A:TYR:HE2	1:151:A:LYS:HE2	19	0.94
(1,1993)	1:130:A:GLU:HB2	1:128:A:TRP:HE3	13	0.94
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	13	0.94
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	19	0.94
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	12	0.94
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	7	0.94
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	11	0.94
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	11	0.94
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	11	0.94
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	11	0.94
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	4	0.94
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	8	0.94
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	10	0.94
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	12	0.94
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	13	0.94
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	14	0.94
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	16	0.94
(1,1111)	1:117:A:ARG:HD3	1:116:A:MET:HA	8	0.94
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	15	0.94
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	15	0.94
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	15	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	15	0.94
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	15	0.94
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	15	0.94
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	15	0.94
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	15	0.94
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	15	0.94
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	2	0.94
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	2	0.94
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	2	0.94
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	1	0.94
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	1	0.94
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	1	0.94
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	15	0.94
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	15	0.94
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	15	0.94
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD2	19	0.94
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD2	19	0.94
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD2	19	0.94
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD3	19	0.94
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD3	19	0.94
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD3	19	0.94
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	3	0.94
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	3	0.94
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	9	0.94
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	9	0.94
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	19	0.94
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	19	0.94
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	15	0.94
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	20	0.94
(1,324)	1:142:A:VAL:HG21	1:114:A:ARG:HB2	17	0.94
(1,324)	1:142:A:VAL:HG22	1:114:A:ARG:HB2	17	0.94
(1,324)	1:142:A:VAL:HG23	1:114:A:ARG:HB2	17	0.94
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	4	0.94
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	4	0.94
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	4	0.94
(1,279)	1:67:A:THR:HB	1:69:A:ILE:HG13	17	0.94
(1,256)	1:86:A:ILE:H	1:81:A:MET:HG2	16	0.94
(1,245)	1:81:A:MET:HG3	1:85:A:LYS:HB3	17	0.94
(1,194)	1:123:A:GLN:HG3	1:123:A:GLN:H	8	0.94
(1,152)	1:104:A:LYS:H	1:103:A:GLU:HG2	5	0.94
(1,140)	1:25:A:LEU:HD11	1:32:A:PHE:HB3	4	0.94
(1,140)	1:25:A:LEU:HD12	1:32:A:PHE:HB3	4	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,140)	1:25:A:LEU:HD13	1:32:A:PHE:HB3	4	0.94
(1,76)	1:140:A:ASP:HB2	1:135:A:CYS:HA	12	0.94
(1,48)	1:86:A:ILE:HG21	1:89:A:LYS:HE3	17	0.94
(1,48)	1:86:A:ILE:HG22	1:89:A:LYS:HE3	17	0.94
(1,48)	1:86:A:ILE:HG23	1:89:A:LYS:HE3	17	0.94
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD1	13	0.93
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD2	13	0.93
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	18	0.93
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	6	0.93
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	6	0.93
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	6	0.93
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	2	0.93
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	2	0.93
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	5	0.93
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	6	0.93
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	18	0.93
(1,1277)	1:128:A:TRP:HE1	1:127:A:SER:HB2	16	0.93
(1,1244)	1:7:A:PRO:HD2	1:6:A:ARG:HD2	7	0.93
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE1	12	0.93
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE2	12	0.93
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE3	12	0.93
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	20	0.93
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	20	0.93
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	20	0.93
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD11	11	0.93
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD12	11	0.93
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD13	11	0.93
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	11	0.93
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	7	0.93
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	9	0.93
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	14	0.93
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	7	0.93
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	18	0.93
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	18	0.93
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	18	0.93
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	6	0.93
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	6	0.93
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	6	0.93
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	1	0.92
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	18	0.92
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD1	20	0.92
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD2	20	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	19	0.92
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	19	0.92
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	19	0.92
(1,1323)	1:46:A:LEU:HB3	1:46:A:LEU:H	11	0.92
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	4	0.92
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	6	0.92
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	6	0.92
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	6	0.92
(1,1163)	1:13:A:VAL:HG11	1:101:A:LYS:HA	17	0.92
(1,1163)	1:13:A:VAL:HG12	1:101:A:LYS:HA	17	0.92
(1,1163)	1:13:A:VAL:HG13	1:101:A:LYS:HA	17	0.92
(1,1105)	1:103:A:GLU:HA	1:104:A:LYS:HG2	15	0.92
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB1	20	0.92
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB2	20	0.92
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB3	20	0.92
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	15	0.92
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	19	0.92
(1,224)	1:119:A:ALA:HA	1:122:A:LYS:HB2	14	0.92
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	11	0.92
(1,209)	1:67:A:THR:HG21	1:68:A:LYS:HB3	12	0.92
(1,209)	1:67:A:THR:HG22	1:68:A:LYS:HB3	12	0.92
(1,209)	1:67:A:THR:HG23	1:68:A:LYS:HB3	12	0.92
(1,118)	1:19:A:ASN:HB3	1:16:A:GLU:HA	5	0.92
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	9	0.92
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	9	0.92
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	9	0.92
(1,3)	1:15:A:LYS:HD3	1:8:A:GLY:HA2	10	0.92
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	1	0.91
(1,1969)	1:24:A:SER:HB3	1:44:A:PHE:HZ	14	0.91
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	16	0.91
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	16	0.91
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	14	0.91
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	18	0.91
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	18	0.91
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	18	0.91
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	8	0.91
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	6	0.91
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	7	0.91
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	7	0.91
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	7	0.91
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	15	0.91
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	15	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	15	0.91
(1,869)	1:13:A:VAL:HG21	1:55:A:LEU:HB2	16	0.91
(1,869)	1:13:A:VAL:HG22	1:55:A:LEU:HB2	16	0.91
(1,869)	1:13:A:VAL:HG23	1:55:A:LEU:HB2	16	0.91
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	5	0.91
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	5	0.91
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	5	0.91
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	16	0.91
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	16	0.91
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	16	0.91
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	16	0.91
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	16	0.91
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	16	0.91
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	17	0.91
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	17	0.91
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	17	0.91
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	13	0.91
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	13	0.91
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	13	0.91
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	14	0.91
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	14	0.91
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	14	0.91
(1,549)	1:34:A:LEU:HB3	1:33:A:SER:HB3	16	0.91
(1,532)	1:92:A:LYS:HB3	1:92:A:LYS:HD3	11	0.91
(1,531)	1:92:A:LYS:HD3	1:92:A:LYS:HB2	17	0.91
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	5	0.91
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	5	0.91
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	5	0.91
(1,441)	1:113:A:LEU:HD21	1:146:A:GLN:HG3	1	0.91
(1,441)	1:113:A:LEU:HD22	1:146:A:GLN:HG3	1	0.91
(1,441)	1:113:A:LEU:HD23	1:146:A:GLN:HG3	1	0.91
(1,441)	1:113:A:LEU:HD21	1:146:A:GLN:HG3	8	0.91
(1,441)	1:113:A:LEU:HD22	1:146:A:GLN:HG3	8	0.91
(1,441)	1:113:A:LEU:HD23	1:146:A:GLN:HG3	8	0.91
(1,324)	1:142:A:VAL:HG21	1:114:A:ARG:HB2	18	0.91
(1,324)	1:142:A:VAL:HG22	1:114:A:ARG:HB2	18	0.91
(1,324)	1:142:A:VAL:HG23	1:114:A:ARG:HB2	18	0.91
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	15	0.91
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	15	0.91
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	15	0.91
(1,138)	1:42:A:ILE:HD11	1:38:A:GLU:HG2	3	0.91
(1,138)	1:42:A:ILE:HD12	1:38:A:GLU:HG2	3	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:42:A:ILE:HD13	1:38:A:GLU:HG2	3	0.91
(1,76)	1:140:A:ASP:HB2	1:135:A:CYS:HA	3	0.91
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	6	0.91
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	3	0.9
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	6	0.9
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	3	0.9
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	7	0.9
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	16	0.9
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	17	0.9
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	9	0.9
(1,1277)	1:128:A:TRP:HE1	1:127:A:SER:HB2	4	0.9
(1,1243)	1:148:A:LEU:HA	1:150:A:PRO:HD3	4	0.9
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE1	19	0.9
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE2	19	0.9
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE3	19	0.9
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	20	0.9
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	20	0.9
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	20	0.9
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	10	0.9
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	10	0.9
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	10	0.9
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	2	0.9
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	2	0.9
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	2	0.9
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG21	1	0.9
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG22	1	0.9
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG23	1	0.9
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG21	1	0.9
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG22	1	0.9
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG23	1	0.9
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG21	1	0.9
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG22	1	0.9
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG23	1	0.9
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG21	1	0.9
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG22	1	0.9
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG23	1	0.9
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG21	1	0.9
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG22	1	0.9
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG23	1	0.9
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG21	1	0.9
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG22	1	0.9
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG23	1	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG21	14	0.9
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG22	14	0.9
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG23	14	0.9
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG21	14	0.9
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG22	14	0.9
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG23	14	0.9
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG21	14	0.9
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG22	14	0.9
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG23	14	0.9
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG21	14	0.9
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG22	14	0.9
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG23	14	0.9
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG21	14	0.9
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG22	14	0.9
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG23	14	0.9
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG21	14	0.9
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG22	14	0.9
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG23	14	0.9
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG21	18	0.9
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG22	18	0.9
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG23	18	0.9
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG21	18	0.9
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG22	18	0.9
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG23	18	0.9
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG21	18	0.9
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG22	18	0.9
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG23	18	0.9
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG21	18	0.9
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG22	18	0.9
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG23	18	0.9
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG21	18	0.9
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG22	18	0.9
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG23	18	0.9
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG21	18	0.9
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG22	18	0.9
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG23	18	0.9
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD11	8	0.9
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD12	8	0.9
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD13	8	0.9
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	13	0.9
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	13	0.9
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	13	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	12	0.9
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	12	0.9
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	12	0.9
(1,506)	1:93:A:LEU:H	1:92:A:LYS:HG2	12	0.9
(1,441)	1:113:A:LEU:HD21	1:146:A:GLN:HG3	17	0.9
(1,441)	1:113:A:LEU:HD22	1:146:A:GLN:HG3	17	0.9
(1,441)	1:113:A:LEU:HD23	1:146:A:GLN:HG3	17	0.9
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	16	0.9
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	16	0.9
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	16	0.9
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	20	0.9
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	20	0.9
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	20	0.9
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	6	0.9
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	6	0.9
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	6	0.9
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	8	0.9
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	8	0.9
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	8	0.9
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG21	16	0.9
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG22	16	0.9
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG23	16	0.9
(1,52)	1:118:A:VAL:HG21	1:138:A:LYS:HE2	15	0.9
(1,52)	1:118:A:VAL:HG22	1:138:A:LYS:HE2	15	0.9
(1,52)	1:118:A:VAL:HG23	1:138:A:LYS:HE2	15	0.9
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	12	0.89
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	20	0.89
(1,1871)	1:8:A:GLY:H	1:7:A:PRO:HG3	11	0.89
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	20	0.89
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	20	0.89
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	20	0.89
(1,1810)	1:91:A:LYS:HB3	1:92:A:LYS:H	19	0.89
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	6	0.89
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG11	17	0.89
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG12	17	0.89
(1,1632)	1:141:A:TYR:H	1:142:A:VAL:HG13	17	0.89
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	20	0.89
(1,1147)	1:83:A:ALA:HA	1:86:A:ILE:HG12	1	0.89
(1,1106)	1:104:A:LYS:HG3	1:103:A:GLU:HA	7	0.89
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	8	0.89
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	8	0.89
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	8	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	20	0.89
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	20	0.89
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	20	0.89
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD2	10	0.89
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD2	10	0.89
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD2	10	0.89
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD3	10	0.89
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD3	10	0.89
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD3	10	0.89
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	11	0.89
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	11	0.89
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	14	0.89
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	14	0.89
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	1	0.89
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	1	0.89
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	1	0.89
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	10	0.89
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	10	0.89
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	10	0.89
(1,244)	1:85:A:LYS:HB3	1:81:A:MET:HG2	17	0.89
(1,205)	1:158:A:LYS:HB2	1:158:A:LYS:HE2	17	0.89
(1,152)	1:104:A:LYS:H	1:103:A:GLU:HG2	17	0.89
(1,138)	1:42:A:ILE:HD11	1:38:A:GLU:HG2	17	0.89
(1,138)	1:42:A:ILE:HD12	1:38:A:GLU:HG2	17	0.89
(1,138)	1:42:A:ILE:HD13	1:38:A:GLU:HG2	17	0.89
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	20	0.88
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	20	0.88
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	19	0.88
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	19	0.88
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	9	0.88
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	6	0.88
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	3	0.88
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	3	0.88
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	3	0.88
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	15	0.88
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	15	0.88
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	15	0.88
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	15	0.88
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	16	0.88
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	16	0.88
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	16	0.88
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	15	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD11	14	0.88
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD12	14	0.88
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD13	14	0.88
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	11	0.88
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	11	0.88
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	11	0.88
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	8	0.88
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	8	0.88
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	8	0.88
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	17	0.88
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	17	0.88
(1,205)	1:158:A:LYS:HB2	1:158:A:LYS:HE2	15	0.88
(1,153)	1:103:A:GLU:HG3	1:104:A:LYS:H	18	0.88
(1,48)	1:86:A:ILE:HG21	1:89:A:LYS:HE3	11	0.88
(1,48)	1:86:A:ILE:HG22	1:89:A:LYS:HE3	11	0.88
(1,48)	1:86:A:ILE:HG23	1:89:A:LYS:HE3	11	0.88
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	17	0.87
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	10	0.87
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	10	0.87
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	12	0.87
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	12	0.87
(1,1907)	1:64:A:ASP:HB3	1:57:A:TYR:HD1	11	0.87
(1,1907)	1:64:A:ASP:HB3	1:57:A:TYR:HD2	11	0.87
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	6	0.87
(1,1810)	1:91:A:LYS:HB3	1:92:A:LYS:H	7	0.87
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	3	0.87
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	16	0.87
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	10	0.87
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	19	0.87
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	14	0.87
(1,1147)	1:83:A:ALA:HA	1:86:A:ILE:HG12	12	0.87
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	6	0.87
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	6	0.87
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	6	0.87
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	19	0.87
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	19	0.87
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	19	0.87
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	15	0.87
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	15	0.87
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	15	0.87
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	7	0.87
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	7	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	7	0.87
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	14	0.87
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	14	0.87
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	14	0.87
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	7	0.87
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	7	0.87
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	7	0.87
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	5	0.87
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	5	0.87
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	5	0.87
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	7	0.87
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	7	0.87
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	11	0.87
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	11	0.87
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	11	0.87
(1,418)	1:6:A:ARG:H	1:6:A:ARG:HG2	13	0.87
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	3	0.87
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	3	0.87
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	3	0.87
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	13	0.87
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	13	0.87
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	13	0.87
(1,256)	1:86:A:ILE:H	1:81:A:MET:HG2	14	0.87
(1,202)	1:79:A:VAL:HG21	1:81:A:MET:HB3	3	0.87
(1,202)	1:79:A:VAL:HG22	1:81:A:MET:HB3	3	0.87
(1,202)	1:79:A:VAL:HG23	1:81:A:MET:HB3	3	0.87
(1,175)	1:137:A:GLU:HG3	1:137:A:GLU:H	5	0.87
(1,11)	1:8:A:GLY:HA3	1:15:A:LYS:HE3	9	0.87
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	2	0.87
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	4	0.86
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	4	0.86
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	17	0.86
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	17	0.86
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	18	0.86
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	20	0.86
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	15	0.86
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	12	0.86
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	9	0.86
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	6	0.86
(1,1423)	1:121:A:LEU:H	1:121:A:LEU:HG	3	0.86
(1,1244)	1:7:A:PRO:HD2	1:6:A:ARG:HD2	14	0.86
(1,1017)	1:84:A:MET:HE1	1:15:A:LYS:HE2	3	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:84:A:MET:HE2	1:15:A:LYS:HE2	3	0.86
(1,1017)	1:84:A:MET:HE3	1:15:A:LYS:HE2	3	0.86
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	9	0.86
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	7	0.86
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	7	0.86
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	7	0.86
(1,927)	1:23:A:LYS:HA	1:22:A:TYR:HB2	1	0.86
(1,927)	1:23:A:LYS:HA	1:22:A:TYR:HB2	2	0.86
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	4	0.86
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	4	0.86
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	4	0.86
(1,858)	1:111:A:VAL:HG21	1:107:A:ASP:HA	17	0.86
(1,858)	1:111:A:VAL:HG22	1:107:A:ASP:HA	17	0.86
(1,858)	1:111:A:VAL:HG23	1:107:A:ASP:HA	17	0.86
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	20	0.86
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	20	0.86
(1,696)	1:71:A:SER:HB3	1:75:A:ARG:HD2	17	0.86
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	15	0.86
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	15	0.86
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	15	0.86
(1,142)	1:88:A:GLU:HG3	1:89:A:LYS:H	10	0.86
(1,1993)	1:130:A:GLU:HB2	1:128:A:TRP:HE3	15	0.85
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	19	0.85
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	13	0.85
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	13	0.85
(1,1907)	1:64:A:ASP:HB3	1:57:A:TYR:HD1	4	0.85
(1,1907)	1:64:A:ASP:HB3	1:57:A:TYR:HD2	4	0.85
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	13	0.85
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	13	0.85
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	13	0.85
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	19	0.85
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	12	0.85
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	1	0.85
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	14	0.85
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	16	0.85
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD11	19	0.85
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD12	19	0.85
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD13	19	0.85
(1,1147)	1:83:A:ALA:HA	1:86:A:ILE:HG12	10	0.85
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	13	0.85
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	13	0.85
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	13	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	9	0.85
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	9	0.85
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	9	0.85
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	9	0.85
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	9	0.85
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	9	0.85
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	9	0.85
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	9	0.85
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	9	0.85
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	11	0.85
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	11	0.85
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	11	0.85
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	5	0.85
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	5	0.85
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	5	0.85
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG11	15	0.85
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG12	15	0.85
(1,847)	1:122:A:LYS:H	1:118:A:VAL:HG13	15	0.85
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	6	0.85
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	6	0.85
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	6	0.85
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	12	0.85
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	12	0.85
(1,786)	1:75:A:ARG:HA	1:75:A:ARG:HD2	6	0.85
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	3	0.85
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	3	0.85
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	3	0.85
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	5	0.85
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	5	0.85
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	5	0.85
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	6	0.85
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	6	0.85
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	6	0.85
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	3	0.85
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	14	0.85
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	14	0.85
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	14	0.85
(1,419)	1:6:A:ARG:HG3	1:6:A:ARG:H	20	0.85
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	6	0.85
(1,279)	1:67:A:THR:HB	1:69:A:ILE:HG13	2	0.85
(1,263)	1:86:A:ILE:H	1:85:A:LYS:HB2	1	0.85
(1,263)	1:86:A:ILE:H	1:85:A:LYS:HB2	2	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:86:A:ILE:H	1:81:A:MET:HG2	2	0.85
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	16	0.85
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	16	0.85
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	16	0.85
(1,136)	1:38:A:GLU:HG3	1:74:A:THR:HG21	7	0.85
(1,136)	1:38:A:GLU:HG3	1:74:A:THR:HG22	7	0.85
(1,136)	1:38:A:GLU:HG3	1:74:A:THR:HG23	7	0.85
(1,76)	1:140:A:ASP:HB2	1:135:A:CYS:HA	19	0.85
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE1	3	0.84
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE2	3	0.84
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	1	0.84
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	1	0.84
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	20	0.84
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	20	0.84
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	12	0.84
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	17	0.84
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	16	0.84
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	18	0.84
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	6	0.84
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	6	0.84
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	6	0.84
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	7	0.84
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	17	0.84
(1,1221)	1:65:A:ALA:HA	1:57:A:TYR:HD1	1	0.84
(1,1221)	1:65:A:ALA:HA	1:57:A:TYR:HD2	1	0.84
(1,1147)	1:83:A:ALA:HA	1:86:A:ILE:HG12	19	0.84
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE1	5	0.84
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE2	5	0.84
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE3	5	0.84
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	17	0.84
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	17	0.84
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	17	0.84
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	12	0.84
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	14	0.84
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	6	0.84
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	11	0.84
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	16	0.84
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	1	0.84
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	1	0.84
(1,907)	1:18:A:LEU:HB3	1:83:A:ALA:HB1	3	0.84
(1,907)	1:18:A:LEU:HB3	1:83:A:ALA:HB2	3	0.84
(1,907)	1:18:A:LEU:HB3	1:83:A:ALA:HB3	3	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	6	0.84
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	6	0.84
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	6	0.84
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	20	0.84
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	20	0.84
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	20	0.84
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD2	3	0.84
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD2	3	0.84
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD2	3	0.84
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD3	3	0.84
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD3	3	0.84
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD3	3	0.84
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	20	0.84
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	20	0.84
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	20	0.84
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	4	0.84
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	4	0.84
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	8	0.84
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	8	0.84
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	18	0.84
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	18	0.84
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	1	0.84
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	1	0.84
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	1	0.84
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	4	0.84
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	4	0.84
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	4	0.84
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	8	0.84
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	8	0.84
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	8	0.84
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	10	0.84
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	10	0.84
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	10	0.84
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	11	0.84
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	11	0.84
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	11	0.84
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	13	0.84
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	13	0.84
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	13	0.84
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	14	0.84
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	14	0.84
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	14	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	15	0.84
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	15	0.84
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	15	0.84
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	16	0.84
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	16	0.84
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	16	0.84
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	10	0.84
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	10	0.84
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	10	0.84
(1,441)	1:113:A:LEU:HD21	1:146:A:GLN:HG3	7	0.84
(1,441)	1:113:A:LEU:HD22	1:146:A:GLN:HG3	7	0.84
(1,441)	1:113:A:LEU:HD23	1:146:A:GLN:HG3	7	0.84
(1,441)	1:113:A:LEU:HD21	1:146:A:GLN:HG3	14	0.84
(1,441)	1:113:A:LEU:HD22	1:146:A:GLN:HG3	14	0.84
(1,441)	1:113:A:LEU:HD23	1:146:A:GLN:HG3	14	0.84
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	12	0.84
(1,324)	1:142:A:VAL:HG21	1:114:A:ARG:HB2	4	0.84
(1,324)	1:142:A:VAL:HG22	1:114:A:ARG:HB2	4	0.84
(1,324)	1:142:A:VAL:HG23	1:114:A:ARG:HB2	4	0.84
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB2	1	0.84
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB3	1	0.84
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB2	9	0.84
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB3	9	0.84
(1,256)	1:86:A:ILE:H	1:81:A:MET:HG2	9	0.84
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	1	0.84
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	9	0.84
(1,145)	1:85:A:LYS:HA	1:88:A:GLU:HG2	5	0.84
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	10	0.83
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	10	0.83
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	10	0.83
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	10	0.83
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	7	0.83
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	7	0.83
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	7	0.83
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	1	0.83
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	8	0.83
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	14	0.83
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	11	0.83
(1,1158)	1:101:A:LYS:HD3	1:101:A:LYS:HA	13	0.83
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	20	0.83
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	20	0.83
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	20	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:84:A:MET:HE1	1:15:A:LYS:HE2	4	0.83
(1,1017)	1:84:A:MET:HE2	1:15:A:LYS:HE2	4	0.83
(1,1017)	1:84:A:MET:HE3	1:15:A:LYS:HE2	4	0.83
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	4	0.83
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	4	0.83
(1,861)	1:111:A:VAL:HG21	1:111:A:VAL:H	18	0.83
(1,861)	1:111:A:VAL:HG22	1:111:A:VAL:H	18	0.83
(1,861)	1:111:A:VAL:HG23	1:111:A:VAL:H	18	0.83
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	19	0.83
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	19	0.83
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	19	0.83
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	6	0.83
(1,687)	1:17:A:PHE:HA	1:20:A:ARG:HB2	14	0.83
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	2	0.83
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	2	0.83
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	2	0.83
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	9	0.83
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	9	0.83
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	9	0.83
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	18	0.83
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	18	0.83
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	18	0.83
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	19	0.83
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	19	0.83
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	19	0.83
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	8	0.83
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	8	0.83
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	8	0.83
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	17	0.83
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	17	0.83
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	17	0.83
(1,507)	1:92:A:LYS:HG3	1:93:A:LEU:H	2	0.83
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	5	0.83
(1,263)	1:86:A:ILE:H	1:85:A:LYS:HB2	12	0.83
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	13	0.83
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	13	0.83
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	13	0.83
(1,2012)	1:152:A:TYR:HE1	1:151:A:LYS:HE2	4	0.82
(1,2012)	1:152:A:TYR:HE2	1:151:A:LYS:HE2	4	0.82
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD1	3	0.82
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD2	3	0.82
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	15	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	15	0.82
(1,1871)	1:8:A:GLY:H	1:7:A:PRO:HG3	7	0.82
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	7	0.82
(1,1810)	1:91:A:LYS:HB3	1:92:A:LYS:H	17	0.82
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	2	0.82
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	20	0.82
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	15	0.82
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	14	0.82
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	20	0.82
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	19	0.82
(1,1147)	1:83:A:ALA:HA	1:86:A:ILE:HG12	11	0.82
(1,1105)	1:103:A:GLU:HA	1:104:A:LYS:HG2	16	0.82
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE1	14	0.82
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE2	14	0.82
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE3	14	0.82
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE1	19	0.82
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE2	19	0.82
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE3	19	0.82
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	20	0.82
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	20	0.82
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	7	0.82
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	7	0.82
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	7	0.82
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	13	0.82
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	13	0.82
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	13	0.82
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	12	0.82
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	12	0.82
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	12	0.82
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	20	0.82
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	20	0.82
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	20	0.82
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	19	0.82
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	19	0.82
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	19	0.82
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	19	0.82
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	19	0.82
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	19	0.82
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	19	0.82
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	19	0.82
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	19	0.82
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD11	17	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD12	17	0.82
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD13	17	0.82
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	4	0.82
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	4	0.82
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	4	0.82
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	18	0.82
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	18	0.82
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	18	0.82
(1,506)	1:93:A:LEU:H	1:92:A:LYS:HG2	3	0.82
(1,418)	1:6:A:ARG:H	1:6:A:ARG:HG2	19	0.82
(1,313)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	7	0.82
(1,76)	1:140:A:ASP:HB2	1:135:A:CYS:HA	10	0.82
(1,26)	1:117:A:ARG:HB3	1:117:A:ARG:HD2	18	0.82
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	3	0.82
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	3	0.82
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	3	0.82
(1,2)	1:8:A:GLY:HA2	1:15:A:LYS:HD2	8	0.82
(1,2)	1:8:A:GLY:HA3	1:15:A:LYS:HD2	8	0.82
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	10	0.81
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	12	0.81
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	20	0.81
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	20	0.81
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	20	0.81
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	13	0.81
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	9	0.81
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	4	0.81
(1,1106)	1:104:A:LYS:HG3	1:103:A:GLU:HA	16	0.81
(1,1105)	1:103:A:GLU:HA	1:104:A:LYS:HG2	6	0.81
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	13	0.81
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	13	0.81
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	13	0.81
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	16	0.81
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	16	0.81
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	16	0.81
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	15	0.81
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	15	0.81
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	15	0.81
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	6	0.81
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	6	0.81
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	6	0.81
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG21	7	0.81
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG22	7	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:146:A:GLN:HG3	1:142:A:VAL:HG23	7	0.81
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	17	0.81
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	17	0.81
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	17	0.81
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	8	0.81
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	8	0.81
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	8	0.81
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	7	0.81
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	7	0.81
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	7	0.81
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	3	0.81
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	3	0.81
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	3	0.81
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	19	0.81
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	19	0.81
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	19	0.81
(1,558)	1:158:A:LYS:HG2	1:158:A:LYS:HE2	9	0.81
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	19	0.81
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	19	0.81
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	19	0.81
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	4	0.81
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	9	0.81
(1,380)	1:81:A:MET:HG3	1:86:A:ILE:HG12	4	0.81
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	19	0.81
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	19	0.81
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	19	0.81
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG21	6	0.81
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG22	6	0.81
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG23	6	0.81
(1,26)	1:117:A:ARG:HB3	1:117:A:ARG:HD2	12	0.81
(1,26)	1:117:A:ARG:HB3	1:117:A:ARG:HD2	14	0.81
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	20	0.8
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	9	0.8
(1,1899)	1:69:A:ILE:HG12	1:60:A:GLY:H	17	0.8
(1,1860)	1:139:A:THR:H	1:137:A:GLU:HB3	16	0.8
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	4	0.8
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	5	0.8
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	17	0.8
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	8	0.8
(1,1381)	1:158:A:LYS:H	1:158:A:LYS:HG3	4	0.8
(1,1147)	1:83:A:ALA:HA	1:86:A:ILE:HG12	9	0.8
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	8	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	8	0.8
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	8	0.8
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	1	0.8
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	1	0.8
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	1	0.8
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	5	0.8
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	5	0.8
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	5	0.8
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	9	0.8
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	9	0.8
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	9	0.8
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	7	0.8
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	7	0.8
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	7	0.8
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	1	0.8
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	1	0.8
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	2	0.8
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	2	0.8
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	2	0.8
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	12	0.8
(1,670)	1:142:A:VAL:HG11	1:142:A:VAL:H	7	0.8
(1,670)	1:142:A:VAL:HG12	1:142:A:VAL:H	7	0.8
(1,670)	1:142:A:VAL:HG13	1:142:A:VAL:H	7	0.8
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	3	0.8
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	3	0.8
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	3	0.8
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	3	0.8
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	3	0.8
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	3	0.8
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	3	0.8
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	3	0.8
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	3	0.8
(1,573)	1:106:A:LEU:HD21	1:108:A:LEU:HA	13	0.8
(1,573)	1:106:A:LEU:HD22	1:108:A:LEU:HA	13	0.8
(1,573)	1:106:A:LEU:HD23	1:108:A:LEU:HA	13	0.8
(1,531)	1:92:A:LYS:HD3	1:92:A:LYS:HB2	11	0.8
(1,418)	1:6:A:ARG:H	1:6:A:ARG:HG2	16	0.8
(1,380)	1:81:A:MET:HG3	1:86:A:ILE:HG12	8	0.8
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD2	6	0.8
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD3	6	0.8
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD2	8	0.8
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD3	8	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,313)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	1	0.8
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB2	15	0.8
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB3	15	0.8
(1,244)	1:85:A:LYS:HB3	1:81:A:MET:HG2	14	0.8
(1,26)	1:117:A:ARG:HB3	1:117:A:ARG:HD2	7	0.8
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	8	0.79
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD1	20	0.79
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD2	20	0.79
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	11	0.79
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	11	0.79
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	15	0.79
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	9	0.79
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	1	0.79
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	2	0.79
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	10	0.79
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	13	0.79
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	19	0.79
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	17	0.79
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	17	0.79
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	17	0.79
(1,1110)	1:116:A:MET:HA	1:117:A:ARG:HD2	4	0.79
(1,1085)	1:56:A:CYS:HB3	1:53:A:ASN:HA	11	0.79
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	19	0.79
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	19	0.79
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	19	0.79
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	2	0.79
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	2	0.79
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	2	0.79
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	2	0.79
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	2	0.79
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	2	0.79
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	2	0.79
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	2	0.79
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	2	0.79
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	12	0.79
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	12	0.79
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	12	0.79
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	19	0.79
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	19	0.79
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	19	0.79
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	4	0.79
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	4	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	4	0.79
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	10	0.79
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	10	0.79
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	10	0.79
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG21	7	0.79
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG22	7	0.79
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG23	7	0.79
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG21	7	0.79
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG22	7	0.79
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG23	7	0.79
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG21	7	0.79
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG22	7	0.79
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG23	7	0.79
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG21	7	0.79
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG22	7	0.79
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG23	7	0.79
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG21	7	0.79
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG22	7	0.79
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG23	7	0.79
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG21	7	0.79
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG22	7	0.79
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG23	7	0.79
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	9	0.79
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	9	0.79
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	9	0.79
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	9	0.79
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	9	0.79
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	9	0.79
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	8	0.79
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	8	0.79
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	8	0.79
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD11	19	0.79
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD12	19	0.79
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD13	19	0.79
(1,558)	1:158:A:LYS:HG2	1:158:A:LYS:HE2	10	0.79
(1,552)	1:31:A:ASN:HD21	1:33:A:SER:HB2	13	0.79
(1,531)	1:92:A:LYS:HD3	1:92:A:LYS:HB2	6	0.79
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	3	0.79
(1,93)	1:64:A:ASP:HB3	1:57:A:TYR:HD1	11	0.79
(1,93)	1:64:A:ASP:HB3	1:57:A:TYR:HD2	11	0.79
(1,26)	1:117:A:ARG:HB3	1:117:A:ARG:HD2	2	0.79
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB1	7	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB2	7	0.79
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB3	7	0.79
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	19	0.79
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	5	0.78
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	5	0.78
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	6	0.78
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	6	0.78
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	8	0.78
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	8	0.78
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	4	0.78
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	4	0.78
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	4	0.78
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	10	0.78
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	7	0.78
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	6	0.78
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	7	0.78
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	3	0.78
(1,1490)	1:140:A:ASP:H	1:137:A:GLU:HB3	12	0.78
(1,1183)	1:86:A:ILE:HD11	1:76:A:PRO:HG3	3	0.78
(1,1183)	1:86:A:ILE:HD12	1:76:A:PRO:HG3	3	0.78
(1,1183)	1:86:A:ILE:HD13	1:76:A:PRO:HG3	3	0.78
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	19	0.78
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	19	0.78
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	19	0.78
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	19	0.78
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	19	0.78
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	19	0.78
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	19	0.78
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	19	0.78
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	19	0.78
(1,1085)	1:56:A:CYS:HB3	1:53:A:ASN:HA	13	0.78
(1,1017)	1:84:A:MET:HE1	1:15:A:LYS:HE2	9	0.78
(1,1017)	1:84:A:MET:HE2	1:15:A:LYS:HE2	9	0.78
(1,1017)	1:84:A:MET:HE3	1:15:A:LYS:HE2	9	0.78
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	6	0.78
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	6	0.78
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	6	0.78
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	6	0.78
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	6	0.78
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	6	0.78
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	6	0.78
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	6	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	6	0.78
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	17	0.78
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	17	0.78
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	2	0.78
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	2	0.78
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	2	0.78
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	20	0.78
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	20	0.78
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	20	0.78
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	14	0.78
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	14	0.78
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	14	0.78
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	20	0.78
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	20	0.78
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	20	0.78
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	9	0.78
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	9	0.78
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	9	0.78
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	16	0.78
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	16	0.78
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	16	0.78
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	18	0.78
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	18	0.78
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	18	0.78
(1,506)	1:93:A:LEU:H	1:92:A:LYS:HG2	18	0.78
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	1	0.78
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	5	0.78
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD11	2	0.78
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD12	2	0.78
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD13	2	0.78
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	17	0.78
(1,48)	1:86:A:ILE:HG21	1:89:A:LYS:HE3	8	0.78
(1,48)	1:86:A:ILE:HG22	1:89:A:LYS:HE3	8	0.78
(1,48)	1:86:A:ILE:HG23	1:89:A:LYS:HE3	8	0.78
(1,1969)	1:24:A:SER:HB3	1:44:A:PHE:HZ	2	0.77
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	9	0.77
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	9	0.77
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	12	0.77
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	6	0.77
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	1	0.77
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	1	0.77
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	1	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1277)	1:128:A:TRP:HE1	1:127:A:SER:HB2	7	0.77
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	2	0.77
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	2	0.77
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	2	0.77
(1,1138)	1:141:A:TYR:HB2	1:145:A:ILE:HD11	14	0.77
(1,1138)	1:141:A:TYR:HB2	1:145:A:ILE:HD12	14	0.77
(1,1138)	1:141:A:TYR:HB2	1:145:A:ILE:HD13	14	0.77
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	17	0.77
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	17	0.77
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	17	0.77
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	17	0.77
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	17	0.77
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	17	0.77
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	17	0.77
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	17	0.77
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	17	0.77
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	1	0.77
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	1	0.77
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	1	0.77
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	15	0.77
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	15	0.77
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	15	0.77
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	11	0.77
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	11	0.77
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	11	0.77
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	11	0.77
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	11	0.77
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	11	0.77
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	11	0.77
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	11	0.77
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	11	0.77
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	6	0.77
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	6	0.77
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	6	0.77
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	15	0.77
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	15	0.77
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	15	0.77
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	17	0.77
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	17	0.77
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	17	0.77
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	1	0.77
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	1	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	1	0.77
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	5	0.77
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	5	0.77
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	5	0.77
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	7	0.77
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	7	0.77
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	7	0.77
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	11	0.77
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	11	0.77
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	11	0.77
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	17	0.77
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	17	0.77
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	17	0.77
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	1	0.77
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	1	0.77
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	1	0.77
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	9	0.77
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	17	0.77
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	17	0.77
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	17	0.77
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	9	0.77
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	9	0.77
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	9	0.77
(1,573)	1:106:A:LEU:HD21	1:108:A:LEU:HA	14	0.77
(1,573)	1:106:A:LEU:HD22	1:108:A:LEU:HA	14	0.77
(1,573)	1:106:A:LEU:HD23	1:108:A:LEU:HA	14	0.77
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD11	8	0.77
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD12	8	0.77
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD13	8	0.77
(1,558)	1:158:A:LYS:HG2	1:158:A:LYS:HE2	4	0.77
(1,558)	1:158:A:LYS:HG2	1:158:A:LYS:HE2	6	0.77
(1,532)	1:92:A:LYS:HB3	1:92:A:LYS:HD3	3	0.77
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	9	0.77
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	9	0.77
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	9	0.77
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	20	0.77
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	20	0.77
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	20	0.77
(1,431)	1:141:A:TYR:HB3	1:121:A:LEU:HD21	2	0.77
(1,431)	1:141:A:TYR:HB3	1:121:A:LEU:HD22	2	0.77
(1,431)	1:141:A:TYR:HB3	1:121:A:LEU:HD23	2	0.77
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	11	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	11	0.77
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	11	0.77
(1,209)	1:67:A:THR:HG21	1:68:A:LYS:HB3	4	0.77
(1,209)	1:67:A:THR:HG22	1:68:A:LYS:HB3	4	0.77
(1,209)	1:67:A:THR:HG23	1:68:A:LYS:HB3	4	0.77
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	5	0.77
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	5	0.77
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	5	0.77
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG21	15	0.77
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG22	15	0.77
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG23	15	0.77
(1,93)	1:64:A:ASP:HB3	1:57:A:TYR:HD1	4	0.77
(1,93)	1:64:A:ASP:HB3	1:57:A:TYR:HD2	4	0.77
(1,76)	1:140:A:ASP:HB2	1:135:A:CYS:HA	15	0.77
(1,61)	1:122:A:LYS:HE3	1:141:A:TYR:HE1	6	0.77
(1,61)	1:122:A:LYS:HE3	1:141:A:TYR:HE2	6	0.77
(1,2008)	1:64:A:ASP:HB3	1:57:A:TYR:HE1	9	0.76
(1,2008)	1:64:A:ASP:HB3	1:57:A:TYR:HE2	9	0.76
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	17	0.76
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	3	0.76
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	3	0.76
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	13	0.76
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	13	0.76
(1,1871)	1:8:A:GLY:H	1:7:A:PRO:HG3	1	0.76
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	13	0.76
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	16	0.76
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	16	0.76
(1,1126)	1:104:A:LYS:HG3	1:104:A:LYS:HA	16	0.76
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	12	0.76
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	12	0.76
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	14	0.76
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	14	0.76
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	14	0.76
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	18	0.76
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	18	0.76
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	18	0.76
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	11	0.76
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	11	0.76
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	11	0.76
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	3	0.76
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	3	0.76
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	3	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	3	0.76
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	3	0.76
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	3	0.76
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	10	0.76
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	10	0.76
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	10	0.76
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	13	0.76
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	13	0.76
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	13	0.76
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB2	15	0.76
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB3	15	0.76
(1,558)	1:158:A:LYS:HG2	1:158:A:LYS:HE2	1	0.76
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	13	0.76
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	13	0.76
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	12	0.76
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	12	0.76
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	12	0.76
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	18	0.76
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	18	0.76
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	18	0.76
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB2	6	0.76
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB3	6	0.76
(1,263)	1:86:A:ILE:H	1:85:A:LYS:HB2	4	0.76
(1,263)	1:86:A:ILE:H	1:85:A:LYS:HB2	6	0.76
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	10	0.76
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	10	0.76
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	10	0.76
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD21	11	0.76
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD22	11	0.76
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD23	11	0.76
(1,206)	1:158:A:LYS:HE3	1:158:A:LYS:HB2	4	0.76
(1,192)	1:111:A:VAL:HG11	1:116:A:MET:HG3	5	0.76
(1,192)	1:111:A:VAL:HG12	1:116:A:MET:HG3	5	0.76
(1,192)	1:111:A:VAL:HG13	1:116:A:MET:HG3	5	0.76
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	9	0.76
(1,20)	1:114:A:ARG:HB2	1:114:A:ARG:HD2	20	0.76
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB1	1	0.76
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB2	1	0.76
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB3	1	0.76
(1,1987)	1:157:A:PRO:HD2	1:156:A:HIS:HD2	5	0.75
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	8	0.75
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	8	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	2	0.75
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	2	0.75
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	3	0.75
(1,1646)	1:88:A:GLU:HB3	1:87:A:CYS:H	10	0.75
(1,1157)	1:101:A:LYS:HA	1:101:A:LYS:HD2	5	0.75
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	4	0.75
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	4	0.75
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	4	0.75
(1,1085)	1:56:A:CYS:HB3	1:53:A:ASN:HA	2	0.75
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	16	0.75
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	16	0.75
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	16	0.75
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	12	0.75
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	12	0.75
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	12	0.75
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	12	0.75
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	12	0.75
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	12	0.75
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	12	0.75
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	12	0.75
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	12	0.75
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	7	0.75
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	7	0.75
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	10	0.75
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	10	0.75
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	10	0.75
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	11	0.75
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	11	0.75
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	11	0.75
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG11	20	0.75
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG12	20	0.75
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG13	20	0.75
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	9	0.75
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	9	0.75
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	9	0.75
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	12	0.75
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	12	0.75
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	12	0.75
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	10	0.75
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	12	0.75
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	12	0.75
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	12	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	8	0.75
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	8	0.75
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	8	0.75
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	8	0.75
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	8	0.75
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	8	0.75
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD11	3	0.75
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD12	3	0.75
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD13	3	0.75
(1,558)	1:158:A:LYS:HG2	1:158:A:LYS:HE2	13	0.75
(1,558)	1:158:A:LYS:HG2	1:158:A:LYS:HE2	14	0.75
(1,558)	1:158:A:LYS:HG2	1:158:A:LYS:HE2	16	0.75
(1,531)	1:92:A:LYS:HD3	1:92:A:LYS:HB2	9	0.75
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	2	0.75
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	2	0.75
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	2	0.75
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB2	13	0.75
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB3	13	0.75
(1,263)	1:86:A:ILE:H	1:85:A:LYS:HB2	13	0.75
(1,153)	1:103:A:GLU:HG3	1:104:A:LYS:H	13	0.75
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG21	5	0.75
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG22	5	0.75
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG23	5	0.75
(1,27)	1:117:A:ARG:HD3	1:117:A:ARG:HB3	3	0.75
(1,21)	1:114:A:ARG:HD3	1:114:A:ARG:HB2	9	0.75
(1,20)	1:114:A:ARG:HB2	1:114:A:ARG:HD2	17	0.75
(1,11)	1:8:A:GLY:HA3	1:15:A:LYS:HE3	17	0.75
(1,9)	1:8:A:GLY:HA2	1:15:A:LYS:HE2	6	0.75
(1,9)	1:8:A:GLY:HA3	1:15:A:LYS:HE2	6	0.75
(1,1993)	1:130:A:GLU:HB2	1:128:A:TRP:HE3	8	0.74
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	4	0.74
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	4	0.74
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	12	0.74
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	12	0.74
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD1	16	0.74
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD2	16	0.74
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	3	0.74
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	3	0.74
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	3	0.74
(1,1319)	1:8:A:GLY:HA3	1:9:A:ALA:H	13	0.74
(1,1085)	1:56:A:CYS:HB3	1:53:A:ASN:HA	4	0.74
(1,1085)	1:56:A:CYS:HB3	1:53:A:ASN:HA	7	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	1	0.74
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	1	0.74
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	1	0.74
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	8	0.74
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	8	0.74
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	10	0.74
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	10	0.74
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	10	0.74
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	12	0.74
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	12	0.74
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	12	0.74
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG11	11	0.74
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG12	11	0.74
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG13	11	0.74
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	10	0.74
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	15	0.74
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	15	0.74
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	15	0.74
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	19	0.74
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	19	0.74
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	19	0.74
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	1	0.74
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	1	0.74
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	1	0.74
(1,605)	1:107:A:ASP:HB3	1:110:A:SER:HB3	15	0.74
(1,573)	1:106:A:LEU:HD21	1:108:A:LEU:HA	20	0.74
(1,573)	1:106:A:LEU:HD22	1:108:A:LEU:HA	20	0.74
(1,573)	1:106:A:LEU:HD23	1:108:A:LEU:HA	20	0.74
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	9	0.74
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	9	0.74
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	9	0.74
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	14	0.74
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	14	0.74
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	14	0.74
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	16	0.74
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	16	0.74
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	16	0.74
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	16	0.74
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	16	0.74
(1,313)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	15	0.74
(1,263)	1:86:A:ILE:H	1:85:A:LYS:HB2	8	0.74
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG21	18	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG22	18	0.74
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG23	18	0.74
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	6	0.73
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	6	0.73
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	6	0.73
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	3	0.73
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	18	0.73
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	18	0.73
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	18	0.73
(1,1319)	1:8:A:GLY:HA3	1:9:A:ALA:H	9	0.73
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	11	0.73
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	16	0.73
(1,1277)	1:128:A:TRP:HE1	1:127:A:SER:HB2	2	0.73
(1,1157)	1:101:A:LYS:HA	1:101:A:LYS:HD2	14	0.73
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	18	0.73
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	18	0.73
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	18	0.73
(1,1101)	1:158:A:LYS:HA	1:158:A:LYS:HG3	19	0.73
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	8	0.73
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	8	0.73
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	8	0.73
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	18	0.73
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	18	0.73
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	18	0.73
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	4	0.73
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	4	0.73
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	4	0.73
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	13	0.73
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	13	0.73
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	3	0.73
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	3	0.73
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	3	0.73
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB1	1	0.73
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB2	1	0.73
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB3	1	0.73
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	9	0.73
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	9	0.73
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	9	0.73
(1,868)	1:13:A:VAL:HG21	1:52:A:GLU:HG2	14	0.73
(1,868)	1:13:A:VAL:HG22	1:52:A:GLU:HG2	14	0.73
(1,868)	1:13:A:VAL:HG23	1:52:A:GLU:HG2	14	0.73
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE1	17	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,792)	1:57:A:TYR:HA	1:57:A:TYR:HE2	17	0.73
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	14	0.73
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	14	0.73
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	14	0.73
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	18	0.73
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	18	0.73
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	18	0.73
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	19	0.73
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	20	0.73
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	20	0.73
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	20	0.73
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	20	0.73
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	20	0.73
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	20	0.73
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	8	0.73
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	8	0.73
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	8	0.73
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	11	0.73
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	11	0.73
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	11	0.73
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	17	0.73
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	17	0.73
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	17	0.73
(1,559)	1:158:A:LYS:HE3	1:158:A:LYS:HG2	5	0.73
(1,530)	1:92:A:LYS:HB3	1:92:A:LYS:HD2	18	0.73
(1,530)	1:92:A:LYS:HB2	1:92:A:LYS:HD2	18	0.73
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	13	0.73
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	13	0.73
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	13	0.73
(1,507)	1:92:A:LYS:HG3	1:93:A:LEU:H	9	0.73
(1,418)	1:6:A:ARG:H	1:6:A:ARG:HG2	6	0.73
(1,362)	1:75:A:ARG:HB2	1:75:A:ARG:HD2	11	0.73
(1,243)	1:81:A:MET:HG3	1:85:A:LYS:HB2	6	0.73
(1,243)	1:81:A:MET:HG2	1:85:A:LYS:HB2	6	0.73
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	11	0.73
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	11	0.73
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	11	0.73
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD11	10	0.73
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD12	10	0.73
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD13	10	0.73
(1,21)	1:114:A:ARG:HD3	1:114:A:ARG:HB2	2	0.73
(1,20)	1:114:A:ARG:HB2	1:114:A:ARG:HD2	12	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	18	0.72
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	18	0.72
(1,1839)	1:114:A:ARG:H	1:114:A:ARG:HG3	16	0.72
(1,1838)	1:114:A:ARG:HB3	1:114:A:ARG:H	2	0.72
(1,1838)	1:114:A:ARG:HB3	1:114:A:ARG:H	11	0.72
(1,1810)	1:91:A:LYS:HB3	1:92:A:LYS:H	3	0.72
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	7	0.72
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	10	0.72
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	12	0.72
(1,1380)	1:158:A:LYS:HB2	1:158:A:LYS:H	20	0.72
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	15	0.72
(1,1017)	1:84:A:MET:HE1	1:15:A:LYS:HE2	2	0.72
(1,1017)	1:84:A:MET:HE2	1:15:A:LYS:HE2	2	0.72
(1,1017)	1:84:A:MET:HE3	1:15:A:LYS:HE2	2	0.72
(1,1017)	1:84:A:MET:HE1	1:15:A:LYS:HE2	7	0.72
(1,1017)	1:84:A:MET:HE2	1:15:A:LYS:HE2	7	0.72
(1,1017)	1:84:A:MET:HE3	1:15:A:LYS:HE2	7	0.72
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	2	0.72
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	2	0.72
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	2	0.72
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	13	0.72
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	13	0.72
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	13	0.72
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	4	0.72
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	4	0.72
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	4	0.72
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	17	0.72
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	17	0.72
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	17	0.72
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	8	0.72
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	8	0.72
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	8	0.72
(1,696)	1:71:A:SER:HB3	1:75:A:ARG:HD2	12	0.72
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	15	0.72
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	15	0.72
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	15	0.72
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	15	0.72
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	15	0.72
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	15	0.72
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	1	0.72
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	1	0.72
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	1	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	9	0.72
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	9	0.72
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	9	0.72
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	11	0.72
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	11	0.72
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	11	0.72
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	15	0.72
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	15	0.72
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	15	0.72
(1,605)	1:107:A:ASP:HB3	1:110:A:SER:HB3	9	0.72
(1,605)	1:107:A:ASP:HB3	1:110:A:SER:HB3	11	0.72
(1,605)	1:107:A:ASP:HB3	1:110:A:SER:HB3	16	0.72
(1,558)	1:158:A:LYS:HG2	1:158:A:LYS:HE2	20	0.72
(1,532)	1:92:A:LYS:HB3	1:92:A:LYS:HD3	12	0.72
(1,532)	1:92:A:LYS:HB3	1:92:A:LYS:HD3	18	0.72
(1,531)	1:92:A:LYS:HD3	1:92:A:LYS:HB2	20	0.72
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	6	0.72
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	6	0.72
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	6	0.72
(1,484)	1:142:A:VAL:HG11	1:139:A:THR:HA	14	0.72
(1,484)	1:142:A:VAL:HG12	1:139:A:THR:HA	14	0.72
(1,484)	1:142:A:VAL:HG13	1:139:A:THR:HA	14	0.72
(1,418)	1:6:A:ARG:H	1:6:A:ARG:HG2	3	0.72
(1,243)	1:81:A:MET:HG3	1:85:A:LYS:HB2	17	0.72
(1,243)	1:81:A:MET:HG2	1:85:A:LYS:HB2	17	0.72
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	3	0.72
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	3	0.72
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	3	0.72
(1,136)	1:38:A:GLU:HG3	1:74:A:THR:HG21	3	0.72
(1,136)	1:38:A:GLU:HG3	1:74:A:THR:HG22	3	0.72
(1,136)	1:38:A:GLU:HG3	1:74:A:THR:HG23	3	0.72
(1,5)	1:9:A:ALA:HB1	1:8:A:GLY:HA2	5	0.72
(1,5)	1:9:A:ALA:HB2	1:8:A:GLY:HA2	5	0.72
(1,5)	1:9:A:ALA:HB3	1:8:A:GLY:HA2	5	0.72
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	11	0.71
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	16	0.71
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	16	0.71
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD1	18	0.71
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD2	18	0.71
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	16	0.71
(1,1716)	1:143:A:ASN:HB3	1:143:A:ASN:H	15	0.71
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	6	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	11	0.71
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	19	0.71
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	7	0.71
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	12	0.71
(1,1319)	1:8:A:GLY:HA3	1:9:A:ALA:H	8	0.71
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	7	0.71
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	12	0.71
(1,1272)	1:106:A:LEU:HD21	1:128:A:TRP:HE1	8	0.71
(1,1272)	1:106:A:LEU:HD22	1:128:A:TRP:HE1	8	0.71
(1,1272)	1:106:A:LEU:HD23	1:128:A:TRP:HE1	8	0.71
(1,1157)	1:101:A:LYS:HA	1:101:A:LYS:HD2	3	0.71
(1,1105)	1:103:A:GLU:HA	1:104:A:LYS:HG2	18	0.71
(1,1102)	1:158:A:LYS:HG2	1:158:A:LYS:HA	7	0.71
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	15	0.71
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	15	0.71
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	15	0.71
(1,944)	1:79:A:VAL:HG21	1:79:A:VAL:H	8	0.71
(1,944)	1:79:A:VAL:HG22	1:79:A:VAL:H	8	0.71
(1,944)	1:79:A:VAL:HG23	1:79:A:VAL:H	8	0.71
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	14	0.71
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	14	0.71
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	14	0.71
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	6	0.71
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	6	0.71
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	6	0.71
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	12	0.71
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	12	0.71
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	12	0.71
(1,786)	1:75:A:ARG:HA	1:75:A:ARG:HD2	20	0.71
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	1	0.71
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	1	0.71
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	1	0.71
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	13	0.71
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	13	0.71
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	13	0.71
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	20	0.71
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	20	0.71
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	20	0.71
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	8	0.71
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	8	0.71
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	8	0.71
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	16	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	16	0.71
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	16	0.71
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	2	0.71
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	2	0.71
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	2	0.71
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	11	0.71
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	11	0.71
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	11	0.71
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	2	0.71
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	2	0.71
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	2	0.71
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	9	0.71
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	9	0.71
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	9	0.71
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	12	0.71
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	12	0.71
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	12	0.71
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	14	0.71
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	14	0.71
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	14	0.71
(1,605)	1:107:A:ASP:HB3	1:110:A:SER:HB3	7	0.71
(1,558)	1:158:A:LYS:HG2	1:158:A:LYS:HE2	5	0.71
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	20	0.71
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	20	0.71
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	20	0.71
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	11	0.71
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	11	0.71
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	11	0.71
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	4	0.71
(1,353)	1:139:A:THR:HB	1:137:A:GLU:HG2	18	0.71
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	12	0.71
(1,183)	1:101:A:LYS:HB2	1:102:A:TYR:HA	17	0.71
(1,142)	1:88:A:GLU:HG3	1:89:A:LYS:H	20	0.71
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD11	5	0.71
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD12	5	0.71
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD13	5	0.71
(1,122)	1:94:A:ASP:HB3	1:97:A:ILE:HB	2	0.71
(1,3)	1:15:A:LYS:HD3	1:8:A:GLY:HA2	6	0.71
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	4	0.7
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE1	7	0.7
(1,1941)	1:17:A:PHE:HA	1:17:A:PHE:HE2	7	0.7
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	2	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	20	0.7
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	17	0.7
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	7	0.7
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	7	0.7
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	7	0.7
(1,1319)	1:8:A:GLY:HA3	1:9:A:ALA:H	16	0.7
(1,1318)	1:9:A:ALA:H	1:8:A:GLY:HA2	3	0.7
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	8	0.7
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	10	0.7
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	19	0.7
(1,1244)	1:7:A:PRO:HD2	1:6:A:ARG:HD2	10	0.7
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	7	0.7
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	7	0.7
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	7	0.7
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	7	0.7
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	7	0.7
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	7	0.7
(1,1158)	1:101:A:LYS:HD3	1:101:A:LYS:HA	2	0.7
(1,1157)	1:101:A:LYS:HA	1:101:A:LYS:HD2	18	0.7
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	13	0.7
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	13	0.7
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	13	0.7
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	13	0.7
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	13	0.7
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	13	0.7
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	13	0.7
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	13	0.7
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	13	0.7
(1,1102)	1:158:A:LYS:HG2	1:158:A:LYS:HA	18	0.7
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	14	0.7
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	14	0.7
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	14	0.7
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB1	4	0.7
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB2	4	0.7
(1,980)	1:122:A:LYS:HD3	1:119:A:ALA:HB3	4	0.7
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	9	0.7
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	9	0.7
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB1	8	0.7
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB2	8	0.7
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB3	8	0.7
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD2	2	0.7
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD2	2	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD2	2	0.7
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD3	2	0.7
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD3	2	0.7
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD3	2	0.7
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	15	0.7
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	15	0.7
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	15	0.7
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	11	0.7
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	14	0.7
(1,716)	1:148:A:LEU:HD21	1:147:A:GLU:HG2	2	0.7
(1,716)	1:148:A:LEU:HD22	1:147:A:GLU:HG2	2	0.7
(1,716)	1:148:A:LEU:HD23	1:147:A:GLU:HG2	2	0.7
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG21	17	0.7
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG22	17	0.7
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG23	17	0.7
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG21	17	0.7
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG22	17	0.7
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG23	17	0.7
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG21	17	0.7
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG22	17	0.7
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG23	17	0.7
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG21	17	0.7
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG22	17	0.7
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG23	17	0.7
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG21	17	0.7
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG22	17	0.7
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG23	17	0.7
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG21	17	0.7
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG22	17	0.7
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG23	17	0.7
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	5	0.7
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	7	0.7
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	7	0.7
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	7	0.7
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	7	0.7
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	7	0.7
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	7	0.7
(1,608)	1:111:A:VAL:HG21	1:110:A:SER:HB2	16	0.7
(1,608)	1:111:A:VAL:HG22	1:110:A:SER:HB2	16	0.7
(1,608)	1:111:A:VAL:HG23	1:110:A:SER:HB2	16	0.7
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD11	5	0.7
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD12	5	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD13	5	0.7
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD11	9	0.7
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD12	9	0.7
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD13	9	0.7
(1,441)	1:113:A:LEU:HD21	1:146:A:GLN:HG3	20	0.7
(1,441)	1:113:A:LEU:HD22	1:146:A:GLN:HG3	20	0.7
(1,441)	1:113:A:LEU:HD23	1:146:A:GLN:HG3	20	0.7
(1,436)	1:6:A:ARG:HG3	1:7:A:PRO:HD2	18	0.7
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	14	0.7
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	14	0.7
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	17	0.7
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	17	0.7
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	17	0.7
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	17	0.7
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	17	0.7
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	17	0.7
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	2	0.7
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	17	0.7
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	17	0.7
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	17	0.7
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	11	0.69
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	17	0.69
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	7	0.69
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	18	0.69
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	6	0.69
(1,1412)	1:124:A:ILE:H	1:123:A:GLN:HB2	8	0.69
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	1	0.69
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	2	0.69
(1,1277)	1:128:A:TRP:HE1	1:127:A:SER:HB2	15	0.69
(1,1102)	1:158:A:LYS:HG2	1:158:A:LYS:HA	2	0.69
(1,1102)	1:158:A:LYS:HG2	1:158:A:LYS:HA	12	0.69
(1,1085)	1:56:A:CYS:HB3	1:53:A:ASN:HA	10	0.69
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	7	0.69
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	7	0.69
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	7	0.69
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	7	0.69
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	7	0.69
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	7	0.69
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	7	0.69
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	7	0.69
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	7	0.69
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	16	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	16	0.69
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	16	0.69
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	16	0.69
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	16	0.69
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	16	0.69
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	16	0.69
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	16	0.69
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	16	0.69
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	17	0.69
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	17	0.69
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	17	0.69
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	17	0.69
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	17	0.69
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	17	0.69
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	17	0.69
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	17	0.69
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	17	0.69
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	18	0.69
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	18	0.69
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	18	0.69
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	18	0.69
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	18	0.69
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	18	0.69
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	18	0.69
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	18	0.69
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	18	0.69
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	3	0.69
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	3	0.69
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	4	0.69
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	4	0.69
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	4	0.69
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	14	0.69
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	14	0.69
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	14	0.69
(1,798)	1:138:A:LYS:HG3	1:138:A:LYS:HA	1	0.69
(1,798)	1:138:A:LYS:HG3	1:138:A:LYS:HA	14	0.69
(1,798)	1:138:A:LYS:HG3	1:138:A:LYS:HA	18	0.69
(1,787)	1:75:A:ARG:HD3	1:75:A:ARG:HA	10	0.69
(1,786)	1:75:A:ARG:HA	1:75:A:ARG:HD2	12	0.69
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	3	0.69
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	3	0.69
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	3	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	16	0.69
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	16	0.69
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	16	0.69
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	20	0.69
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	20	0.69
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	20	0.69
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	10	0.69
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	10	0.69
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	10	0.69
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	1	0.69
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	1	0.69
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	1	0.69
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	7	0.69
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	7	0.69
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	7	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD11	1	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD12	1	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD13	1	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD11	3	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD12	3	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD13	3	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD11	4	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD12	4	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD13	4	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD11	13	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD12	13	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD13	13	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD11	14	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD12	14	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD13	14	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD11	15	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD12	15	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD13	15	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD11	16	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD12	16	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD13	16	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD11	17	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD12	17	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD13	17	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD11	19	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD12	19	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD13	19	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD11	20	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD12	20	0.69
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD13	20	0.69
(1,573)	1:106:A:LEU:HD21	1:108:A:LEU:HA	5	0.69
(1,573)	1:106:A:LEU:HD22	1:108:A:LEU:HA	5	0.69
(1,573)	1:106:A:LEU:HD23	1:108:A:LEU:HA	5	0.69
(1,559)	1:158:A:LYS:HE3	1:158:A:LYS:HG2	17	0.69
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	6	0.69
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	6	0.69
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	6	0.69
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	1	0.69
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	1	0.69
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	1	0.69
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	7	0.69
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	7	0.69
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	7	0.69
(1,243)	1:81:A:MET:HG3	1:85:A:LYS:HB2	2	0.69
(1,243)	1:81:A:MET:HG2	1:85:A:LYS:HB2	2	0.69
(1,136)	1:38:A:GLU:HG3	1:74:A:THR:HG21	17	0.69
(1,136)	1:38:A:GLU:HG3	1:74:A:THR:HG22	17	0.69
(1,136)	1:38:A:GLU:HG3	1:74:A:THR:HG23	17	0.69
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	3	0.69
(1,21)	1:114:A:ARG:HD3	1:114:A:ARG:HB2	11	0.69
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	6	0.68
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	6	0.68
(1,1939)	1:55:A:LEU:HD21	1:17:A:PHE:HE1	3	0.68
(1,1939)	1:55:A:LEU:HD21	1:17:A:PHE:HE2	3	0.68
(1,1939)	1:55:A:LEU:HD22	1:17:A:PHE:HE1	3	0.68
(1,1939)	1:55:A:LEU:HD22	1:17:A:PHE:HE2	3	0.68
(1,1939)	1:55:A:LEU:HD23	1:17:A:PHE:HE1	3	0.68
(1,1939)	1:55:A:LEU:HD23	1:17:A:PHE:HE2	3	0.68
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	3	0.68
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	3	0.68
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	3	0.68
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	13	0.68
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	15	0.68
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	14	0.68
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	3	0.68
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	5	0.68
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	9	0.68
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	17	0.68
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD11	3	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD12	3	0.68
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD13	3	0.68
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	11	0.68
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	11	0.68
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	11	0.68
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	1	0.68
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	1	0.68
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	1	0.68
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	6	0.68
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	6	0.68
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	6	0.68
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	11	0.68
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	11	0.68
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	11	0.68
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE1	20	0.68
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE2	20	0.68
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE3	20	0.68
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	11	0.68
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	11	0.68
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	11	0.68
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	19	0.68
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	19	0.68
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	18	0.68
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	18	0.68
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	18	0.68
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	19	0.68
(1,798)	1:138:A:LYS:HG3	1:138:A:LYS:HA	5	0.68
(1,798)	1:138:A:LYS:HG3	1:138:A:LYS:HA	7	0.68
(1,798)	1:138:A:LYS:HG3	1:138:A:LYS:HA	10	0.68
(1,798)	1:138:A:LYS:HG3	1:138:A:LYS:HA	13	0.68
(1,786)	1:75:A:ARG:HA	1:75:A:ARG:HD2	9	0.68
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	11	0.68
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	11	0.68
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	11	0.68
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	19	0.68
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	19	0.68
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	19	0.68
(1,740)	1:30:A:VAL:HG11	1:30:A:VAL:H	6	0.68
(1,740)	1:30:A:VAL:HG12	1:30:A:VAL:H	6	0.68
(1,740)	1:30:A:VAL:HG13	1:30:A:VAL:H	6	0.68
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG21	6	0.68
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG22	6	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG23	6	0.68
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG21	6	0.68
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG22	6	0.68
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG23	6	0.68
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG21	6	0.68
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG22	6	0.68
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG23	6	0.68
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG21	6	0.68
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG22	6	0.68
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG23	6	0.68
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG21	6	0.68
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG22	6	0.68
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG23	6	0.68
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG21	6	0.68
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG22	6	0.68
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG23	6	0.68
(1,687)	1:17:A:PHE:HA	1:20:A:ARG:HB2	3	0.68
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	1	0.68
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	1	0.68
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	1	0.68
(1,605)	1:107:A:ASP:HB3	1:110:A:SER:HB3	12	0.68
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD11	2	0.68
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD12	2	0.68
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD13	2	0.68
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD11	7	0.68
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD12	7	0.68
(1,599)	1:106:A:LEU:HB3	1:106:A:LEU:HD13	7	0.68
(1,568)	1:34:A:LEU:HD11	1:75:A:ARG:HD2	20	0.68
(1,568)	1:34:A:LEU:HD12	1:75:A:ARG:HD2	20	0.68
(1,568)	1:34:A:LEU:HD13	1:75:A:ARG:HD2	20	0.68
(1,532)	1:92:A:LYS:HB3	1:92:A:LYS:HD3	17	0.68
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	17	0.68
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	17	0.68
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	17	0.68
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	1	0.68
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	1	0.68
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	18	0.68
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	18	0.68
(1,362)	1:75:A:ARG:HB2	1:75:A:ARG:HD2	4	0.68
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	8	0.68
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	8	0.68
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	8	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	8	0.68
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	8	0.68
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	8	0.68
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	8	0.68
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	8	0.68
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	8	0.68
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB2	17	0.68
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB3	17	0.68
(1,193)	1:123:A:GLN:HA	1:123:A:GLN:HG3	8	0.68
(1,168)	1:17:A:PHE:H	1:16:A:GLU:HG2	9	0.68
(1,142)	1:88:A:GLU:HG3	1:89:A:LYS:H	9	0.68
(1,20)	1:114:A:ARG:HB2	1:114:A:ARG:HD2	16	0.68
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	5	0.67
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	5	0.67
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	5	0.67
(1,1878)	1:5:A:GLY:H	1:4:A:GLY:HA2	2	0.67
(1,1878)	1:5:A:GLY:H	1:4:A:GLY:HA2	19	0.67
(1,1837)	1:114:A:ARG:H	1:114:A:ARG:HB2	9	0.67
(1,1716)	1:143:A:ASN:HB3	1:143:A:ASN:H	7	0.67
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	4	0.67
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	14	0.67
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	15	0.67
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	11	0.67
(1,1646)	1:88:A:GLU:HB3	1:87:A:CYS:H	9	0.67
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	5	0.67
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	5	0.67
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	5	0.67
(1,1319)	1:8:A:GLY:HA3	1:9:A:ALA:H	12	0.67
(1,1318)	1:9:A:ALA:H	1:8:A:GLY:HA2	5	0.67
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	13	0.67
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	13	0.67
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	13	0.67
(1,1157)	1:101:A:LYS:HA	1:101:A:LYS:HD2	7	0.67
(1,1157)	1:101:A:LYS:HA	1:101:A:LYS:HD2	20	0.67
(1,1147)	1:83:A:ALA:HA	1:86:A:ILE:HG12	17	0.67
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	20	0.67
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	20	0.67
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	20	0.67
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	20	0.67
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	20	0.67
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	20	0.67
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	20	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	20	0.67
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	20	0.67
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	11	0.67
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	11	0.67
(1,911)	1:9:A:ALA:HB1	1:15:A:LYS:HD2	11	0.67
(1,911)	1:9:A:ALA:HB2	1:15:A:LYS:HD2	11	0.67
(1,911)	1:9:A:ALA:HB3	1:15:A:LYS:HD2	11	0.67
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	11	0.67
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	11	0.67
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	11	0.67
(1,798)	1:138:A:LYS:HG3	1:138:A:LYS:HA	4	0.67
(1,639)	1:73:A:VAL:HG11	1:72:A:GLU:HA	12	0.67
(1,639)	1:73:A:VAL:HG12	1:72:A:GLU:HA	12	0.67
(1,639)	1:73:A:VAL:HG13	1:72:A:GLU:HA	12	0.67
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	15	0.67
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	15	0.67
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	15	0.67
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	16	0.67
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	16	0.67
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	16	0.67
(1,441)	1:113:A:LEU:HD21	1:146:A:GLN:HG3	19	0.67
(1,441)	1:113:A:LEU:HD22	1:146:A:GLN:HG3	19	0.67
(1,441)	1:113:A:LEU:HD23	1:146:A:GLN:HG3	19	0.67
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	17	0.67
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	17	0.67
(1,400)	1:59:A:LEU:HA	1:69:A:ILE:HG12	1	0.67
(1,380)	1:81:A:MET:HG3	1:86:A:ILE:HG12	15	0.67
(1,299)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	13	0.67
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	9	0.67
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	9	0.67
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	9	0.67
(1,243)	1:81:A:MET:HG3	1:85:A:LYS:HB2	9	0.67
(1,243)	1:81:A:MET:HG2	1:85:A:LYS:HB2	9	0.67
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	9	0.67
(1,168)	1:17:A:PHE:H	1:16:A:GLU:HG2	14	0.67
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB1	10	0.67
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB2	10	0.67
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB3	10	0.67
(1,1879)	1:4:A:GLY:HA3	1:5:A:GLY:H	20	0.66
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	18	0.66
(1,1646)	1:88:A:GLU:HB3	1:87:A:CYS:H	17	0.66
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	15	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	13	0.66
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	13	0.66
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	13	0.66
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	9	0.66
(1,1380)	1:158:A:LYS:HB2	1:158:A:LYS:H	1	0.66
(1,1292)	1:108:A:LEU:HB3	1:108:A:LEU:H	13	0.66
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	18	0.66
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	18	0.66
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	18	0.66
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	19	0.66
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	19	0.66
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	19	0.66
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	18	0.66
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	18	0.66
(1,911)	1:9:A:ALA:HB1	1:15:A:LYS:HD2	12	0.66
(1,911)	1:9:A:ALA:HB2	1:15:A:LYS:HD2	12	0.66
(1,911)	1:9:A:ALA:HB3	1:15:A:LYS:HD2	12	0.66
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	6	0.66
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	6	0.66
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	6	0.66
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	17	0.66
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	17	0.66
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	17	0.66
(1,798)	1:138:A:LYS:HG3	1:138:A:LYS:HA	19	0.66
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	18	0.66
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	18	0.66
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	18	0.66
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	6	0.66
(1,716)	1:148:A:LEU:HD21	1:147:A:GLU:HG2	1	0.66
(1,716)	1:148:A:LEU:HD22	1:147:A:GLU:HG2	1	0.66
(1,716)	1:148:A:LEU:HD23	1:147:A:GLU:HG2	1	0.66
(1,687)	1:17:A:PHE:HA	1:20:A:ARG:HB2	10	0.66
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	10	0.66
(1,605)	1:107:A:ASP:HB3	1:110:A:SER:HB3	13	0.66
(1,531)	1:92:A:LYS:HD3	1:92:A:LYS:HB2	2	0.66
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	7	0.66
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	7	0.66
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	7	0.66
(1,418)	1:6:A:ARG:H	1:6:A:ARG:HG2	4	0.66
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	18	0.66
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD2	16	0.66
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD3	16	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,324)	1:142:A:VAL:HG21	1:114:A:ARG:HB2	20	0.66
(1,324)	1:142:A:VAL:HG22	1:114:A:ARG:HB2	20	0.66
(1,324)	1:142:A:VAL:HG23	1:114:A:ARG:HB2	20	0.66
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	5	0.66
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	5	0.66
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	5	0.66
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	4	0.66
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	4	0.66
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	4	0.66
(1,153)	1:103:A:GLU:HG3	1:104:A:LYS:H	8	0.66
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD11	20	0.66
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD12	20	0.66
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD13	20	0.66
(1,138)	1:42:A:ILE:HD11	1:38:A:GLU:HG2	11	0.66
(1,138)	1:42:A:ILE:HD12	1:38:A:GLU:HG2	11	0.66
(1,138)	1:42:A:ILE:HD13	1:38:A:GLU:HG2	11	0.66
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	19	0.66
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	10	0.66
(1,2012)	1:152:A:TYR:HE1	1:151:A:LYS:HE2	10	0.65
(1,2012)	1:152:A:TYR:HE2	1:151:A:LYS:HE2	10	0.65
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	19	0.65
(1,1878)	1:5:A:GLY:H	1:4:A:GLY:HA2	1	0.65
(1,1878)	1:5:A:GLY:H	1:4:A:GLY:HA2	16	0.65
(1,1716)	1:143:A:ASN:HB3	1:143:A:ASN:H	14	0.65
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	7	0.65
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	15	0.65
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	7	0.65
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	14	0.65
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	10	0.65
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	10	0.65
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	10	0.65
(1,1319)	1:8:A:GLY:HA3	1:9:A:ALA:H	10	0.65
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	7	0.65
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	7	0.65
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	7	0.65
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	7	0.65
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	7	0.65
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	7	0.65
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	7	0.65
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	7	0.65
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	7	0.65
(1,1055)	1:92:A:LYS:HG3	1:92:A:LYS:HA	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE1	6	0.65
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE2	6	0.65
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE3	6	0.65
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	16	0.65
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	16	0.65
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	16	0.65
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	16	0.65
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	16	0.65
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB1	5	0.65
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB2	5	0.65
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB3	5	0.65
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	7	0.65
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	7	0.65
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	7	0.65
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	19	0.65
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	19	0.65
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	19	0.65
(1,869)	1:13:A:VAL:HG21	1:55:A:LEU:HB2	9	0.65
(1,869)	1:13:A:VAL:HG22	1:55:A:LEU:HB2	9	0.65
(1,869)	1:13:A:VAL:HG23	1:55:A:LEU:HB2	9	0.65
(1,823)	1:142:A:VAL:HG21	1:146:A:GLN:HE21	16	0.65
(1,823)	1:142:A:VAL:HG22	1:146:A:GLN:HE21	16	0.65
(1,823)	1:142:A:VAL:HG23	1:146:A:GLN:HE21	16	0.65
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	5	0.65
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	5	0.65
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	5	0.65
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	7	0.65
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	7	0.65
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	7	0.65
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	3	0.65
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	3	0.65
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	3	0.65
(1,605)	1:107:A:ASP:HB3	1:110:A:SER:HB3	1	0.65
(1,552)	1:31:A:ASN:HD21	1:33:A:SER:HB2	9	0.65
(1,506)	1:93:A:LEU:H	1:92:A:LYS:HG2	10	0.65
(1,506)	1:93:A:LEU:H	1:92:A:LYS:HG2	13	0.65
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	2	0.65
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	2	0.65
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	8	0.65
(1,299)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	19	0.65
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	10	0.65
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	10	0.65
(1,168)	1:17:A:PHE:H	1:16:A:GLU:HG2	2	0.65
(1,1969)	1:24:A:SER:HB3	1:44:A:PHE:HZ	16	0.64
(1,1879)	1:4:A:GLY:HA3	1:5:A:GLY:H	15	0.64
(1,1708)	1:115:A:LYS:H	1:115:A:LYS:HB2	14	0.64
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	13	0.64
(1,1543)	1:117:A:ARG:HB3	1:119:A:ALA:H	15	0.64
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	5	0.64
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	10	0.64
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	18	0.64
(1,1522)	1:131:A:GLU:H	1:130:A:GLU:HB3	19	0.64
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	4	0.64
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	4	0.64
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	4	0.64
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	8	0.64
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	8	0.64
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	8	0.64
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	13	0.64
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	13	0.64
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	13	0.64
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	17	0.64
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	17	0.64
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	17	0.64
(1,1319)	1:8:A:GLY:HA3	1:9:A:ALA:H	15	0.64
(1,1319)	1:8:A:GLY:HA3	1:9:A:ALA:H	17	0.64
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	10	0.64
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	10	0.64
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	10	0.64
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	15	0.64
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	15	0.64
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	15	0.64
(1,1058)	1:54:A:ARG:HA	1:54:A:ARG:HD3	4	0.64
(1,927)	1:23:A:LYS:HA	1:22:A:TYR:HB2	12	0.64
(1,911)	1:9:A:ALA:HB1	1:15:A:LYS:HD2	2	0.64
(1,911)	1:9:A:ALA:HB2	1:15:A:LYS:HD2	2	0.64
(1,911)	1:9:A:ALA:HB3	1:15:A:LYS:HD2	2	0.64
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	9	0.64
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	9	0.64
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	9	0.64
(1,786)	1:75:A:ARG:HA	1:75:A:ARG:HD2	17	0.64
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	4	0.64
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	4	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	4	0.64
(1,716)	1:148:A:LEU:HD21	1:147:A:GLU:HG2	15	0.64
(1,716)	1:148:A:LEU:HD22	1:147:A:GLU:HG2	15	0.64
(1,716)	1:148:A:LEU:HD23	1:147:A:GLU:HG2	15	0.64
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	2	0.64
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	2	0.64
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	2	0.64
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	1	0.64
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	17	0.64
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	3	0.64
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	3	0.64
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	3	0.64
(1,559)	1:158:A:LYS:HE3	1:158:A:LYS:HG2	15	0.64
(1,558)	1:158:A:LYS:HG2	1:158:A:LYS:HE2	19	0.64
(1,484)	1:142:A:VAL:HG11	1:139:A:THR:HA	9	0.64
(1,484)	1:142:A:VAL:HG12	1:139:A:THR:HA	9	0.64
(1,484)	1:142:A:VAL:HG13	1:139:A:THR:HA	9	0.64
(1,470)	1:36:A:THR:HA	1:35:A:ASP:HB2	20	0.64
(1,419)	1:6:A:ARG:HG3	1:6:A:ARG:H	15	0.64
(1,362)	1:75:A:ARG:HB2	1:75:A:ARG:HD2	5	0.64
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD2	10	0.64
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD3	10	0.64
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD2	17	0.64
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD3	17	0.64
(1,183)	1:101:A:LYS:HB2	1:102:A:TYR:HA	20	0.64
(1,168)	1:17:A:PHE:H	1:16:A:GLU:HG2	5	0.64
(1,168)	1:17:A:PHE:H	1:16:A:GLU:HG2	7	0.64
(1,121)	1:97:A:ILE:HB	1:94:A:ASP:HB2	18	0.64
(1,3)	1:15:A:LYS:HD3	1:8:A:GLY:HA2	7	0.64
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	6	0.63
(1,1878)	1:5:A:GLY:H	1:4:A:GLY:HA2	6	0.63
(1,1859)	1:142:A:VAL:HG11	1:139:A:THR:H	17	0.63
(1,1859)	1:142:A:VAL:HG12	1:139:A:THR:H	17	0.63
(1,1859)	1:142:A:VAL:HG13	1:139:A:THR:H	17	0.63
(1,1708)	1:115:A:LYS:H	1:115:A:LYS:HB2	10	0.63
(1,1708)	1:115:A:LYS:H	1:115:A:LYS:HB2	18	0.63
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	13	0.63
(1,1552)	1:125:A:LEU:HB3	1:130:A:GLU:H	9	0.63
(1,1522)	1:131:A:GLU:H	1:130:A:GLU:HB3	7	0.63
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	20	0.63
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	20	0.63
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	20	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	2	0.63
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	2	0.63
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	2	0.63
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	2	0.63
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	2	0.63
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	2	0.63
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	2	0.63
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	2	0.63
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	2	0.63
(1,1055)	1:92:A:LYS:HG3	1:92:A:LYS:HA	20	0.63
(1,814)	1:38:A:GLU:HA	1:38:A:GLU:HG2	17	0.63
(1,798)	1:138:A:LYS:HG3	1:138:A:LYS:HA	12	0.63
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	5	0.63
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	9	0.63
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD21	16	0.63
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD22	16	0.63
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD23	16	0.63
(1,716)	1:148:A:LEU:HD21	1:147:A:GLU:HG2	20	0.63
(1,716)	1:148:A:LEU:HD22	1:147:A:GLU:HG2	20	0.63
(1,716)	1:148:A:LEU:HD23	1:147:A:GLU:HG2	20	0.63
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	7	0.63
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB2	5	0.63
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB3	5	0.63
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	9	0.63
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	18	0.63
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	12	0.63
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	12	0.63
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	12	0.63
(1,605)	1:107:A:ASP:HB3	1:110:A:SER:HB3	10	0.63
(1,484)	1:142:A:VAL:HG11	1:139:A:THR:HA	11	0.63
(1,484)	1:142:A:VAL:HG12	1:139:A:THR:HA	11	0.63
(1,484)	1:142:A:VAL:HG13	1:139:A:THR:HA	11	0.63
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD2	19	0.63
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD3	19	0.63
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB2	11	0.63
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB3	11	0.63
(1,264)	1:85:A:LYS:HB3	1:86:A:ILE:H	5	0.63
(1,263)	1:86:A:ILE:H	1:85:A:LYS:HB2	9	0.63
(1,194)	1:123:A:GLN:HG3	1:123:A:GLN:H	14	0.63
(1,183)	1:101:A:LYS:HB2	1:102:A:TYR:HA	10	0.63
(1,183)	1:101:A:LYS:HB2	1:102:A:TYR:HA	18	0.63
(1,118)	1:19:A:ASN:HB3	1:16:A:GLU:HA	20	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	1	0.63
(1,27)	1:117:A:ARG:HD3	1:117:A:ARG:HB3	6	0.63
(1,1992)	1:126:A:HIS:HB3	1:126:A:HIS:HD2	6	0.62
(1,1992)	1:126:A:HIS:HB3	1:126:A:HIS:HD2	9	0.62
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD1	10	0.62
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD2	10	0.62
(1,1879)	1:4:A:GLY:HA3	1:5:A:GLY:H	3	0.62
(1,1878)	1:5:A:GLY:H	1:4:A:GLY:HA2	11	0.62
(1,1708)	1:115:A:LYS:H	1:115:A:LYS:HB2	5	0.62
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	14	0.62
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	10	0.62
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	17	0.62
(1,1553)	1:93:A:LEU:H	1:92:A:LYS:HB2	11	0.62
(1,1553)	1:93:A:LEU:H	1:92:A:LYS:HB2	17	0.62
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	14	0.62
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	14	0.62
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	14	0.62
(1,1381)	1:158:A:LYS:H	1:158:A:LYS:HG3	15	0.62
(1,1381)	1:158:A:LYS:H	1:158:A:LYS:HG3	20	0.62
(1,1380)	1:158:A:LYS:HB2	1:158:A:LYS:H	2	0.62
(1,1319)	1:8:A:GLY:HA3	1:9:A:ALA:H	2	0.62
(1,1318)	1:9:A:ALA:H	1:8:A:GLY:HA2	4	0.62
(1,1318)	1:9:A:ALA:H	1:8:A:GLY:HA2	11	0.62
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	15	0.62
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	4	0.62
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	4	0.62
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	4	0.62
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	8	0.62
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	8	0.62
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	8	0.62
(1,1157)	1:101:A:LYS:HA	1:101:A:LYS:HD2	6	0.62
(1,1106)	1:104:A:LYS:HG3	1:103:A:GLU:HA	14	0.62
(1,1104)	1:103:A:GLU:HG3	1:103:A:GLU:HA	7	0.62
(1,1055)	1:92:A:LYS:HG3	1:92:A:LYS:HA	9	0.62
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	5	0.62
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	5	0.62
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	5	0.62
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	5	0.62
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	5	0.62
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	5	0.62
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	5	0.62
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	5	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	5	0.62
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG11	10	0.62
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG12	10	0.62
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG13	10	0.62
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	10	0.62
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	11	0.62
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	14	0.62
(1,605)	1:107:A:ASP:HB3	1:110:A:SER:HB3	2	0.62
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	7	0.62
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	7	0.62
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	7	0.62
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD21	9	0.62
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD22	9	0.62
(1,520)	1:37:A:ILE:HG13	1:25:A:LEU:HD23	9	0.62
(1,506)	1:93:A:LEU:H	1:92:A:LYS:HG2	15	0.62
(1,506)	1:93:A:LEU:H	1:92:A:LYS:HG2	19	0.62
(1,484)	1:142:A:VAL:HG11	1:139:A:THR:HA	1	0.62
(1,484)	1:142:A:VAL:HG12	1:139:A:THR:HA	1	0.62
(1,484)	1:142:A:VAL:HG13	1:139:A:THR:HA	1	0.62
(1,311)	1:91:A:LYS:HD3	1:95:A:SER:HA	17	0.62
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	15	0.62
(1,279)	1:67:A:THR:HB	1:69:A:ILE:HG13	6	0.62
(1,168)	1:17:A:PHE:H	1:16:A:GLU:HG2	17	0.62
(1,164)	1:2:A:GLU:HG3	1:2:A:GLU:HA	5	0.62
(1,164)	1:2:A:GLU:HG3	1:2:A:GLU:HA	18	0.62
(1,164)	1:2:A:GLU:HG3	1:2:A:GLU:HA	19	0.62
(1,145)	1:85:A:LYS:HA	1:88:A:GLU:HG2	11	0.62
(1,145)	1:85:A:LYS:HA	1:88:A:GLU:HG2	14	0.62
(1,142)	1:88:A:GLU:HG3	1:89:A:LYS:H	7	0.62
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD11	4	0.62
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD12	4	0.62
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD13	4	0.62
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG21	20	0.62
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG22	20	0.62
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG23	20	0.62
(1,84)	1:47:A:ASP:HB3	1:48:A:THR:HG21	17	0.62
(1,84)	1:47:A:ASP:HB3	1:48:A:THR:HG22	17	0.62
(1,84)	1:47:A:ASP:HB3	1:48:A:THR:HG23	17	0.62
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	14	0.62
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	14	0.62
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	14	0.62
(1,1)	1:49:A:LYS:HB3	1:50:A:GLY:HA2	8	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1992)	1:126:A:HIS:HB3	1:126:A:HIS:HD2	15	0.61
(1,1992)	1:126:A:HIS:HB3	1:126:A:HIS:HD2	19	0.61
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	2	0.61
(1,1937)	1:58:A:TYR:HD1	1:97:A:ILE:HG13	14	0.61
(1,1937)	1:58:A:TYR:HD2	1:97:A:ILE:HG13	14	0.61
(1,1878)	1:5:A:GLY:H	1:4:A:GLY:HA2	13	0.61
(1,1810)	1:91:A:LYS:HB3	1:92:A:LYS:H	6	0.61
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	8	0.61
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	8	0.61
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	8	0.61
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	8	0.61
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	12	0.61
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	5	0.61
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	12	0.61
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	12	0.61
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	12	0.61
(1,1319)	1:8:A:GLY:HA3	1:9:A:ALA:H	7	0.61
(1,1277)	1:128:A:TRP:HE1	1:127:A:SER:HB2	19	0.61
(1,1019)	1:84:A:MET:HE1	1:15:A:LYS:HD2	10	0.61
(1,1019)	1:84:A:MET:HE2	1:15:A:LYS:HD2	10	0.61
(1,1019)	1:84:A:MET:HE3	1:15:A:LYS:HD2	10	0.61
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	8	0.61
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	8	0.61
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	8	0.61
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	8	0.61
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	8	0.61
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	8	0.61
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	8	0.61
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	8	0.61
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	8	0.61
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	20	0.61
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	20	0.61
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	20	0.61
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	2	0.61
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	2	0.61
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	2	0.61
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	18	0.61
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	18	0.61
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	18	0.61
(1,797)	1:138:A:LYS:HA	1:138:A:LYS:HG2	3	0.61
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	15	0.61
(1,716)	1:148:A:LEU:HD21	1:147:A:GLU:HG2	11	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,716)	1:148:A:LEU:HD22	1:147:A:GLU:HG2	11	0.61
(1,716)	1:148:A:LEU:HD23	1:147:A:GLU:HG2	11	0.61
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	6	0.61
(1,506)	1:93:A:LEU:H	1:92:A:LYS:HG2	1	0.61
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	6	0.61
(1,263)	1:86:A:ILE:H	1:85:A:LYS:HB2	15	0.61
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	2	0.61
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	2	0.61
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	2	0.61
(1,214)	1:82:A:PRO:HB3	1:85:A:LYS:H	10	0.61
(1,164)	1:2:A:GLU:HG3	1:2:A:GLU:HA	7	0.61
(1,164)	1:2:A:GLU:HG3	1:2:A:GLU:HA	8	0.61
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	20	0.61
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	1	0.61
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	1	0.61
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	1	0.61
(1,1992)	1:126:A:HIS:HB3	1:126:A:HIS:HD2	1	0.6
(1,1992)	1:126:A:HIS:HB3	1:126:A:HIS:HD2	14	0.6
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	13	0.6
(1,1969)	1:24:A:SER:HB3	1:44:A:PHE:HZ	3	0.6
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	15	0.6
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	15	0.6
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	15	0.6
(1,1810)	1:91:A:LYS:HB3	1:92:A:LYS:H	1	0.6
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	15	0.6
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	12	0.6
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	16	0.6
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	18	0.6
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	1	0.6
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	20	0.6
(1,1580)	1:127:A:SER:H	1:126:A:HIS:HB2	14	0.6
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	8	0.6
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	3	0.6
(1,1319)	1:8:A:GLY:HA3	1:9:A:ALA:H	1	0.6
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	16	0.6
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	16	0.6
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	16	0.6
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	1	0.6
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	1	0.6
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	1	0.6
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	18	0.6
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	18	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	18	0.6
(1,1104)	1:103:A:GLU:HG3	1:103:A:GLU:HA	4	0.6
(1,1104)	1:103:A:GLU:HG3	1:103:A:GLU:HA	6	0.6
(1,1104)	1:103:A:GLU:HG3	1:103:A:GLU:HA	9	0.6
(1,1103)	1:103:A:GLU:HA	1:103:A:GLU:HG2	5	0.6
(1,798)	1:138:A:LYS:HG3	1:138:A:LYS:HA	16	0.6
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	8	0.6
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	8	0.6
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	8	0.6
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD21	18	0.6
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD22	18	0.6
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD23	18	0.6
(1,696)	1:71:A:SER:HB3	1:75:A:ARG:HD2	15	0.6
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	2	0.6
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	6	0.6
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	8	0.6
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	6	0.6
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	6	0.6
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	6	0.6
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	6	0.6
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	6	0.6
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	6	0.6
(1,507)	1:92:A:LYS:HG3	1:93:A:LEU:H	20	0.6
(1,506)	1:93:A:LEU:H	1:92:A:LYS:HG2	8	0.6
(1,441)	1:113:A:LEU:HD21	1:146:A:GLN:HG3	18	0.6
(1,441)	1:113:A:LEU:HD22	1:146:A:GLN:HG3	18	0.6
(1,441)	1:113:A:LEU:HD23	1:146:A:GLN:HG3	18	0.6
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	7	0.6
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	7	0.6
(1,385)	1:121:A:LEU:HB3	1:118:A:VAL:HA	10	0.6
(1,324)	1:142:A:VAL:HG21	1:114:A:ARG:HB2	11	0.6
(1,324)	1:142:A:VAL:HG22	1:114:A:ARG:HB2	11	0.6
(1,324)	1:142:A:VAL:HG23	1:114:A:ARG:HB2	11	0.6
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	6	0.6
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	6	0.6
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	6	0.6
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	15	0.6
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	10	0.6
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	10	0.6
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	10	0.6
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	16	0.6
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	16	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	16	0.6
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD21	1	0.6
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD22	1	0.6
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD23	1	0.6
(1,193)	1:123:A:GLN:HA	1:123:A:GLN:HG3	10	0.6
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	2	0.6
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	2	0.6
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	2	0.6
(1,164)	1:2:A:GLU:HG3	1:2:A:GLU:HA	4	0.6
(1,164)	1:2:A:GLU:HG3	1:2:A:GLU:HA	9	0.6
(1,164)	1:2:A:GLU:HG3	1:2:A:GLU:HA	14	0.6
(1,164)	1:2:A:GLU:HG3	1:2:A:GLU:HA	17	0.6
(1,152)	1:104:A:LYS:H	1:103:A:GLU:HG2	10	0.6
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG21	8	0.6
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG22	8	0.6
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG23	8	0.6
(1,21)	1:114:A:ARG:HD3	1:114:A:ARG:HB2	3	0.6
(1,21)	1:114:A:ARG:HD3	1:114:A:ARG:HB2	18	0.6
(1,1993)	1:130:A:GLU:HB2	1:128:A:TRP:HE3	3	0.59
(1,1992)	1:126:A:HIS:HB3	1:126:A:HIS:HD2	16	0.59
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	11	0.59
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	11	0.59
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	11	0.59
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	17	0.59
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	17	0.59
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	17	0.59
(1,1708)	1:115:A:LYS:H	1:115:A:LYS:HB2	11	0.59
(1,1708)	1:115:A:LYS:H	1:115:A:LYS:HB2	12	0.59
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	1	0.59
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	9	0.59
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	11	0.59
(1,1646)	1:88:A:GLU:HB3	1:87:A:CYS:H	7	0.59
(1,1580)	1:127:A:SER:H	1:126:A:HIS:HB2	8	0.59
(1,1580)	1:127:A:SER:H	1:126:A:HIS:HB2	15	0.59
(1,1522)	1:131:A:GLU:H	1:130:A:GLU:HB3	4	0.59
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	20	0.59
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	20	0.59
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	20	0.59
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	10	0.59
(1,1380)	1:158:A:LYS:HB2	1:158:A:LYS:H	8	0.59
(1,1380)	1:158:A:LYS:HB2	1:158:A:LYS:H	12	0.59
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	11	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	5	0.59
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	5	0.59
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	5	0.59
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	19	0.59
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	19	0.59
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	19	0.59
(1,1055)	1:92:A:LYS:HG3	1:92:A:LYS:HA	7	0.59
(1,1054)	1:92:A:LYS:HA	1:92:A:LYS:HG2	3	0.59
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	10	0.59
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	10	0.59
(1,880)	1:122:A:LYS:HG3	1:122:A:LYS:HA	14	0.59
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	2	0.59
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	16	0.59
(1,719)	1:144:A:LEU:HB2	1:141:A:TYR:HA	7	0.59
(1,605)	1:107:A:ASP:HB3	1:110:A:SER:HB3	3	0.59
(1,573)	1:106:A:LEU:HD21	1:108:A:LEU:HA	9	0.59
(1,573)	1:106:A:LEU:HD22	1:108:A:LEU:HA	9	0.59
(1,573)	1:106:A:LEU:HD23	1:108:A:LEU:HA	9	0.59
(1,507)	1:92:A:LYS:HG3	1:93:A:LEU:H	18	0.59
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	19	0.59
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	19	0.59
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	10	0.59
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	10	0.59
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	10	0.59
(1,263)	1:86:A:ILE:H	1:85:A:LYS:HB2	14	0.59
(1,261)	1:28:A:ARG:HB3	1:29:A:GLY:H	4	0.59
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	3	0.59
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	3	0.59
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	3	0.59
(1,168)	1:17:A:PHE:H	1:16:A:GLU:HG2	6	0.59
(1,164)	1:2:A:GLU:HG3	1:2:A:GLU:HA	10	0.59
(1,149)	1:49:A:LYS:HB3	1:53:A:ASN:HB3	20	0.59
(1,142)	1:88:A:GLU:HG3	1:89:A:LYS:H	18	0.59
(1,1992)	1:126:A:HIS:HB3	1:126:A:HIS:HD2	2	0.58
(1,1992)	1:126:A:HIS:HB3	1:126:A:HIS:HD2	18	0.58
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	14	0.58
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	3	0.58
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	5	0.58
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	17	0.58
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	19	0.58
(1,1580)	1:127:A:SER:H	1:126:A:HIS:HB2	1	0.58
(1,1580)	1:127:A:SER:H	1:126:A:HIS:HB2	19	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	7	0.58
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	11	0.58
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	12	0.58
(1,1380)	1:158:A:LYS:HB2	1:158:A:LYS:H	19	0.58
(1,1157)	1:101:A:LYS:HA	1:101:A:LYS:HD2	17	0.58
(1,1104)	1:103:A:GLU:HG3	1:103:A:GLU:HA	15	0.58
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE1	3	0.58
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE2	3	0.58
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE3	3	0.58
(1,1008)	1:85:A:LYS:HA	1:88:A:GLU:HB3	13	0.58
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	7	0.58
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	7	0.58
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	7	0.58
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	6	0.58
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	6	0.58
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	6	0.58
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	14	0.58
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	14	0.58
(1,911)	1:9:A:ALA:HB1	1:15:A:LYS:HD2	7	0.58
(1,911)	1:9:A:ALA:HB2	1:15:A:LYS:HD2	7	0.58
(1,911)	1:9:A:ALA:HB3	1:15:A:LYS:HD2	7	0.58
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB1	3	0.58
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB2	3	0.58
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB3	3	0.58
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	7	0.58
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	12	0.58
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	17	0.58
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	20	0.58
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	20	0.58
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	18	0.58
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	18	0.58
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	18	0.58
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	18	0.58
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	18	0.58
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	18	0.58
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD2	3	0.58
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD3	3	0.58
(1,299)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	18	0.58
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB2	5	0.58
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB3	5	0.58
(1,164)	1:2:A:GLU:HG3	1:2:A:GLU:HA	13	0.58
(1,153)	1:103:A:GLU:HG3	1:104:A:LYS:H	4	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,142)	1:88:A:GLU:HG3	1:89:A:LYS:H	1	0.58
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB1	2	0.58
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB2	2	0.58
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB3	2	0.58
(1,1992)	1:126:A:HIS:HB3	1:126:A:HIS:HD2	8	0.57
(1,1992)	1:126:A:HIS:HB3	1:126:A:HIS:HD2	20	0.57
(1,1991)	1:126:A:HIS:HD2	1:126:A:HIS:HB2	11	0.57
(1,1878)	1:5:A:GLY:H	1:4:A:GLY:HA2	18	0.57
(1,1871)	1:8:A:GLY:H	1:7:A:PRO:HG3	15	0.57
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	16	0.57
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	3	0.57
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	14	0.57
(1,1600)	1:123:A:GLN:H	1:122:A:LYS:HB2	14	0.57
(1,1580)	1:127:A:SER:H	1:126:A:HIS:HB2	6	0.57
(1,1580)	1:127:A:SER:H	1:126:A:HIS:HB2	9	0.57
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	18	0.57
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	1	0.57
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	1	0.57
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	1	0.57
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	1	0.57
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	5	0.57
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	5	0.57
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	5	0.57
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	12	0.57
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	14	0.57
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	2	0.57
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	9	0.57
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	18	0.57
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	17	0.57
(1,1146)	1:115:A:LYS:HA	1:115:A:LYS:HG2	8	0.57
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	8	0.57
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	8	0.57
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	8	0.57
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	8	0.57
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	8	0.57
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	8	0.57
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	8	0.57
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	8	0.57
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	8	0.57
(1,1104)	1:103:A:GLU:HG3	1:103:A:GLU:HA	8	0.57
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE1	5	0.57
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE2	5	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE3	5	0.57
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE1	13	0.57
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE2	13	0.57
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE3	13	0.57
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	5	0.57
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	5	0.57
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	5	0.57
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB1	7	0.57
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB2	7	0.57
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB3	7	0.57
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	3	0.57
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	3	0.57
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	3	0.57
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG11	17	0.57
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG12	17	0.57
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG13	17	0.57
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	8	0.57
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	8	0.57
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	8	0.57
(1,716)	1:148:A:LEU:HD21	1:147:A:GLU:HG2	17	0.57
(1,716)	1:148:A:LEU:HD22	1:147:A:GLU:HG2	17	0.57
(1,716)	1:148:A:LEU:HD23	1:147:A:GLU:HG2	17	0.57
(1,557)	1:158:A:LYS:HE3	1:158:A:LYS:HG3	19	0.57
(1,557)	1:158:A:LYS:HE2	1:158:A:LYS:HG3	19	0.57
(1,535)	1:86:A:ILE:HA	1:89:A:LYS:HG2	9	0.57
(1,506)	1:93:A:LEU:H	1:92:A:LYS:HG2	16	0.57
(1,363)	1:75:A:ARG:HD3	1:75:A:ARG:HB2	5	0.57
(1,362)	1:75:A:ARG:HB2	1:75:A:ARG:HD2	12	0.57
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	4	0.57
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	5	0.57
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	5	0.57
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	5	0.57
(1,264)	1:85:A:LYS:HB3	1:86:A:ILE:H	18	0.57
(1,263)	1:86:A:ILE:H	1:85:A:LYS:HB2	17	0.57
(1,243)	1:81:A:MET:HG3	1:85:A:LYS:HB2	1	0.57
(1,243)	1:81:A:MET:HG2	1:85:A:LYS:HB2	1	0.57
(1,204)	1:158:A:LYS:HE3	1:158:A:LYS:HB3	10	0.57
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	6	0.57
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	6	0.57
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	6	0.57
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	15	0.57
(1,164)	1:2:A:GLU:HG3	1:2:A:GLU:HA	15	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,145)	1:85:A:LYS:HA	1:88:A:GLU:HG2	16	0.57
(1,48)	1:86:A:ILE:HG21	1:89:A:LYS:HE3	4	0.57
(1,48)	1:86:A:ILE:HG22	1:89:A:LYS:HE3	4	0.57
(1,48)	1:86:A:ILE:HG23	1:89:A:LYS:HE3	4	0.57
(1,1992)	1:126:A:HIS:HB3	1:126:A:HIS:HD2	10	0.56
(1,1991)	1:126:A:HIS:HD2	1:126:A:HIS:HB2	7	0.56
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	18	0.56
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE1	11	0.56
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE2	11	0.56
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE1	13	0.56
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE2	13	0.56
(1,1879)	1:4:A:GLY:HA3	1:5:A:GLY:H	7	0.56
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	19	0.56
(1,1708)	1:115:A:LYS:H	1:115:A:LYS:HB2	9	0.56
(1,1708)	1:115:A:LYS:H	1:115:A:LYS:HB2	13	0.56
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	6	0.56
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	8	0.56
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	2	0.56
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	20	0.56
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	19	0.56
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	19	0.56
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	19	0.56
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	15	0.56
(1,1380)	1:158:A:LYS:HB2	1:158:A:LYS:H	18	0.56
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	11	0.56
(1,1277)	1:128:A:TRP:HE1	1:127:A:SER:HB2	1	0.56
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	9	0.56
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	9	0.56
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	9	0.56
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	16	0.56
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	16	0.56
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	16	0.56
(1,1158)	1:101:A:LYS:HD3	1:101:A:LYS:HA	9	0.56
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE1	8	0.56
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE2	8	0.56
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE3	8	0.56
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE1	10	0.56
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE2	10	0.56
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE3	10	0.56
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE1	18	0.56
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE2	18	0.56
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE3	18	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	2	0.56
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	2	0.56
(1,798)	1:138:A:LYS:HG3	1:138:A:LYS:HA	2	0.56
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	16	0.56
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	10	0.56
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	17	0.56
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	17	0.56
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	17	0.56
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	17	0.56
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	17	0.56
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	17	0.56
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	10	0.56
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	10	0.56
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	10	0.56
(1,506)	1:93:A:LEU:H	1:92:A:LYS:HG2	14	0.56
(1,484)	1:142:A:VAL:HG11	1:139:A:THR:HA	16	0.56
(1,484)	1:142:A:VAL:HG12	1:139:A:THR:HA	16	0.56
(1,484)	1:142:A:VAL:HG13	1:139:A:THR:HA	16	0.56
(1,385)	1:121:A:LEU:HB3	1:118:A:VAL:HA	4	0.56
(1,355)	1:137:A:GLU:HB3	1:139:A:THR:HB	16	0.56
(1,324)	1:142:A:VAL:HG21	1:114:A:ARG:HB2	16	0.56
(1,324)	1:142:A:VAL:HG22	1:114:A:ARG:HB2	16	0.56
(1,324)	1:142:A:VAL:HG23	1:114:A:ARG:HB2	16	0.56
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	12	0.56
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	12	0.56
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	12	0.56
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	17	0.56
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	17	0.56
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	17	0.56
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	17	0.56
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	17	0.56
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	17	0.56
(1,164)	1:2:A:GLU:HG3	1:2:A:GLU:HA	20	0.56
(1,43)	1:51:A:LYS:HE2	1:51:A:LYS:HG2	13	0.56
(1,11)	1:8:A:GLY:HA3	1:15:A:LYS:HE3	6	0.56
(1,2)	1:8:A:GLY:HA2	1:15:A:LYS:HD2	7	0.56
(1,2)	1:8:A:GLY:HA3	1:15:A:LYS:HD2	7	0.56
(1,1991)	1:126:A:HIS:HD2	1:126:A:HIS:HB2	12	0.55
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	14	0.55
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	14	0.55
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	6	0.55
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	5	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1708)	1:115:A:LYS:H	1:115:A:LYS:HB2	15	0.55
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	12	0.55
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	16	0.55
(1,1656)	1:122:A:LYS:H	1:122:A:LYS:HG2	4	0.55
(1,1580)	1:127:A:SER:H	1:126:A:HIS:HB2	20	0.55
(1,1554)	1:92:A:LYS:HB3	1:93:A:LEU:H	4	0.55
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	13	0.55
(1,1522)	1:131:A:GLU:H	1:130:A:GLU:HB3	10	0.55
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	9	0.55
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	9	0.55
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	9	0.55
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	19	0.55
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	19	0.55
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	19	0.55
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	10	0.55
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	8	0.55
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	14	0.55
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	14	0.55
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	14	0.55
(1,1147)	1:83:A:ALA:HA	1:86:A:ILE:HG12	5	0.55
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	11	0.55
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	11	0.55
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	11	0.55
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	11	0.55
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	11	0.55
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	11	0.55
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	11	0.55
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	11	0.55
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	11	0.55
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	18	0.55
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	18	0.55
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	18	0.55
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	20	0.55
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	5	0.55
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	5	0.55
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	5	0.55
(1,797)	1:138:A:LYS:HA	1:138:A:LYS:HG2	8	0.55
(1,763)	1:155:A:THR:HG21	1:156:A:HIS:HB2	7	0.55
(1,763)	1:155:A:THR:HG22	1:156:A:HIS:HB2	7	0.55
(1,763)	1:155:A:THR:HG23	1:156:A:HIS:HB2	7	0.55
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	2	0.55
(1,696)	1:71:A:SER:HB3	1:75:A:ARG:HD2	5	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	16	0.55
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	16	0.55
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	16	0.55
(1,605)	1:107:A:ASP:HB3	1:110:A:SER:HB3	14	0.55
(1,439)	1:147:A:GLU:HG2	1:144:A:LEU:HG	15	0.55
(1,263)	1:86:A:ILE:H	1:85:A:LYS:HB2	11	0.55
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	8	0.55
(1,61)	1:122:A:LYS:HE3	1:141:A:TYR:HE1	18	0.55
(1,61)	1:122:A:LYS:HE3	1:141:A:TYR:HE2	18	0.55
(1,18)	1:28:A:ARG:HA	1:28:A:ARG:HD2	16	0.55
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	8	0.55
(1,1992)	1:126:A:HIS:HB3	1:126:A:HIS:HD2	13	0.54
(1,1969)	1:24:A:SER:HB3	1:44:A:PHE:HZ	10	0.54
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	18	0.54
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	18	0.54
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	16	0.54
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	16	0.54
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	16	0.54
(1,1835)	1:114:A:ARG:H	1:114:A:ARG:HD2	14	0.54
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	5	0.54
(1,1700)	1:23:A:LYS:HB3	1:23:A:LYS:H	20	0.54
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	9	0.54
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	20	0.54
(1,1628)	1:148:A:LEU:H	1:147:A:GLU:HG2	11	0.54
(1,1580)	1:127:A:SER:H	1:126:A:HIS:HB2	16	0.54
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	10	0.54
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	10	0.54
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	10	0.54
(1,1319)	1:8:A:GLY:HA3	1:9:A:ALA:H	19	0.54
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	1	0.54
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	9	0.54
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	9	0.54
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	9	0.54
(1,1221)	1:65:A:ALA:HA	1:57:A:TYR:HD1	18	0.54
(1,1221)	1:65:A:ALA:HA	1:57:A:TYR:HD2	18	0.54
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	10	0.54
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	10	0.54
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	10	0.54
(1,1146)	1:115:A:LYS:HA	1:115:A:LYS:HG2	1	0.54
(1,1146)	1:115:A:LYS:HA	1:115:A:LYS:HG2	4	0.54
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD11	2	0.54
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD12	2	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD13	2	0.54
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	20	0.54
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	20	0.54
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	20	0.54
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	20	0.54
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	20	0.54
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	20	0.54
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	20	0.54
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	20	0.54
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	20	0.54
(1,1085)	1:56:A:CYS:HB3	1:53:A:ASN:HA	15	0.54
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE1	9	0.54
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE2	9	0.54
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE3	9	0.54
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE1	19	0.54
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE2	19	0.54
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE3	19	0.54
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	3	0.54
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	3	0.54
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	3	0.54
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	3	0.54
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	3	0.54
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	3	0.54
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	3	0.54
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	3	0.54
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	3	0.54
(1,911)	1:9:A:ALA:HB1	1:15:A:LYS:HD2	10	0.54
(1,911)	1:9:A:ALA:HB2	1:15:A:LYS:HD2	10	0.54
(1,911)	1:9:A:ALA:HB3	1:15:A:LYS:HD2	10	0.54
(1,879)	1:122:A:LYS:HA	1:122:A:LYS:HG2	14	0.54
(1,869)	1:13:A:VAL:HG21	1:55:A:LEU:HB2	3	0.54
(1,869)	1:13:A:VAL:HG22	1:55:A:LEU:HB2	3	0.54
(1,869)	1:13:A:VAL:HG23	1:55:A:LEU:HB2	3	0.54
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	6	0.54
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	6	0.54
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	6	0.54
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	2	0.54
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	2	0.54
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	2	0.54
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	16	0.54
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	16	0.54
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	16	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,814)	1:38:A:GLU:HA	1:38:A:GLU:HG2	7	0.54
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	7	0.54
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	7	0.54
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	7	0.54
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	10	0.54
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	10	0.54
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	10	0.54
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	14	0.54
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	14	0.54
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	14	0.54
(1,731)	1:148:A:LEU:HD21	1:151:A:LYS:HE2	4	0.54
(1,731)	1:148:A:LEU:HD22	1:151:A:LYS:HE2	4	0.54
(1,731)	1:148:A:LEU:HD23	1:151:A:LYS:HE2	4	0.54
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	8	0.54
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	8	0.54
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	8	0.54
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	8	0.54
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	8	0.54
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	8	0.54
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	8	0.54
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	8	0.54
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	8	0.54
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	16	0.54
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	16	0.54
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	16	0.54
(1,419)	1:6:A:ARG:HG3	1:6:A:ARG:H	17	0.54
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	15	0.54
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	15	0.54
(1,384)	1:96:A:GLN:HB3	1:58:A:TYR:HD1	9	0.54
(1,384)	1:96:A:GLN:HB3	1:58:A:TYR:HD2	9	0.54
(1,363)	1:75:A:ARG:HD3	1:75:A:ARG:HB2	4	0.54
(1,243)	1:81:A:MET:HG3	1:85:A:LYS:HB2	16	0.54
(1,243)	1:81:A:MET:HG2	1:85:A:LYS:HB2	16	0.54
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	9	0.54
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	9	0.54
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	9	0.54
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	1	0.54
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	1	0.54
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	1	0.54
(1,163)	1:2:A:GLU:HA	1:2:A:GLU:HG2	16	0.54
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	10	0.54
(1,43)	1:51:A:LYS:HE2	1:51:A:LYS:HG2	6	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:51:A:LYS:HE3	1:51:A:LYS:HG2	3	0.54
(1,1991)	1:126:A:HIS:HD2	1:126:A:HIS:HB2	4	0.53
(1,1991)	1:126:A:HIS:HD2	1:126:A:HIS:HB2	5	0.53
(1,1991)	1:126:A:HIS:HD2	1:126:A:HIS:HB2	17	0.53
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	14	0.53
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	10	0.53
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	1	0.53
(1,1661)	1:39:A:LYS:HB3	1:39:A:LYS:H	2	0.53
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	6	0.53
(1,1586)	1:143:A:ASN:HB3	1:142:A:VAL:H	5	0.53
(1,1580)	1:127:A:SER:H	1:126:A:HIS:HB2	10	0.53
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	5	0.53
(1,1548)	1:130:A:GLU:H	1:128:A:TRP:HB3	19	0.53
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	16	0.53
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	3	0.53
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	3	0.53
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	3	0.53
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	6	0.53
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	9	0.53
(1,1380)	1:158:A:LYS:HB2	1:158:A:LYS:H	10	0.53
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	2	0.53
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	19	0.53
(1,1318)	1:9:A:ALA:H	1:8:A:GLY:HA2	6	0.53
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	5	0.53
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	5	0.53
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	5	0.53
(1,1104)	1:103:A:GLU:HG3	1:103:A:GLU:HA	14	0.53
(1,1054)	1:92:A:LYS:HA	1:92:A:LYS:HG2	18	0.53
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE1	12	0.53
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE2	12	0.53
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE3	12	0.53
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE1	14	0.53
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE2	14	0.53
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE3	14	0.53
(1,1017)	1:84:A:MET:HE1	1:15:A:LYS:HE2	10	0.53
(1,1017)	1:84:A:MET:HE2	1:15:A:LYS:HE2	10	0.53
(1,1017)	1:84:A:MET:HE3	1:15:A:LYS:HE2	10	0.53
(1,1008)	1:85:A:LYS:HA	1:88:A:GLU:HB3	5	0.53
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	16	0.53
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	16	0.53
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	16	0.53
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	6	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	6	0.53
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	6	0.53
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	13	0.53
(1,716)	1:148:A:LEU:HD21	1:147:A:GLU:HG2	4	0.53
(1,716)	1:148:A:LEU:HD22	1:147:A:GLU:HG2	4	0.53
(1,716)	1:148:A:LEU:HD23	1:147:A:GLU:HG2	4	0.53
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG21	9	0.53
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG22	9	0.53
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG23	9	0.53
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG21	9	0.53
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG22	9	0.53
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG23	9	0.53
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG21	9	0.53
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG22	9	0.53
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG23	9	0.53
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG21	9	0.53
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG22	9	0.53
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG23	9	0.53
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG21	9	0.53
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG22	9	0.53
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG23	9	0.53
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG21	9	0.53
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG22	9	0.53
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG23	9	0.53
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	6	0.53
(1,687)	1:17:A:PHE:HA	1:20:A:ARG:HB2	8	0.53
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	4	0.53
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	4	0.53
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	4	0.53
(1,584)	1:102:A:TYR:H	1:101:A:LYS:HG2	3	0.53
(1,484)	1:142:A:VAL:HG11	1:139:A:THR:HA	15	0.53
(1,484)	1:142:A:VAL:HG12	1:139:A:THR:HA	15	0.53
(1,484)	1:142:A:VAL:HG13	1:139:A:THR:HA	15	0.53
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	9	0.53
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	9	0.53
(1,400)	1:59:A:LEU:HA	1:69:A:ILE:HG12	15	0.53
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	17	0.53
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	17	0.53
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	17	0.53
(1,263)	1:86:A:ILE:H	1:85:A:LYS:HB2	16	0.53
(1,163)	1:2:A:GLU:HA	1:2:A:GLU:HG2	12	0.53
(1,153)	1:103:A:GLU:HG3	1:104:A:LYS:H	5	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,135)	1:74:A:THR:HG21	1:38:A:GLU:HG2	1	0.53
(1,135)	1:74:A:THR:HG22	1:38:A:GLU:HG2	1	0.53
(1,135)	1:74:A:THR:HG23	1:38:A:GLU:HG2	1	0.53
(1,112)	1:53:A:ASN:H	1:52:A:GLU:HG3	6	0.53
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG21	4	0.53
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG22	4	0.53
(1,106)	1:31:A:ASN:HB3	1:30:A:VAL:HG23	4	0.53
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	4	0.53
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	17	0.53
(1,76)	1:140:A:ASP:HB2	1:135:A:CYS:HA	1	0.53
(1,33)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	4	0.53
(1,1991)	1:126:A:HIS:HD2	1:126:A:HIS:HB2	3	0.52
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	11	0.52
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	11	0.52
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE1	9	0.52
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE2	9	0.52
(1,1879)	1:4:A:GLY:HA3	1:5:A:GLY:H	8	0.52
(1,1865)	1:142:A:VAL:HG21	1:146:A:GLN:HE22	8	0.52
(1,1865)	1:142:A:VAL:HG22	1:146:A:GLN:HE22	8	0.52
(1,1865)	1:142:A:VAL:HG23	1:146:A:GLN:HE22	8	0.52
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	6	0.52
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	9	0.52
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	19	0.52
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	6	0.52
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	10	0.52
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	18	0.52
(1,1602)	1:54:A:ARG:HD2	1:54:A:ARG:H	14	0.52
(1,1581)	1:126:A:HIS:HB3	1:127:A:SER:H	3	0.52
(1,1580)	1:127:A:SER:H	1:126:A:HIS:HB2	13	0.52
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	4	0.52
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	11	0.52
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	19	0.52
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	12	0.52
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	12	0.52
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	12	0.52
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	12	0.52
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	12	0.52
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	12	0.52
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	1	0.52
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	1	0.52
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	1	0.52
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	1	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	1	0.52
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	1	0.52
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	1	0.52
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	1	0.52
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	1	0.52
(1,1111)	1:117:A:ARG:HD3	1:116:A:MET:HA	16	0.52
(1,1085)	1:56:A:CYS:HB3	1:53:A:ASN:HA	9	0.52
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE1	11	0.52
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE2	11	0.52
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE3	11	0.52
(1,936)	1:9:A:ALA:HB1	1:10:A:ASP:HB3	5	0.52
(1,936)	1:9:A:ALA:HB2	1:10:A:ASP:HB3	5	0.52
(1,936)	1:9:A:ALA:HB3	1:10:A:ASP:HB3	5	0.52
(1,927)	1:23:A:LYS:HA	1:22:A:TYR:HB2	16	0.52
(1,869)	1:13:A:VAL:HG21	1:55:A:LEU:HB2	6	0.52
(1,869)	1:13:A:VAL:HG22	1:55:A:LEU:HB2	6	0.52
(1,869)	1:13:A:VAL:HG23	1:55:A:LEU:HB2	6	0.52
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	4	0.52
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	4	0.52
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	4	0.52
(1,727)	1:62:A:THR:HG21	1:56:A:CYS:HB2	8	0.52
(1,727)	1:62:A:THR:HG22	1:56:A:CYS:HB2	8	0.52
(1,727)	1:62:A:THR:HG23	1:56:A:CYS:HB2	8	0.52
(1,716)	1:148:A:LEU:HD21	1:147:A:GLU:HG2	5	0.52
(1,716)	1:148:A:LEU:HD22	1:147:A:GLU:HG2	5	0.52
(1,716)	1:148:A:LEU:HD23	1:147:A:GLU:HG2	5	0.52
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	8	0.52
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	4	0.52
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	20	0.52
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	20	0.52
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	20	0.52
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	20	0.52
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	20	0.52
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	20	0.52
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	20	0.52
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	20	0.52
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	20	0.52
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	20	0.52
(1,385)	1:121:A:LEU:HB3	1:118:A:VAL:HA	13	0.52
(1,362)	1:75:A:ARG:HB2	1:75:A:ARG:HD2	20	0.52
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	2	0.52
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	20	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	2	0.52
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	2	0.52
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	2	0.52
(1,293)	1:37:A:ILE:HG21	1:38:A:GLU:HB3	14	0.52
(1,293)	1:37:A:ILE:HG22	1:38:A:GLU:HB3	14	0.52
(1,293)	1:37:A:ILE:HG23	1:38:A:GLU:HB3	14	0.52
(1,264)	1:85:A:LYS:HB3	1:86:A:ILE:H	3	0.52
(1,244)	1:85:A:LYS:HB3	1:81:A:MET:HG2	9	0.52
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	6	0.52
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	6	0.52
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	6	0.52
(1,209)	1:67:A:THR:HG21	1:68:A:LYS:HB3	17	0.52
(1,209)	1:67:A:THR:HG22	1:68:A:LYS:HB3	17	0.52
(1,209)	1:67:A:THR:HG23	1:68:A:LYS:HB3	17	0.52
(1,178)	1:136:A:ALA:HB1	1:137:A:GLU:HG2	16	0.52
(1,178)	1:136:A:ALA:HB2	1:137:A:GLU:HG2	16	0.52
(1,178)	1:136:A:ALA:HB3	1:137:A:GLU:HG2	16	0.52
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	15	0.52
(1,33)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	6	0.52
(1,32)	1:6:A:ARG:HG3	1:6:A:ARG:HD2	15	0.52
(1,1708)	1:115:A:LYS:H	1:115:A:LYS:HB2	8	0.51
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	20	0.51
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	20	0.51
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	20	0.51
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	10	0.51
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	9	0.51
(1,1580)	1:127:A:SER:H	1:126:A:HIS:HB2	18	0.51
(1,1553)	1:93:A:LEU:H	1:92:A:LYS:HB2	7	0.51
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	3	0.51
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	9	0.51
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	8	0.51
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	16	0.51
(1,1386)	1:103:A:GLU:H	1:102:A:TYR:HB3	16	0.51
(1,1380)	1:158:A:LYS:HB2	1:158:A:LYS:H	11	0.51
(1,1380)	1:158:A:LYS:HB2	1:158:A:LYS:H	13	0.51
(1,1380)	1:158:A:LYS:HB2	1:158:A:LYS:H	16	0.51
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	17	0.51
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	7	0.51
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	15	0.51
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	1	0.51
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	1	0.51
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	1	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1221)	1:65:A:ALA:HA	1:57:A:TYR:HD1	17	0.51
(1,1221)	1:65:A:ALA:HA	1:57:A:TYR:HD2	17	0.51
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	16	0.51
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	16	0.51
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	16	0.51
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	19	0.51
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	19	0.51
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	19	0.51
(1,1158)	1:101:A:LYS:HD3	1:101:A:LYS:HA	14	0.51
(1,1110)	1:116:A:MET:HA	1:117:A:ARG:HD2	13	0.51
(1,1103)	1:103:A:GLU:HA	1:103:A:GLU:HG2	13	0.51
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE1	10	0.51
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE2	10	0.51
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE3	10	0.51
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	18	0.51
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	18	0.51
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	18	0.51
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG11	17	0.51
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG12	17	0.51
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG13	17	0.51
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	4	0.51
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	20	0.51
(1,687)	1:17:A:PHE:HA	1:20:A:ARG:HB2	9	0.51
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	19	0.51
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	20	0.51
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	6	0.51
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	6	0.51
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	6	0.51
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	5	0.51
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	5	0.51
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	5	0.51
(1,437)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	11	0.51
(1,437)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	15	0.51
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	4	0.51
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	4	0.51
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	12	0.51
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	12	0.51
(1,363)	1:75:A:ARG:HD3	1:75:A:ARG:HB2	10	0.51
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	1	0.51
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	7	0.51
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	7	0.51
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	7	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	7	0.51
(1,209)	1:67:A:THR:HG21	1:68:A:LYS:HB3	2	0.51
(1,209)	1:67:A:THR:HG22	1:68:A:LYS:HB3	2	0.51
(1,209)	1:67:A:THR:HG23	1:68:A:LYS:HB3	2	0.51
(1,142)	1:88:A:GLU:HG3	1:89:A:LYS:H	15	0.51
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	7	0.51
(1,69)	1:87:A:CYS:HA	1:90:A:LEU:HB3	19	0.51
(1,33)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	16	0.51
(1,33)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	17	0.51
(1,18)	1:28:A:ARG:HA	1:28:A:ARG:HD2	1	0.51
(1,9)	1:8:A:GLY:HA2	1:15:A:LYS:HE2	16	0.51
(1,9)	1:8:A:GLY:HA3	1:15:A:LYS:HE2	16	0.51
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	1	0.5
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	1	0.5
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD1	15	0.5
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD2	15	0.5
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	11	0.5
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	17	0.5
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	16	0.5
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	1	0.5
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	8	0.5
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	19	0.5
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	15	0.5
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	20	0.5
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	20	0.5
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	20	0.5
(1,1462)	1:107:A:ASP:HB3	1:109:A:ALA:H	17	0.5
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	6	0.5
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	6	0.5
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	6	0.5
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	13	0.5
(1,1380)	1:158:A:LYS:HB2	1:158:A:LYS:H	14	0.5
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	6	0.5
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	11	0.5
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	18	0.5
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	18	0.5
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	18	0.5
(1,1055)	1:92:A:LYS:HG3	1:92:A:LYS:HA	2	0.5
(1,1054)	1:92:A:LYS:HA	1:92:A:LYS:HG2	12	0.5
(1,1008)	1:85:A:LYS:HA	1:88:A:GLU:HB3	9	0.5
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	1	0.5
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	1	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	1	0.5
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	1	0.5
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	1	0.5
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	1	0.5
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	1	0.5
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	1	0.5
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	1	0.5
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	16	0.5
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	16	0.5
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	16	0.5
(1,812)	1:41:A:LEU:HB3	1:38:A:GLU:HA	5	0.5
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	5	0.5
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	13	0.5
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	13	0.5
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	13	0.5
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	14	0.5
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	15	0.5
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	14	0.5
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	14	0.5
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	14	0.5
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	14	0.5
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	14	0.5
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	14	0.5
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	14	0.5
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	14	0.5
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	14	0.5
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	12	0.5
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	13	0.5
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	6	0.5
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	15	0.5
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	15	0.5
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	15	0.5
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	12	0.5
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	16	0.5
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	18	0.5
(1,438)	1:6:A:ARG:HG3	1:6:A:ARG:HB3	9	0.5
(1,438)	1:6:A:ARG:HG3	1:6:A:ARG:HB3	17	0.5
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	8	0.5
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	8	0.5
(1,299)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	12	0.5
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	5	0.5
(1,33)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	2	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	9	0.5
(1,33)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	20	0.5
(1,32)	1:6:A:ARG:HG3	1:6:A:ARG:HD2	7	0.5
(1,27)	1:117:A:ARG:HD3	1:117:A:ARG:HB3	11	0.5
(1,19)	1:28:A:ARG:HD3	1:28:A:ARG:HA	5	0.5
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	4	0.49
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE1	15	0.49
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE2	15	0.49
(1,1810)	1:91:A:LYS:HB3	1:92:A:LYS:H	8	0.49
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	7	0.49
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	14	0.49
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	7	0.49
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	7	0.49
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	7	0.49
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	10	0.49
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	1	0.49
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	10	0.49
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	11	0.49
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	15	0.49
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD11	17	0.49
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD12	17	0.49
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD13	17	0.49
(1,1244)	1:7:A:PRO:HD2	1:6:A:ARG:HD2	11	0.49
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	20	0.49
(1,1233)	1:26:A:ILE:HD11	1:23:A:LYS:H	4	0.49
(1,1233)	1:26:A:ILE:HD12	1:23:A:LYS:H	4	0.49
(1,1233)	1:26:A:ILE:HD13	1:23:A:LYS:H	4	0.49
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	10	0.49
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	10	0.49
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	10	0.49
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	14	0.49
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	14	0.49
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	14	0.49
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	6	0.49
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	6	0.49
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	6	0.49
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	6	0.49
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	6	0.49
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	6	0.49
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	6	0.49
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	6	0.49
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	6	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1055)	1:92:A:LYS:HG3	1:92:A:LYS:HA	17	0.49
(1,1054)	1:92:A:LYS:HA	1:92:A:LYS:HG2	11	0.49
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	10	0.49
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	10	0.49
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	10	0.49
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	10	0.49
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	10	0.49
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	10	0.49
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	10	0.49
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	10	0.49
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	10	0.49
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	19	0.49
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	19	0.49
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	19	0.49
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	19	0.49
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	19	0.49
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	19	0.49
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	19	0.49
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	19	0.49
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	19	0.49
(1,787)	1:75:A:ARG:HD3	1:75:A:ARG:HA	19	0.49
(1,763)	1:155:A:THR:HG21	1:156:A:HIS:HB2	3	0.49
(1,763)	1:155:A:THR:HG22	1:156:A:HIS:HB2	3	0.49
(1,763)	1:155:A:THR:HG23	1:156:A:HIS:HB2	3	0.49
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	8	0.49
(1,716)	1:148:A:LEU:HD21	1:147:A:GLU:HG2	13	0.49
(1,716)	1:148:A:LEU:HD22	1:147:A:GLU:HG2	13	0.49
(1,716)	1:148:A:LEU:HD23	1:147:A:GLU:HG2	13	0.49
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG21	20	0.49
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG22	20	0.49
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG23	20	0.49
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG21	20	0.49
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG22	20	0.49
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG23	20	0.49
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG21	20	0.49
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG22	20	0.49
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG23	20	0.49
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG21	20	0.49
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG22	20	0.49
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG23	20	0.49
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG21	20	0.49
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG22	20	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG23	20	0.49
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG21	20	0.49
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG22	20	0.49
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG23	20	0.49
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	7	0.49
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	17	0.49
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	16	0.49
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	19	0.49
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	19	0.49
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	19	0.49
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	13	0.49
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	13	0.49
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	13	0.49
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	15	0.49
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	15	0.49
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	15	0.49
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	18	0.49
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	18	0.49
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	18	0.49
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	4	0.49
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	8	0.49
(1,438)	1:6:A:ARG:HG3	1:6:A:ARG:HB3	2	0.49
(1,438)	1:6:A:ARG:HG3	1:6:A:ARG:HB3	3	0.49
(1,437)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	1	0.49
(1,437)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	10	0.49
(1,437)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	14	0.49
(1,437)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	20	0.49
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	13	0.49
(1,362)	1:75:A:ARG:HB2	1:75:A:ARG:HD2	6	0.49
(1,362)	1:75:A:ARG:HB2	1:75:A:ARG:HD2	17	0.49
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	19	0.49
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	13	0.49
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	13	0.49
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	13	0.49
(1,209)	1:67:A:THR:HG21	1:68:A:LYS:HB3	10	0.49
(1,209)	1:67:A:THR:HG22	1:68:A:LYS:HB3	10	0.49
(1,209)	1:67:A:THR:HG23	1:68:A:LYS:HB3	10	0.49
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	9	0.49
(1,112)	1:53:A:ASN:H	1:52:A:GLU:HG3	3	0.49
(1,92)	1:64:A:ASP:HB3	1:57:A:TYR:HE1	9	0.49
(1,92)	1:64:A:ASP:HB3	1:57:A:TYR:HE2	9	0.49
(1,9)	1:8:A:GLY:HA2	1:15:A:LYS:HE2	17	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:8:A:GLY:HA3	1:15:A:LYS:HE2	17	0.49
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	2	0.49
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	2	0.49
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	2	0.49
(1,1969)	1:24:A:SER:HB3	1:44:A:PHE:HZ	11	0.48
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD1	17	0.48
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD2	17	0.48
(1,1871)	1:8:A:GLY:H	1:7:A:PRO:HG3	14	0.48
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	17	0.48
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	17	0.48
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	17	0.48
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	13	0.48
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	15	0.48
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	11	0.48
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	12	0.48
(1,1581)	1:126:A:HIS:HB3	1:127:A:SER:H	12	0.48
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	7	0.48
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	2	0.48
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	2	0.48
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	2	0.48
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	19	0.48
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	7	0.48
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	19	0.48
(1,1221)	1:65:A:ALA:HA	1:57:A:TYR:HD1	20	0.48
(1,1221)	1:65:A:ALA:HA	1:57:A:TYR:HD2	20	0.48
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	4	0.48
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	4	0.48
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	4	0.48
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	8	0.48
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	8	0.48
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	8	0.48
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	18	0.48
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	18	0.48
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	18	0.48
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	18	0.48
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	18	0.48
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	18	0.48
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	18	0.48
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	18	0.48
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	18	0.48
(1,1106)	1:104:A:LYS:HG3	1:103:A:GLU:HA	8	0.48
(1,1085)	1:56:A:CYS:HB3	1:53:A:ASN:HA	12	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	1:92:A:LYS:HA	1:92:A:LYS:HG2	17	0.48
(1,1047)	1:77:A:MET:HE1	1:22:A:TYR:HB3	20	0.48
(1,1047)	1:77:A:MET:HE2	1:22:A:TYR:HB3	20	0.48
(1,1047)	1:77:A:MET:HE3	1:22:A:TYR:HB3	20	0.48
(1,1008)	1:85:A:LYS:HA	1:88:A:GLU:HB3	3	0.48
(1,1008)	1:85:A:LYS:HA	1:88:A:GLU:HB3	7	0.48
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	17	0.48
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	17	0.48
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	17	0.48
(1,890)	1:65:A:ALA:HB1	1:64:A:ASP:HB2	5	0.48
(1,890)	1:65:A:ALA:HB2	1:64:A:ASP:HB2	5	0.48
(1,890)	1:65:A:ALA:HB3	1:64:A:ASP:HB2	5	0.48
(1,887)	1:65:A:ALA:HB1	1:57:A:TYR:HE1	2	0.48
(1,887)	1:65:A:ALA:HB1	1:57:A:TYR:HE2	2	0.48
(1,887)	1:65:A:ALA:HB2	1:57:A:TYR:HE1	2	0.48
(1,887)	1:65:A:ALA:HB2	1:57:A:TYR:HE2	2	0.48
(1,887)	1:65:A:ALA:HB3	1:57:A:TYR:HE1	2	0.48
(1,887)	1:65:A:ALA:HB3	1:57:A:TYR:HE2	2	0.48
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	1	0.48
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	1	0.48
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	1	0.48
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	2	0.48
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	4	0.48
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	13	0.48
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	16	0.48
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG2	11	0.48
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG2	11	0.48
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG2	11	0.48
(1,651)	1:118:A:VAL:HG21	1:138:A:LYS:HG3	11	0.48
(1,651)	1:118:A:VAL:HG22	1:138:A:LYS:HG3	11	0.48
(1,651)	1:118:A:VAL:HG23	1:138:A:LYS:HG3	11	0.48
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	6	0.48
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	6	0.48
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	6	0.48
(1,573)	1:106:A:LEU:HD21	1:108:A:LEU:HA	16	0.48
(1,573)	1:106:A:LEU:HD22	1:108:A:LEU:HA	16	0.48
(1,573)	1:106:A:LEU:HD23	1:108:A:LEU:HA	16	0.48
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	6	0.48
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	13	0.48
(1,437)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	5	0.48
(1,363)	1:75:A:ARG:HD3	1:75:A:ARG:HB2	11	0.48
(1,264)	1:85:A:LYS:HB3	1:86:A:ILE:H	17	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	14	0.48
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	14	0.48
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	14	0.48
(1,175)	1:137:A:GLU:HG3	1:137:A:GLU:H	16	0.48
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	18	0.48
(1,144)	1:12:A:GLU:HA	1:12:A:GLU:HG3	3	0.48
(1,48)	1:86:A:ILE:HG21	1:89:A:LYS:HE3	12	0.48
(1,48)	1:86:A:ILE:HG22	1:89:A:LYS:HE3	12	0.48
(1,48)	1:86:A:ILE:HG23	1:89:A:LYS:HE3	12	0.48
(1,33)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	10	0.48
(1,32)	1:6:A:ARG:HG3	1:6:A:ARG:HD2	1	0.48
(1,21)	1:114:A:ARG:HD3	1:114:A:ARG:HB2	14	0.48
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	17	0.47
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	17	0.47
(1,1708)	1:115:A:LYS:H	1:115:A:LYS:HB2	1	0.47
(1,1708)	1:115:A:LYS:H	1:115:A:LYS:HB2	4	0.47
(1,1655)	1:122:A:LYS:H	1:122:A:LYS:HB2	14	0.47
(1,1646)	1:88:A:GLU:HB3	1:87:A:CYS:H	5	0.47
(1,1646)	1:88:A:GLU:HB3	1:87:A:CYS:H	20	0.47
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	13	0.47
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	14	0.47
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	18	0.47
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	3	0.47
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	20	0.47
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	2	0.47
(1,1462)	1:107:A:ASP:HB3	1:109:A:ALA:H	5	0.47
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	4	0.47
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	4	0.47
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	4	0.47
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	8	0.47
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	8	0.47
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	8	0.47
(1,1427)	1:63:A:LYS:HB3	1:63:A:LYS:H	2	0.47
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	1	0.47
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	3	0.47
(1,1380)	1:158:A:LYS:HB2	1:158:A:LYS:H	9	0.47
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	1	0.47
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	4	0.47
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	17	0.47
(1,1158)	1:101:A:LYS:HD3	1:101:A:LYS:HA	18	0.47
(1,1158)	1:101:A:LYS:HD3	1:101:A:LYS:HA	20	0.47
(1,1146)	1:115:A:LYS:HA	1:115:A:LYS:HG2	15	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE1	17	0.47
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE2	17	0.47
(1,1022)	1:84:A:MET:HG3	1:84:A:MET:HE3	17	0.47
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	14	0.47
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	14	0.47
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	14	0.47
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	14	0.47
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	14	0.47
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	14	0.47
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	14	0.47
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	14	0.47
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	14	0.47
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	12	0.47
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	12	0.47
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	12	0.47
(1,911)	1:9:A:ALA:HB1	1:15:A:LYS:HD2	1	0.47
(1,911)	1:9:A:ALA:HB2	1:15:A:LYS:HD2	1	0.47
(1,911)	1:9:A:ALA:HB3	1:15:A:LYS:HD2	1	0.47
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	4	0.47
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	4	0.47
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	4	0.47
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	16	0.47
(1,787)	1:75:A:ARG:HD3	1:75:A:ARG:HA	2	0.47
(1,787)	1:75:A:ARG:HD3	1:75:A:ARG:HA	15	0.47
(1,716)	1:148:A:LEU:HD21	1:147:A:GLU:HG2	16	0.47
(1,716)	1:148:A:LEU:HD22	1:147:A:GLU:HG2	16	0.47
(1,716)	1:148:A:LEU:HD23	1:147:A:GLU:HG2	16	0.47
(1,711)	1:139:A:THR:HG21	1:143:A:ASN:HB2	16	0.47
(1,711)	1:139:A:THR:HG22	1:143:A:ASN:HB2	16	0.47
(1,711)	1:139:A:THR:HG23	1:143:A:ASN:HB2	16	0.47
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	3	0.47
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	12	0.47
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	11	0.47
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	11	0.47
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	11	0.47
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD11	20	0.47
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD12	20	0.47
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD13	20	0.47
(1,559)	1:158:A:LYS:HE3	1:158:A:LYS:HG2	8	0.47
(1,557)	1:158:A:LYS:HE3	1:158:A:LYS:HG3	13	0.47
(1,557)	1:158:A:LYS:HE2	1:158:A:LYS:HG3	13	0.47
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	5	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,418)	1:6:A:ARG:H	1:6:A:ARG:HG2	15	0.47
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	9	0.47
(1,282)	1:20:A:ARG:HB3	1:20:A:ARG:HD3	15	0.47
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD11	3	0.47
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD12	3	0.47
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD13	3	0.47
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	20	0.47
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	20	0.47
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	20	0.47
(1,232)	1:91:A:LYS:H	1:91:A:LYS:HB3	14	0.47
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG21	12	0.47
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG22	12	0.47
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG23	12	0.47
(1,112)	1:53:A:ASN:H	1:52:A:GLU:HG3	4	0.47
(1,33)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	14	0.47
(1,19)	1:28:A:ARG:HD3	1:28:A:ARG:HA	10	0.47
(1,2)	1:8:A:GLY:HA2	1:15:A:LYS:HD2	19	0.47
(1,2)	1:8:A:GLY:HA3	1:15:A:LYS:HD2	19	0.47
(1,2013)	1:151:A:LYS:HE3	1:152:A:TYR:HE1	10	0.46
(1,2013)	1:151:A:LYS:HE3	1:152:A:TYR:HE2	10	0.46
(1,1878)	1:5:A:GLY:H	1:4:A:GLY:HA2	9	0.46
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	17	0.46
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	20	0.46
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	1	0.46
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	1	0.46
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	1	0.46
(1,1669)	1:93:A:LEU:HB3	1:94:A:ASP:H	3	0.46
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	6	0.46
(1,1628)	1:148:A:LEU:H	1:147:A:GLU:HG2	1	0.46
(1,1628)	1:148:A:LEU:H	1:147:A:GLU:HG2	15	0.46
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	12	0.46
(1,1522)	1:131:A:GLU:H	1:130:A:GLU:HB3	20	0.46
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	17	0.46
(1,1363)	1:27:A:ASP:H	1:27:A:ASP:HB3	15	0.46
(1,1363)	1:27:A:ASP:H	1:27:A:ASP:HB3	17	0.46
(1,1358)	1:65:A:ALA:H	1:63:A:LYS:HB2	5	0.46
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	3	0.46
(1,1146)	1:115:A:LYS:HA	1:115:A:LYS:HG2	5	0.46
(1,1146)	1:115:A:LYS:HA	1:115:A:LYS:HG2	9	0.46
(1,1058)	1:54:A:ARG:HA	1:54:A:ARG:HD3	3	0.46
(1,1058)	1:54:A:ARG:HA	1:54:A:ARG:HD3	13	0.46
(1,1058)	1:54:A:ARG:HA	1:54:A:ARG:HD3	19	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	19	0.46
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	19	0.46
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	19	0.46
(1,869)	1:13:A:VAL:HG21	1:55:A:LEU:HB2	18	0.46
(1,869)	1:13:A:VAL:HG22	1:55:A:LEU:HB2	18	0.46
(1,869)	1:13:A:VAL:HG23	1:55:A:LEU:HB2	18	0.46
(1,859)	1:111:A:VAL:HG21	1:108:A:LEU:H	4	0.46
(1,859)	1:111:A:VAL:HG22	1:108:A:LEU:H	4	0.46
(1,859)	1:111:A:VAL:HG23	1:108:A:LEU:H	4	0.46
(1,826)	1:111:A:VAL:HG11	1:116:A:MET:HE1	4	0.46
(1,826)	1:111:A:VAL:HG11	1:116:A:MET:HE2	4	0.46
(1,826)	1:111:A:VAL:HG11	1:116:A:MET:HE3	4	0.46
(1,826)	1:111:A:VAL:HG12	1:116:A:MET:HE1	4	0.46
(1,826)	1:111:A:VAL:HG12	1:116:A:MET:HE2	4	0.46
(1,826)	1:111:A:VAL:HG12	1:116:A:MET:HE3	4	0.46
(1,826)	1:111:A:VAL:HG13	1:116:A:MET:HE1	4	0.46
(1,826)	1:111:A:VAL:HG13	1:116:A:MET:HE2	4	0.46
(1,826)	1:111:A:VAL:HG13	1:116:A:MET:HE3	4	0.46
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	14	0.46
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	14	0.46
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	14	0.46
(1,787)	1:75:A:ARG:HD3	1:75:A:ARG:HA	8	0.46
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG21	4	0.46
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG22	4	0.46
(1,772)	1:31:A:ASN:HB2	1:30:A:VAL:HG23	4	0.46
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	15	0.46
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	15	0.46
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	15	0.46
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	12	0.46
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	15	0.46
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	15	0.46
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	15	0.46
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	15	0.46
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	15	0.46
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	15	0.46
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	15	0.46
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	15	0.46
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	15	0.46
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	19	0.46
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	19	0.46
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	19	0.46
(1,507)	1:92:A:LYS:HG3	1:93:A:LEU:H	3	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:6:A:ARG:HG3	1:6:A:ARG:HB3	8	0.46
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	5	0.46
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	5	0.46
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	19	0.46
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	19	0.46
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	19	0.46
(1,33)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	5	0.46
(1,33)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	8	0.46
(1,33)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	11	0.46
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	19	0.46
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	19	0.46
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	19	0.46
(1,1993)	1:130:A:GLU:HB2	1:128:A:TRP:HE3	20	0.45
(1,1969)	1:24:A:SER:HB3	1:44:A:PHE:HZ	15	0.45
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD1	8	0.45
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD2	8	0.45
(1,1871)	1:8:A:GLY:H	1:7:A:PRO:HG3	20	0.45
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	19	0.45
(1,1581)	1:126:A:HIS:HB3	1:127:A:SER:H	11	0.45
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	10	0.45
(1,1522)	1:131:A:GLU:H	1:130:A:GLU:HB3	11	0.45
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	7	0.45
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	15	0.45
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	18	0.45
(1,1380)	1:158:A:LYS:HB2	1:158:A:LYS:H	6	0.45
(1,1380)	1:158:A:LYS:HB2	1:158:A:LYS:H	7	0.45
(1,1363)	1:27:A:ASP:H	1:27:A:ASP:HB3	8	0.45
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	8	0.45
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	13	0.45
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	7	0.45
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	11	0.45
(1,1181)	1:86:A:ILE:HD11	1:82:A:PRO:HD3	2	0.45
(1,1181)	1:86:A:ILE:HD12	1:82:A:PRO:HD3	2	0.45
(1,1181)	1:86:A:ILE:HD13	1:82:A:PRO:HD3	2	0.45
(1,1146)	1:115:A:LYS:HA	1:115:A:LYS:HG2	10	0.45
(1,1146)	1:115:A:LYS:HA	1:115:A:LYS:HG2	13	0.45
(1,1146)	1:115:A:LYS:HA	1:115:A:LYS:HG2	18	0.45
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	12	0.45
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	12	0.45
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	12	0.45
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	12	0.45
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	12	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	12	0.45
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	12	0.45
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	12	0.45
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	12	0.45
(1,1085)	1:56:A:CYS:HB3	1:53:A:ASN:HA	16	0.45
(1,1058)	1:54:A:ARG:HA	1:54:A:ARG:HD3	10	0.45
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	8	0.45
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	8	0.45
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	8	0.45
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	12	0.45
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	12	0.45
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	12	0.45
(1,787)	1:75:A:ARG:HD3	1:75:A:ARG:HA	7	0.45
(1,787)	1:75:A:ARG:HD3	1:75:A:ARG:HA	16	0.45
(1,786)	1:75:A:ARG:HA	1:75:A:ARG:HD2	3	0.45
(1,763)	1:155:A:THR:HG21	1:156:A:HIS:HB2	19	0.45
(1,763)	1:155:A:THR:HG22	1:156:A:HIS:HB2	19	0.45
(1,763)	1:155:A:THR:HG23	1:156:A:HIS:HB2	19	0.45
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	18	0.45
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	11	0.45
(1,530)	1:92:A:LYS:HB3	1:92:A:LYS:HD2	19	0.45
(1,530)	1:92:A:LYS:HB2	1:92:A:LYS:HD2	19	0.45
(1,507)	1:92:A:LYS:HG3	1:93:A:LEU:H	6	0.45
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	3	0.45
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	17	0.45
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	19	0.45
(1,437)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	7	0.45
(1,385)	1:121:A:LEU:HB3	1:118:A:VAL:HA	1	0.45
(1,264)	1:85:A:LYS:HB3	1:86:A:ILE:H	2	0.45
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD11	5	0.45
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD12	5	0.45
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD13	5	0.45
(1,193)	1:123:A:GLN:HA	1:123:A:GLN:HG3	7	0.45
(1,142)	1:88:A:GLU:HG3	1:89:A:LYS:H	2	0.45
(1,135)	1:74:A:THR:HG21	1:38:A:GLU:HG2	17	0.45
(1,135)	1:74:A:THR:HG22	1:38:A:GLU:HG2	17	0.45
(1,135)	1:74:A:THR:HG23	1:38:A:GLU:HG2	17	0.45
(1,18)	1:28:A:ARG:HA	1:28:A:ARG:HD2	9	0.45
(1,2008)	1:64:A:ASP:HB3	1:57:A:TYR:HE1	4	0.44
(1,2008)	1:64:A:ASP:HB3	1:57:A:TYR:HE2	4	0.44
(1,1937)	1:58:A:TYR:HD1	1:97:A:ILE:HG13	10	0.44
(1,1937)	1:58:A:TYR:HD2	1:97:A:ILE:HG13	10	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1646)	1:88:A:GLU:HB3	1:87:A:CYS:H	4	0.44
(1,1628)	1:148:A:LEU:H	1:147:A:GLU:HG2	20	0.44
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	11	0.44
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	13	0.44
(1,1586)	1:143:A:ASN:HB3	1:142:A:VAL:H	3	0.44
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	2	0.44
(1,1538)	1:116:A:MET:H	1:116:A:MET:HB2	17	0.44
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	5	0.44
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	20	0.44
(1,1386)	1:103:A:GLU:H	1:102:A:TYR:HB3	18	0.44
(1,1386)	1:103:A:GLU:H	1:102:A:TYR:HB3	19	0.44
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	10	0.44
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	18	0.44
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD11	5	0.44
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD12	5	0.44
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD13	5	0.44
(1,1239)	1:82:A:PRO:HD3	1:81:A:MET:HG2	4	0.44
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	3	0.44
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	3	0.44
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	3	0.44
(1,1158)	1:101:A:LYS:HD3	1:101:A:LYS:HA	3	0.44
(1,1146)	1:115:A:LYS:HA	1:115:A:LYS:HG2	14	0.44
(1,1126)	1:104:A:LYS:HG3	1:104:A:LYS:HA	13	0.44
(1,1110)	1:116:A:MET:HA	1:117:A:ARG:HD2	8	0.44
(1,1054)	1:92:A:LYS:HA	1:92:A:LYS:HG2	7	0.44
(1,1047)	1:77:A:MET:HE1	1:22:A:TYR:HB3	15	0.44
(1,1047)	1:77:A:MET:HE2	1:22:A:TYR:HB3	15	0.44
(1,1047)	1:77:A:MET:HE3	1:22:A:TYR:HB3	15	0.44
(1,1008)	1:85:A:LYS:HA	1:88:A:GLU:HB3	20	0.44
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	13	0.44
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	6	0.44
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	6	0.44
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	12	0.44
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	12	0.44
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	12	0.44
(1,815)	1:38:A:GLU:HG3	1:38:A:GLU:HA	2	0.44
(1,787)	1:75:A:ARG:HD3	1:75:A:ARG:HA	18	0.44
(1,696)	1:71:A:SER:HB3	1:75:A:ARG:HD2	11	0.44
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	1	0.44
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	5	0.44
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	9	0.44
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	18	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	5	0.44
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	13	0.44
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	13	0.44
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	13	0.44
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD11	9	0.44
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD12	9	0.44
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD13	9	0.44
(1,530)	1:92:A:LYS:HB3	1:92:A:LYS:HD2	8	0.44
(1,530)	1:92:A:LYS:HB2	1:92:A:LYS:HD2	8	0.44
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	13	0.44
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	13	0.44
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	13	0.44
(1,506)	1:93:A:LEU:H	1:92:A:LYS:HG2	4	0.44
(1,506)	1:93:A:LEU:H	1:92:A:LYS:HG2	5	0.44
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	10	0.44
(1,362)	1:75:A:ARG:HB2	1:75:A:ARG:HD2	9	0.44
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	2	0.44
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	14	0.44
(1,279)	1:67:A:THR:HB	1:69:A:ILE:HG13	15	0.44
(1,232)	1:91:A:LYS:H	1:91:A:LYS:HB3	19	0.44
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	14	0.44
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	14	0.44
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	14	0.44
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	15	0.44
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	15	0.44
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	15	0.44
(1,193)	1:123:A:GLN:HA	1:123:A:GLN:HG3	4	0.44
(1,193)	1:123:A:GLN:HA	1:123:A:GLN:HG3	16	0.44
(1,165)	1:147:A:GLU:HG2	1:147:A:GLU:HA	1	0.44
(1,165)	1:147:A:GLU:HG2	1:147:A:GLU:HA	2	0.44
(1,165)	1:147:A:GLU:HG2	1:147:A:GLU:HA	15	0.44
(1,165)	1:147:A:GLU:HG2	1:147:A:GLU:HA	20	0.44
(1,152)	1:104:A:LYS:H	1:103:A:GLU:HG2	14	0.44
(1,122)	1:94:A:ASP:HB3	1:97:A:ILE:HB	5	0.44
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG21	17	0.44
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG22	17	0.44
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG23	17	0.44
(1,95)	1:35:A:ASP:HB3	1:34:A:LEU:HB3	1	0.44
(1,18)	1:28:A:ARG:HA	1:28:A:ARG:HD2	19	0.44
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	5	0.44
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	11	0.43
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	3	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1878)	1:5:A:GLY:H	1:4:A:GLY:HA2	14	0.43
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	9	0.43
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	12	0.43
(1,1628)	1:148:A:LEU:H	1:147:A:GLU:HG2	2	0.43
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	16	0.43
(1,1586)	1:143:A:ASN:HB3	1:142:A:VAL:H	10	0.43
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	17	0.43
(1,1565)	1:117:A:ARG:H	1:116:A:MET:HB3	5	0.43
(1,1549)	1:130:A:GLU:H	1:130:A:GLU:HB2	5	0.43
(1,1549)	1:130:A:GLU:H	1:130:A:GLU:HB2	8	0.43
(1,1549)	1:130:A:GLU:H	1:130:A:GLU:HB2	15	0.43
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	17	0.43
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	17	0.43
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	17	0.43
(1,1462)	1:107:A:ASP:HB3	1:109:A:ALA:H	8	0.43
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	18	0.43
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	18	0.43
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	18	0.43
(1,1427)	1:63:A:LYS:HB3	1:63:A:LYS:H	5	0.43
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	13	0.43
(1,1426)	1:63:A:LYS:H	1:63:A:LYS:HB2	20	0.43
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	1	0.43
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	4	0.43
(1,1386)	1:103:A:GLU:H	1:102:A:TYR:HB3	3	0.43
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	14	0.43
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	19	0.43
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD11	9	0.43
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD12	9	0.43
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD13	9	0.43
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD11	16	0.43
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD12	16	0.43
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD13	16	0.43
(1,1241)	1:82:A:PRO:HD2	1:81:A:MET:HA	3	0.43
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	6	0.43
(1,1161)	1:119:A:ALA:HA	1:122:A:LYS:HG2	8	0.43
(1,1146)	1:115:A:LYS:HA	1:115:A:LYS:HG2	11	0.43
(1,1146)	1:115:A:LYS:HA	1:115:A:LYS:HG2	12	0.43
(1,1126)	1:104:A:LYS:HG3	1:104:A:LYS:HA	8	0.43
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	10	0.43
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	10	0.43
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	10	0.43
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	10	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	10	0.43
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	10	0.43
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	10	0.43
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	10	0.43
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	10	0.43
(1,1110)	1:116:A:MET:HA	1:117:A:ARG:HD2	9	0.43
(1,959)	1:24:A:SER:HB3	1:21:A:PHE:HA	10	0.43
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	18	0.43
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	18	0.43
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	18	0.43
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	18	0.43
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	18	0.43
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	18	0.43
(1,815)	1:38:A:GLU:HG3	1:38:A:GLU:HA	9	0.43
(1,814)	1:38:A:GLU:HA	1:38:A:GLU:HG2	18	0.43
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	20	0.43
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	20	0.43
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	20	0.43
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	3	0.43
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	3	0.43
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	3	0.43
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	15	0.43
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	15	0.43
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	15	0.43
(1,787)	1:75:A:ARG:HD3	1:75:A:ARG:HA	1	0.43
(1,763)	1:155:A:THR:HG21	1:156:A:HIS:HB2	9	0.43
(1,763)	1:155:A:THR:HG22	1:156:A:HIS:HB2	9	0.43
(1,763)	1:155:A:THR:HG23	1:156:A:HIS:HB2	9	0.43
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	19	0.43
(1,727)	1:62:A:THR:HG21	1:56:A:CYS:HB2	14	0.43
(1,727)	1:62:A:THR:HG22	1:56:A:CYS:HB2	14	0.43
(1,727)	1:62:A:THR:HG23	1:56:A:CYS:HB2	14	0.43
(1,719)	1:144:A:LEU:HB2	1:141:A:TYR:HA	10	0.43
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	12	0.43
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	1	0.43
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	14	0.43
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	14	0.43
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	14	0.43
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	18	0.43
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	18	0.43
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	18	0.43
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	20	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	20	0.43
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	20	0.43
(1,583)	1:151:A:LYS:HG2	1:151:A:LYS:H	6	0.43
(1,573)	1:106:A:LEU:HD21	1:108:A:LEU:HA	7	0.43
(1,573)	1:106:A:LEU:HD22	1:108:A:LEU:HA	7	0.43
(1,573)	1:106:A:LEU:HD23	1:108:A:LEU:HA	7	0.43
(1,573)	1:106:A:LEU:HD21	1:108:A:LEU:HA	19	0.43
(1,573)	1:106:A:LEU:HD22	1:108:A:LEU:HA	19	0.43
(1,573)	1:106:A:LEU:HD23	1:108:A:LEU:HA	19	0.43
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD11	5	0.43
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD12	5	0.43
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD13	5	0.43
(1,530)	1:92:A:LYS:HB3	1:92:A:LYS:HD2	5	0.43
(1,530)	1:92:A:LYS:HB2	1:92:A:LYS:HD2	5	0.43
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	14	0.43
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	14	0.43
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	14	0.43
(1,484)	1:142:A:VAL:HG11	1:139:A:THR:HA	13	0.43
(1,484)	1:142:A:VAL:HG12	1:139:A:THR:HA	13	0.43
(1,484)	1:142:A:VAL:HG13	1:139:A:THR:HA	13	0.43
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	7	0.43
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	17	0.43
(1,311)	1:91:A:LYS:HD3	1:95:A:SER:HA	7	0.43
(1,245)	1:81:A:MET:HG3	1:85:A:LYS:HB3	20	0.43
(1,232)	1:91:A:LYS:H	1:91:A:LYS:HB3	3	0.43
(1,209)	1:67:A:THR:HG21	1:68:A:LYS:HB3	9	0.43
(1,209)	1:67:A:THR:HG22	1:68:A:LYS:HB3	9	0.43
(1,209)	1:67:A:THR:HG23	1:68:A:LYS:HB3	9	0.43
(1,193)	1:123:A:GLN:HA	1:123:A:GLN:HG3	1	0.43
(1,193)	1:123:A:GLN:HA	1:123:A:GLN:HG3	2	0.43
(1,193)	1:123:A:GLN:HA	1:123:A:GLN:HG3	12	0.43
(1,193)	1:123:A:GLN:HA	1:123:A:GLN:HG3	18	0.43
(1,169)	1:16:A:GLU:HA	1:16:A:GLU:HG2	19	0.43
(1,116)	1:19:A:ASN:H	1:19:A:ASN:HB3	16	0.43
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG21	14	0.43
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG22	14	0.43
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG23	14	0.43
(1,112)	1:53:A:ASN:H	1:52:A:GLU:HG3	16	0.43
(1,9)	1:8:A:GLY:HA2	1:15:A:LYS:HE2	5	0.43
(1,9)	1:8:A:GLY:HA3	1:15:A:LYS:HE2	5	0.43
(1,2007)	1:57:A:TYR:HE1	1:64:A:ASP:HB2	9	0.42
(1,2007)	1:57:A:TYR:HE2	1:64:A:ASP:HB2	9	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	7	0.42
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	7	0.42
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD1	15	0.42
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD2	15	0.42
(1,1835)	1:114:A:ARG:H	1:114:A:ARG:HD2	16	0.42
(1,1810)	1:91:A:LYS:HB3	1:92:A:LYS:H	18	0.42
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	11	0.42
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	20	0.42
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	8	0.42
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	15	0.42
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	1	0.42
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	5	0.42
(1,1586)	1:143:A:ASN:HB3	1:142:A:VAL:H	6	0.42
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	9	0.42
(1,1549)	1:130:A:GLU:H	1:130:A:GLU:HB2	4	0.42
(1,1527)	1:116:A:MET:H	1:115:A:LYS:HB2	13	0.42
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	2	0.42
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	2	0.42
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	2	0.42
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	16	0.42
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	16	0.42
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	16	0.42
(1,1387)	1:103:A:GLU:H	1:103:A:GLU:HB2	5	0.42
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	7	0.42
(1,1363)	1:27:A:ASP:H	1:27:A:ASP:HB3	10	0.42
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	12	0.42
(1,1318)	1:9:A:ALA:H	1:8:A:GLY:HA2	20	0.42
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	17	0.42
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	17	0.42
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	17	0.42
(1,1091)	1:14:A:CYS:HA	1:97:A:ILE:HG21	5	0.42
(1,1091)	1:14:A:CYS:HA	1:97:A:ILE:HG22	5	0.42
(1,1091)	1:14:A:CYS:HA	1:97:A:ILE:HG23	5	0.42
(1,1058)	1:54:A:ARG:HA	1:54:A:ARG:HD3	17	0.42
(1,1008)	1:85:A:LYS:HA	1:88:A:GLU:HB3	18	0.42
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	13	0.42
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	13	0.42
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	13	0.42
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	13	0.42
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	13	0.42
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	13	0.42
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	13	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	13	0.42
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	13	0.42
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	1	0.42
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	1	0.42
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	1	0.42
(1,906)	1:82:A:PRO:HB3	1:83:A:ALA:HB1	17	0.42
(1,906)	1:82:A:PRO:HB3	1:83:A:ALA:HB2	17	0.42
(1,906)	1:82:A:PRO:HB3	1:83:A:ALA:HB3	17	0.42
(1,814)	1:38:A:GLU:HA	1:38:A:GLU:HG2	19	0.42
(1,763)	1:155:A:THR:HG21	1:156:A:HIS:HB2	6	0.42
(1,763)	1:155:A:THR:HG22	1:156:A:HIS:HB2	6	0.42
(1,763)	1:155:A:THR:HG23	1:156:A:HIS:HB2	6	0.42
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	14	0.42
(1,716)	1:148:A:LEU:HD21	1:147:A:GLU:HG2	10	0.42
(1,716)	1:148:A:LEU:HD22	1:147:A:GLU:HG2	10	0.42
(1,716)	1:148:A:LEU:HD23	1:147:A:GLU:HG2	10	0.42
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	19	0.42
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	11	0.42
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	2	0.42
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	4	0.42
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	2	0.42
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	2	0.42
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	2	0.42
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	3	0.42
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	3	0.42
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	3	0.42
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	6	0.42
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	6	0.42
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	6	0.42
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	8	0.42
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	8	0.42
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	8	0.42
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	11	0.42
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	11	0.42
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	11	0.42
(1,585)	1:101:A:LYS:HG3	1:102:A:TYR:H	2	0.42
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	18	0.42
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	18	0.42
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	18	0.42
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	10	0.42
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	10	0.42
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	10	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	17	0.42
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	17	0.42
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	17	0.42
(1,419)	1:6:A:ARG:HG3	1:6:A:ARG:H	9	0.42
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	10	0.42
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	8	0.42
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	11	0.42
(1,193)	1:123:A:GLN:HA	1:123:A:GLN:HG3	9	0.42
(1,193)	1:123:A:GLN:HA	1:123:A:GLN:HG3	11	0.42
(1,193)	1:123:A:GLN:HA	1:123:A:GLN:HG3	19	0.42
(1,165)	1:147:A:GLU:HG2	1:147:A:GLU:HA	14	0.42
(1,152)	1:104:A:LYS:H	1:103:A:GLU:HG2	13	0.42
(1,119)	1:58:A:TYR:HB2	1:97:A:ILE:HD11	9	0.42
(1,119)	1:58:A:TYR:HB2	1:97:A:ILE:HD12	9	0.42
(1,119)	1:58:A:TYR:HB2	1:97:A:ILE:HD13	9	0.42
(1,116)	1:19:A:ASN:H	1:19:A:ASN:HB3	5	0.42
(1,95)	1:35:A:ASP:HB3	1:34:A:LEU:HB3	20	0.42
(1,18)	1:28:A:ARG:HA	1:28:A:ARG:HD2	7	0.42
(1,18)	1:28:A:ARG:HA	1:28:A:ARG:HD2	11	0.42
(1,18)	1:28:A:ARG:HA	1:28:A:ARG:HD2	13	0.42
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	10	0.42
(1,5)	1:9:A:ALA:HB1	1:8:A:GLY:HA2	20	0.42
(1,5)	1:9:A:ALA:HB2	1:8:A:GLY:HA2	20	0.42
(1,5)	1:9:A:ALA:HB3	1:8:A:GLY:HA2	20	0.42
(1,2)	1:8:A:GLY:HA2	1:15:A:LYS:HD2	9	0.42
(1,2)	1:8:A:GLY:HA3	1:15:A:LYS:HD2	9	0.42
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD1	5	0.41
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD2	5	0.41
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	15	0.41
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	8	0.41
(1,1646)	1:88:A:GLU:HB3	1:87:A:CYS:H	13	0.41
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	5	0.41
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	3	0.41
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	8	0.41
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	9	0.41
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	20	0.41
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	6	0.41
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	16	0.41
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	11	0.41
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	19	0.41
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	7	0.41
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	13	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	13	0.41
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	13	0.41
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	15	0.41
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	15	0.41
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	15	0.41
(1,1188)	1:64:A:ASP:HB3	1:64:A:ASP:HA	5	0.41
(1,1058)	1:54:A:ARG:HA	1:54:A:ARG:HD3	2	0.41
(1,1055)	1:92:A:LYS:HG3	1:92:A:LYS:HA	11	0.41
(1,936)	1:9:A:ALA:HB1	1:10:A:ASP:HB3	2	0.41
(1,936)	1:9:A:ALA:HB2	1:10:A:ASP:HB3	2	0.41
(1,936)	1:9:A:ALA:HB3	1:10:A:ASP:HB3	2	0.41
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB1	10	0.41
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB2	10	0.41
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB3	10	0.41
(1,814)	1:38:A:GLU:HA	1:38:A:GLU:HG2	15	0.41
(1,814)	1:38:A:GLU:HA	1:38:A:GLU:HG2	16	0.41
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	6	0.41
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	6	0.41
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	6	0.41
(1,769)	1:30:A:VAL:HG21	1:31:A:ASN:H	6	0.41
(1,769)	1:30:A:VAL:HG22	1:31:A:ASN:H	6	0.41
(1,769)	1:30:A:VAL:HG23	1:31:A:ASN:H	6	0.41
(1,693)	1:43:A:SER:H	1:43:A:SER:HB2	10	0.41
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	13	0.41
(1,677)	1:59:A:LEU:HB3	1:56:A:CYS:HA	10	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	1	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	1	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	1	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	4	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	4	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	4	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	5	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	5	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	5	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	7	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	7	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	7	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	12	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	12	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	12	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	15	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	15	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	15	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	16	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	16	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	16	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	19	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	19	0.41
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	19	0.41
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG21	14	0.41
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG22	14	0.41
(1,645)	1:138:A:LYS:H	1:118:A:VAL:HG23	14	0.41
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG11	20	0.41
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG12	20	0.41
(1,638)	1:73:A:VAL:H	1:73:A:VAL:HG13	20	0.41
(1,619)	1:58:A:TYR:HE1	1:100:A:LEU:HD21	5	0.41
(1,619)	1:58:A:TYR:HE1	1:100:A:LEU:HD22	5	0.41
(1,619)	1:58:A:TYR:HE1	1:100:A:LEU:HD23	5	0.41
(1,619)	1:58:A:TYR:HE2	1:100:A:LEU:HD21	5	0.41
(1,619)	1:58:A:TYR:HE2	1:100:A:LEU:HD22	5	0.41
(1,619)	1:58:A:TYR:HE2	1:100:A:LEU:HD23	5	0.41
(1,605)	1:107:A:ASP:HB3	1:110:A:SER:HB3	4	0.41
(1,585)	1:101:A:LYS:HG3	1:102:A:TYR:H	14	0.41
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD11	19	0.41
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD12	19	0.41
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD13	19	0.41
(1,507)	1:92:A:LYS:HG3	1:93:A:LEU:H	12	0.41
(1,419)	1:6:A:ARG:HG3	1:6:A:ARG:H	3	0.41
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	17	0.41
(1,279)	1:67:A:THR:HB	1:69:A:ILE:HG13	18	0.41
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD11	20	0.41
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD12	20	0.41
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD13	20	0.41
(1,203)	1:158:A:LYS:HB3	1:158:A:LYS:HE2	8	0.41
(1,193)	1:123:A:GLN:HA	1:123:A:GLN:HG3	6	0.41
(1,193)	1:123:A:GLN:HA	1:123:A:GLN:HG3	13	0.41
(1,193)	1:123:A:GLN:HA	1:123:A:GLN:HG3	15	0.41
(1,145)	1:85:A:LYS:HA	1:88:A:GLU:HG2	12	0.41
(1,138)	1:42:A:ILE:HD11	1:38:A:GLU:HG2	20	0.41
(1,138)	1:42:A:ILE:HD12	1:38:A:GLU:HG2	20	0.41
(1,138)	1:42:A:ILE:HD13	1:38:A:GLU:HG2	20	0.41
(1,135)	1:74:A:THR:HG21	1:38:A:GLU:HG2	7	0.41
(1,135)	1:74:A:THR:HG22	1:38:A:GLU:HG2	7	0.41
(1,135)	1:74:A:THR:HG23	1:38:A:GLU:HG2	7	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,112)	1:53:A:ASN:H	1:52:A:GLU:HG3	15	0.41
(1,95)	1:35:A:ASP:HB3	1:34:A:LEU:HB3	7	0.41
(1,27)	1:117:A:ARG:HD3	1:117:A:ARG:HB3	17	0.41
(1,18)	1:28:A:ARG:HA	1:28:A:ARG:HD2	3	0.41
(1,18)	1:28:A:ARG:HA	1:28:A:ARG:HD2	12	0.41
(1,18)	1:28:A:ARG:HA	1:28:A:ARG:HD2	18	0.41
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	11	0.41
(1,5)	1:9:A:ALA:HB1	1:8:A:GLY:HA2	10	0.41
(1,5)	1:9:A:ALA:HB2	1:8:A:GLY:HA2	10	0.41
(1,5)	1:9:A:ALA:HB3	1:8:A:GLY:HA2	10	0.41
(1,1835)	1:114:A:ARG:H	1:114:A:ARG:HD2	6	0.4
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	7	0.4
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	10	0.4
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	13	0.4
(1,1646)	1:88:A:GLU:HB3	1:87:A:CYS:H	18	0.4
(1,1586)	1:143:A:ASN:HB3	1:142:A:VAL:H	13	0.4
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	5	0.4
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	11	0.4
(1,1565)	1:117:A:ARG:H	1:116:A:MET:HB3	2	0.4
(1,1549)	1:130:A:GLU:H	1:130:A:GLU:HB2	11	0.4
(1,1529)	1:131:A:GLU:H	1:131:A:GLU:HB2	7	0.4
(1,1522)	1:131:A:GLU:H	1:130:A:GLU:HB3	5	0.4
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	7	0.4
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	7	0.4
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	7	0.4
(1,1450)	1:96:A:GLN:H	1:94:A:ASP:HB2	4	0.4
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	8	0.4
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	14	0.4
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	18	0.4
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	16	0.4
(1,1316)	1:160:A:GLU:H	1:160:A:GLU:HB2	9	0.4
(1,1245)	1:6:A:ARG:HD3	1:7:A:PRO:HD2	2	0.4
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	8	0.4
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	6	0.4
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	6	0.4
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	6	0.4
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	13	0.4
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	13	0.4
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	13	0.4
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	20	0.4
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	20	0.4
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	20	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1106)	1:104:A:LYS:HG3	1:103:A:GLU:HA	4	0.4
(1,1085)	1:56:A:CYS:HB3	1:53:A:ASN:HA	17	0.4
(1,1047)	1:77:A:MET:HE1	1:22:A:TYR:HB3	5	0.4
(1,1047)	1:77:A:MET:HE2	1:22:A:TYR:HB3	5	0.4
(1,1047)	1:77:A:MET:HE3	1:22:A:TYR:HB3	5	0.4
(1,1047)	1:77:A:MET:HE1	1:22:A:TYR:HB3	17	0.4
(1,1047)	1:77:A:MET:HE2	1:22:A:TYR:HB3	17	0.4
(1,1047)	1:77:A:MET:HE3	1:22:A:TYR:HB3	17	0.4
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	19	0.4
(1,936)	1:9:A:ALA:HB1	1:10:A:ASP:HB3	12	0.4
(1,936)	1:9:A:ALA:HB2	1:10:A:ASP:HB3	12	0.4
(1,936)	1:9:A:ALA:HB3	1:10:A:ASP:HB3	12	0.4
(1,936)	1:9:A:ALA:HB1	1:10:A:ASP:HB3	16	0.4
(1,936)	1:9:A:ALA:HB2	1:10:A:ASP:HB3	16	0.4
(1,936)	1:9:A:ALA:HB3	1:10:A:ASP:HB3	16	0.4
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB1	12	0.4
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB2	12	0.4
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB3	12	0.4
(1,826)	1:111:A:VAL:HG11	1:116:A:MET:HE1	6	0.4
(1,826)	1:111:A:VAL:HG11	1:116:A:MET:HE2	6	0.4
(1,826)	1:111:A:VAL:HG11	1:116:A:MET:HE3	6	0.4
(1,826)	1:111:A:VAL:HG12	1:116:A:MET:HE1	6	0.4
(1,826)	1:111:A:VAL:HG12	1:116:A:MET:HE2	6	0.4
(1,826)	1:111:A:VAL:HG12	1:116:A:MET:HE3	6	0.4
(1,826)	1:111:A:VAL:HG13	1:116:A:MET:HE1	6	0.4
(1,826)	1:111:A:VAL:HG13	1:116:A:MET:HE2	6	0.4
(1,826)	1:111:A:VAL:HG13	1:116:A:MET:HE3	6	0.4
(1,786)	1:75:A:ARG:HA	1:75:A:ARG:HD2	10	0.4
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	7	0.4
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	8	0.4
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	9	0.4
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	9	0.4
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	9	0.4
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	10	0.4
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	10	0.4
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	10	0.4
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD21	17	0.4
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD22	17	0.4
(1,654)	1:108:A:LEU:HB2	1:108:A:LEU:HD23	17	0.4
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD21	9	0.4
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD22	9	0.4
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD23	9	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD21	9	0.4
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD22	9	0.4
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD23	9	0.4
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD21	9	0.4
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD22	9	0.4
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD23	9	0.4
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD21	19	0.4
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD22	19	0.4
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD23	19	0.4
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD21	19	0.4
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD22	19	0.4
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD23	19	0.4
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD21	19	0.4
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD22	19	0.4
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD23	19	0.4
(1,583)	1:151:A:LYS:HG2	1:151:A:LYS:H	7	0.4
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	12	0.4
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	12	0.4
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	12	0.4
(1,484)	1:142:A:VAL:HG11	1:139:A:THR:HA	3	0.4
(1,484)	1:142:A:VAL:HG12	1:139:A:THR:HA	3	0.4
(1,484)	1:142:A:VAL:HG13	1:139:A:THR:HA	3	0.4
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	16	0.4
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	19	0.4
(1,232)	1:91:A:LYS:H	1:91:A:LYS:HB3	9	0.4
(1,232)	1:91:A:LYS:H	1:91:A:LYS:HB3	16	0.4
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	17	0.4
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	17	0.4
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	17	0.4
(1,138)	1:42:A:ILE:HD11	1:38:A:GLU:HG2	12	0.4
(1,138)	1:42:A:ILE:HD12	1:38:A:GLU:HG2	12	0.4
(1,138)	1:42:A:ILE:HD13	1:38:A:GLU:HG2	12	0.4
(1,116)	1:19:A:ASN:H	1:19:A:ASN:HB3	10	0.4
(1,112)	1:53:A:ASN:H	1:52:A:GLU:HG3	19	0.4
(1,95)	1:35:A:ASP:HB3	1:34:A:LEU:HB3	4	0.4
(1,26)	1:117:A:ARG:HB3	1:117:A:ARG:HD2	8	0.4
(1,18)	1:28:A:ARG:HA	1:28:A:ARG:HD2	17	0.4
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	1	0.4
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	20	0.39
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	7	0.39
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	15	0.39
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	19	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	6	0.39
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	9	0.39
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	13	0.39
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	15	0.39
(1,1646)	1:88:A:GLU:HB3	1:87:A:CYS:H	3	0.39
(1,1611)	1:40:A:GLU:H	1:40:A:GLU:HG3	18	0.39
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	17	0.39
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	11	0.39
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	11	0.39
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	11	0.39
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG21	15	0.39
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG22	15	0.39
(1,1456)	1:144:A:LEU:H	1:142:A:VAL:HG23	15	0.39
(1,1381)	1:158:A:LYS:H	1:158:A:LYS:HG3	17	0.39
(1,1379)	1:158:A:LYS:H	1:157:A:PRO:HB3	4	0.39
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	20	0.39
(1,1332)	1:117:A:ARG:HB3	1:118:A:VAL:H	15	0.39
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	19	0.39
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	20	0.39
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	20	0.39
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	20	0.39
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	7	0.39
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	7	0.39
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	7	0.39
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	12	0.39
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	12	0.39
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	12	0.39
(1,1165)	1:117:A:ARG:HD3	1:117:A:ARG:HA	6	0.39
(1,1126)	1:104:A:LYS:HG3	1:104:A:LYS:HA	4	0.39
(1,1126)	1:104:A:LYS:HG3	1:104:A:LYS:HA	20	0.39
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	3	0.39
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	3	0.39
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	3	0.39
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	1	0.39
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	8	0.39
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	8	0.39
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	8	0.39
(1,927)	1:23:A:LYS:HA	1:22:A:TYR:HB2	9	0.39
(1,911)	1:9:A:ALA:HB1	1:15:A:LYS:HD2	9	0.39
(1,911)	1:9:A:ALA:HB2	1:15:A:LYS:HD2	9	0.39
(1,911)	1:9:A:ALA:HB3	1:15:A:LYS:HD2	9	0.39
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	13	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	13	0.39
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	13	0.39
(1,887)	1:65:A:ALA:HB1	1:57:A:TYR:HE1	16	0.39
(1,887)	1:65:A:ALA:HB1	1:57:A:TYR:HE2	16	0.39
(1,887)	1:65:A:ALA:HB2	1:57:A:TYR:HE1	16	0.39
(1,887)	1:65:A:ALA:HB2	1:57:A:TYR:HE2	16	0.39
(1,887)	1:65:A:ALA:HB3	1:57:A:TYR:HE1	16	0.39
(1,887)	1:65:A:ALA:HB3	1:57:A:TYR:HE2	16	0.39
(1,869)	1:13:A:VAL:HG21	1:55:A:LEU:HB2	1	0.39
(1,869)	1:13:A:VAL:HG22	1:55:A:LEU:HB2	1	0.39
(1,869)	1:13:A:VAL:HG23	1:55:A:LEU:HB2	1	0.39
(1,855)	1:61:A:ALA:HB1	1:45:A:CYS:HB3	1	0.39
(1,855)	1:61:A:ALA:HB2	1:45:A:CYS:HB3	1	0.39
(1,855)	1:61:A:ALA:HB3	1:45:A:CYS:HB3	1	0.39
(1,855)	1:61:A:ALA:HB1	1:45:A:CYS:HB3	20	0.39
(1,855)	1:61:A:ALA:HB2	1:45:A:CYS:HB3	20	0.39
(1,855)	1:61:A:ALA:HB3	1:45:A:CYS:HB3	20	0.39
(1,814)	1:38:A:GLU:HA	1:38:A:GLU:HG2	13	0.39
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	8	0.39
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	8	0.39
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	8	0.39
(1,716)	1:148:A:LEU:HD21	1:147:A:GLU:HG2	19	0.39
(1,716)	1:148:A:LEU:HD22	1:147:A:GLU:HG2	19	0.39
(1,716)	1:148:A:LEU:HD23	1:147:A:GLU:HG2	19	0.39
(1,696)	1:71:A:SER:HB3	1:75:A:ARG:HD2	10	0.39
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	19	0.39
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	20	0.39
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	18	0.39
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	10	0.39
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	10	0.39
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	10	0.39
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD21	20	0.39
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD22	20	0.39
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD23	20	0.39
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD21	20	0.39
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD22	20	0.39
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD23	20	0.39
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD21	20	0.39
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD22	20	0.39
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD23	20	0.39
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	2	0.39
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	2	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	2	0.39
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	6	0.39
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	6	0.39
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	6	0.39
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	8	0.39
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	8	0.39
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	8	0.39
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	11	0.39
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	11	0.39
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	11	0.39
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	13	0.39
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	13	0.39
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	13	0.39
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	16	0.39
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	16	0.39
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	16	0.39
(1,583)	1:151:A:LYS:HG2	1:151:A:LYS:H	14	0.39
(1,582)	1:151:A:LYS:H	1:151:A:LYS:HG3	5	0.39
(1,582)	1:151:A:LYS:H	1:151:A:LYS:HG3	13	0.39
(1,543)	1:35:A:ASP:H	1:33:A:SER:HB3	9	0.39
(1,484)	1:142:A:VAL:HG11	1:139:A:THR:HA	18	0.39
(1,484)	1:142:A:VAL:HG12	1:139:A:THR:HA	18	0.39
(1,484)	1:142:A:VAL:HG13	1:139:A:THR:HA	18	0.39
(1,441)	1:113:A:LEU:HD21	1:146:A:GLN:HG3	4	0.39
(1,441)	1:113:A:LEU:HD22	1:146:A:GLN:HG3	4	0.39
(1,441)	1:113:A:LEU:HD23	1:146:A:GLN:HG3	4	0.39
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	10	0.39
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	10	0.39
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	1	0.39
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	12	0.39
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	15	0.39
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	20	0.39
(1,232)	1:91:A:LYS:H	1:91:A:LYS:HB3	7	0.39
(1,153)	1:103:A:GLU:HG3	1:104:A:LYS:H	10	0.39
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG21	1	0.39
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG22	1	0.39
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG23	1	0.39
(1,2004)	1:77:A:MET:HA	1:22:A:TYR:HE1	3	0.38
(1,2004)	1:77:A:MET:HA	1:22:A:TYR:HE2	3	0.38
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE1	2	0.38
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE2	2	0.38
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE1	5	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE2	5	0.38
(1,1835)	1:114:A:ARG:H	1:114:A:ARG:HD2	19	0.38
(1,1807)	1:23:A:LYS:HB3	1:24:A:SER:H	5	0.38
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	1	0.38
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	3	0.38
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	4	0.38
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	6	0.38
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	16	0.38
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	19	0.38
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	20	0.38
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	3	0.38
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	8	0.38
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	7	0.38
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	15	0.38
(1,1669)	1:93:A:LEU:HB3	1:94:A:ASP:H	5	0.38
(1,1462)	1:107:A:ASP:HB3	1:109:A:ALA:H	1	0.38
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	8	0.38
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	14	0.38
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	14	0.38
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	14	0.38
(1,1221)	1:65:A:ALA:HA	1:57:A:TYR:HD1	8	0.38
(1,1221)	1:65:A:ALA:HA	1:57:A:TYR:HD2	8	0.38
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	1	0.38
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	15	0.38
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	17	0.38
(1,1161)	1:119:A:ALA:HA	1:122:A:LYS:HG2	5	0.38
(1,1126)	1:104:A:LYS:HG3	1:104:A:LYS:HA	14	0.38
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE1	3	0.38
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE2	3	0.38
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE3	3	0.38
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	18	0.38
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	7	0.38
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	15	0.38
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	2	0.38
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	2	0.38
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	2	0.38
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	9	0.38
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	9	0.38
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	9	0.38
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	7	0.38
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	7	0.38
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	7	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,887)	1:65:A:ALA:HB1	1:57:A:TYR:HE1	19	0.38
(1,887)	1:65:A:ALA:HB1	1:57:A:TYR:HE2	19	0.38
(1,887)	1:65:A:ALA:HB2	1:57:A:TYR:HE1	19	0.38
(1,887)	1:65:A:ALA:HB2	1:57:A:TYR:HE2	19	0.38
(1,887)	1:65:A:ALA:HB3	1:57:A:TYR:HE1	19	0.38
(1,887)	1:65:A:ALA:HB3	1:57:A:TYR:HE2	19	0.38
(1,787)	1:75:A:ARG:HD3	1:75:A:ARG:HA	14	0.38
(1,716)	1:148:A:LEU:HD21	1:147:A:GLU:HG2	3	0.38
(1,716)	1:148:A:LEU:HD22	1:147:A:GLU:HG2	3	0.38
(1,716)	1:148:A:LEU:HD23	1:147:A:GLU:HG2	3	0.38
(1,696)	1:71:A:SER:HB3	1:75:A:ARG:HD2	8	0.38
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	17	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	1	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	1	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	1	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	3	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	3	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	3	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	4	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	4	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	4	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	5	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	5	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	5	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	7	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	7	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	7	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	10	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	10	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	10	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	12	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	12	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	12	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	15	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	15	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	15	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	17	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	17	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	17	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	19	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	19	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	19	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	20	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	20	0.38
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	20	0.38
(1,589)	1:63:A:LYS:HB3	1:63:A:LYS:HG3	18	0.38
(1,583)	1:151:A:LYS:HG2	1:151:A:LYS:H	12	0.38
(1,582)	1:151:A:LYS:H	1:151:A:LYS:HG3	10	0.38
(1,582)	1:151:A:LYS:H	1:151:A:LYS:HG3	17	0.38
(1,552)	1:31:A:ASN:HD21	1:33:A:SER:HB2	6	0.38
(1,527)	1:93:A:LEU:HD21	1:92:A:LYS:HD2	1	0.38
(1,527)	1:93:A:LEU:HD22	1:92:A:LYS:HD2	1	0.38
(1,527)	1:93:A:LEU:HD23	1:92:A:LYS:HD2	1	0.38
(1,484)	1:142:A:VAL:HG11	1:139:A:THR:HA	8	0.38
(1,484)	1:142:A:VAL:HG12	1:139:A:THR:HA	8	0.38
(1,484)	1:142:A:VAL:HG13	1:139:A:THR:HA	8	0.38
(1,386)	1:77:A:MET:H	1:76:A:PRO:HG3	3	0.38
(1,336)	1:42:A:ILE:H	1:42:A:ILE:HG13	17	0.38
(1,324)	1:142:A:VAL:HG21	1:114:A:ARG:HB2	5	0.38
(1,324)	1:142:A:VAL:HG22	1:114:A:ARG:HB2	5	0.38
(1,324)	1:142:A:VAL:HG23	1:114:A:ARG:HB2	5	0.38
(1,323)	1:114:A:ARG:HB3	1:115:A:LYS:H	18	0.38
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	7	0.38
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	17	0.38
(1,264)	1:85:A:LYS:HB3	1:86:A:ILE:H	19	0.38
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD11	4	0.38
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD12	4	0.38
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD13	4	0.38
(1,232)	1:91:A:LYS:H	1:91:A:LYS:HB3	18	0.38
(1,232)	1:91:A:LYS:H	1:91:A:LYS:HB3	20	0.38
(1,204)	1:158:A:LYS:HE3	1:158:A:LYS:HB3	9	0.38
(1,194)	1:123:A:GLN:HG3	1:123:A:GLN:H	2	0.38
(1,193)	1:123:A:GLN:HA	1:123:A:GLN:HG3	14	0.38
(1,178)	1:136:A:ALA:HB1	1:137:A:GLU:HG2	17	0.38
(1,178)	1:136:A:ALA:HB2	1:137:A:GLU:HG2	17	0.38
(1,178)	1:136:A:ALA:HB3	1:137:A:GLU:HG2	17	0.38
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	3	0.38
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	8	0.38
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	8	0.38
(1,165)	1:147:A:GLU:HG2	1:147:A:GLU:HA	11	0.38
(1,151)	1:103:A:GLU:H	1:103:A:GLU:HG2	2	0.38
(1,151)	1:103:A:GLU:H	1:103:A:GLU:HG3	2	0.38
(1,116)	1:19:A:ASN:H	1:19:A:ASN:HB3	3	0.38
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	20	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:140:A:ASP:HB2	1:135:A:CYS:HA	7	0.38
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	16	0.38
(1,1777)	1:28:A:ARG:H	1:28:A:ARG:HB2	15	0.37
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	11	0.37
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	15	0.37
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	17	0.37
(1,1592)	1:55:A:LEU:H	1:100:A:LEU:HD11	5	0.37
(1,1592)	1:55:A:LEU:H	1:100:A:LEU:HD12	5	0.37
(1,1592)	1:55:A:LEU:H	1:100:A:LEU:HD13	5	0.37
(1,1581)	1:126:A:HIS:HB3	1:127:A:SER:H	17	0.37
(1,1565)	1:117:A:ARG:H	1:116:A:MET:HB3	6	0.37
(1,1549)	1:130:A:GLU:H	1:130:A:GLU:HB2	1	0.37
(1,1549)	1:130:A:GLU:H	1:130:A:GLU:HB2	17	0.37
(1,1450)	1:96:A:GLN:H	1:94:A:ASP:HB2	2	0.37
(1,1423)	1:121:A:LEU:H	1:121:A:LEU:HG	6	0.37
(1,1412)	1:124:A:ILE:H	1:123:A:GLN:HB2	10	0.37
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	17	0.37
(1,1386)	1:103:A:GLU:H	1:102:A:TYR:HB3	9	0.37
(1,1379)	1:158:A:LYS:H	1:157:A:PRO:HB3	17	0.37
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	13	0.37
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	2	0.37
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	3	0.37
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	6	0.37
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	7	0.37
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	8	0.37
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	10	0.37
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	12	0.37
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	13	0.37
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	14	0.37
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	16	0.37
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	18	0.37
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	19	0.37
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	20	0.37
(1,1161)	1:119:A:ALA:HA	1:122:A:LYS:HG2	16	0.37
(1,1157)	1:101:A:LYS:HA	1:101:A:LYS:HD2	2	0.37
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	1	0.37
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	3	0.37
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	5	0.37
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	8	0.37
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	11	0.37
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	12	0.37
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	13	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	14	0.37
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	16	0.37
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	19	0.37
(1,1058)	1:54:A:ARG:HA	1:54:A:ARG:HD3	6	0.37
(1,1017)	1:84:A:MET:HE1	1:15:A:LYS:HE2	6	0.37
(1,1017)	1:84:A:MET:HE2	1:15:A:LYS:HE2	6	0.37
(1,1017)	1:84:A:MET:HE3	1:15:A:LYS:HE2	6	0.37
(1,1008)	1:85:A:LYS:HA	1:88:A:GLU:HB3	10	0.37
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	5	0.37
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	5	0.37
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	5	0.37
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB1	10	0.37
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB2	10	0.37
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB3	10	0.37
(1,814)	1:38:A:GLU:HA	1:38:A:GLU:HG2	11	0.37
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	17	0.37
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	17	0.37
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	17	0.37
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	1	0.37
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	9	0.37
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	14	0.37
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	14	0.37
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	14	0.37
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	18	0.37
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	18	0.37
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	18	0.37
(1,589)	1:63:A:LYS:HB3	1:63:A:LYS:HG3	2	0.37
(1,589)	1:63:A:LYS:HB3	1:63:A:LYS:HG3	3	0.37
(1,589)	1:63:A:LYS:HB3	1:63:A:LYS:HG3	8	0.37
(1,589)	1:63:A:LYS:HB3	1:63:A:LYS:HG3	10	0.37
(1,589)	1:63:A:LYS:HB3	1:63:A:LYS:HG3	17	0.37
(1,589)	1:63:A:LYS:HB3	1:63:A:LYS:HG3	19	0.37
(1,589)	1:63:A:LYS:HB3	1:63:A:LYS:HG3	20	0.37
(1,582)	1:151:A:LYS:H	1:151:A:LYS:HG3	3	0.37
(1,582)	1:151:A:LYS:H	1:151:A:LYS:HG3	6	0.37
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD11	16	0.37
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD12	16	0.37
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD13	16	0.37
(1,543)	1:35:A:ASP:H	1:33:A:SER:HB3	1	0.37
(1,543)	1:35:A:ASP:H	1:33:A:SER:HB3	4	0.37
(1,543)	1:35:A:ASP:H	1:33:A:SER:HB3	6	0.37
(1,484)	1:142:A:VAL:HG11	1:139:A:THR:HA	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:142:A:VAL:HG12	1:139:A:THR:HA	6	0.37
(1,484)	1:142:A:VAL:HG13	1:139:A:THR:HA	6	0.37
(1,419)	1:6:A:ARG:HG3	1:6:A:ARG:H	12	0.37
(1,418)	1:6:A:ARG:H	1:6:A:ARG:HG2	20	0.37
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD2	6	0.37
(1,414)	1:75:A:ARG:HG3	1:76:A:PRO:HD3	6	0.37
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	15	0.37
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	4	0.37
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	18	0.37
(1,244)	1:85:A:LYS:HB3	1:81:A:MET:HG2	13	0.37
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	3	0.37
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	3	0.37
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	3	0.37
(1,194)	1:123:A:GLN:HG3	1:123:A:GLN:H	11	0.37
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	1	0.37
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	7	0.37
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	9	0.37
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	14	0.37
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	15	0.37
(1,176)	1:137:A:GLU:HB3	1:137:A:GLU:HG2	16	0.37
(1,174)	1:137:A:GLU:H	1:137:A:GLU:HG2	20	0.37
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	12	0.37
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	13	0.37
(1,145)	1:85:A:LYS:HA	1:88:A:GLU:HG2	4	0.37
(1,138)	1:42:A:ILE:HD11	1:38:A:GLU:HG2	4	0.37
(1,138)	1:42:A:ILE:HD12	1:38:A:GLU:HG2	4	0.37
(1,138)	1:42:A:ILE:HD13	1:38:A:GLU:HG2	4	0.37
(1,5)	1:9:A:ALA:HB1	1:8:A:GLY:HA2	17	0.37
(1,5)	1:9:A:ALA:HB2	1:8:A:GLY:HA2	17	0.37
(1,5)	1:9:A:ALA:HB3	1:8:A:GLY:HA2	17	0.37
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG11	4	0.36
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG12	4	0.36
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG13	4	0.36
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG11	4	0.36
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG12	4	0.36
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG13	4	0.36
(1,1870)	1:29:A:GLY:H	1:26:A:ILE:HG21	2	0.36
(1,1870)	1:29:A:GLY:H	1:26:A:ILE:HG22	2	0.36
(1,1870)	1:29:A:GLY:H	1:26:A:ILE:HG23	2	0.36
(1,1836)	1:114:A:ARG:HD3	1:114:A:ARG:H	20	0.36
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	2	0.36
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	4	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	5	0.36
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	8	0.36
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	5	0.36
(1,1669)	1:93:A:LEU:HB3	1:94:A:ASP:H	4	0.36
(1,1549)	1:130:A:GLU:H	1:130:A:GLU:HB2	10	0.36
(1,1549)	1:130:A:GLU:H	1:130:A:GLU:HB2	13	0.36
(1,1529)	1:131:A:GLU:H	1:131:A:GLU:HB2	19	0.36
(1,1522)	1:131:A:GLU:H	1:130:A:GLU:HB3	1	0.36
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	2	0.36
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	7	0.36
(1,1363)	1:27:A:ASP:H	1:27:A:ASP:HB3	1	0.36
(1,1363)	1:27:A:ASP:H	1:27:A:ASP:HB3	5	0.36
(1,1363)	1:27:A:ASP:H	1:27:A:ASP:HB3	16	0.36
(1,1316)	1:160:A:GLU:H	1:160:A:GLU:HB2	13	0.36
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	18	0.36
(1,1223)	1:10:A:ASP:H	1:9:A:ALA:HA	10	0.36
(1,1206)	1:108:A:LEU:H	1:107:A:ASP:HA	18	0.36
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	4	0.36
(1,1126)	1:104:A:LYS:HG3	1:104:A:LYS:HA	1	0.36
(1,1106)	1:104:A:LYS:HG3	1:103:A:GLU:HA	15	0.36
(1,1085)	1:56:A:CYS:HB3	1:53:A:ASN:HA	18	0.36
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	6	0.36
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	7	0.36
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	9	0.36
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	17	0.36
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	20	0.36
(1,1051)	1:26:A:ILE:HG21	1:27:A:ASP:HA	4	0.36
(1,1051)	1:26:A:ILE:HG22	1:27:A:ASP:HA	4	0.36
(1,1051)	1:26:A:ILE:HG23	1:27:A:ASP:HA	4	0.36
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	10	0.36
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	17	0.36
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	20	0.36
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	9	0.36
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	9	0.36
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	9	0.36
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	13	0.36
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	13	0.36
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	13	0.36
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB1	2	0.36
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB2	2	0.36
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB3	2	0.36
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG11	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG12	7	0.36
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG13	7	0.36
(1,815)	1:38:A:GLU:HG3	1:38:A:GLU:HA	20	0.36
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	18	0.36
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	12	0.36
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	12	0.36
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	12	0.36
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG21	16	0.36
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG22	16	0.36
(1,714)	1:41:A:LEU:HD11	1:73:A:VAL:HG23	16	0.36
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG21	16	0.36
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG22	16	0.36
(1,714)	1:41:A:LEU:HD12	1:73:A:VAL:HG23	16	0.36
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG21	16	0.36
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG22	16	0.36
(1,714)	1:41:A:LEU:HD13	1:73:A:VAL:HG23	16	0.36
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG21	16	0.36
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG22	16	0.36
(1,714)	1:41:A:LEU:HD21	1:73:A:VAL:HG23	16	0.36
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG21	16	0.36
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG22	16	0.36
(1,714)	1:41:A:LEU:HD22	1:73:A:VAL:HG23	16	0.36
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG21	16	0.36
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG22	16	0.36
(1,714)	1:41:A:LEU:HD23	1:73:A:VAL:HG23	16	0.36
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB2	3	0.36
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB3	3	0.36
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	1	0.36
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	7	0.36
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	20	0.36
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	9	0.36
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	9	0.36
(1,626)	1:46:A:LEU:HB2	1:46:A:LEU:HD23	9	0.36
(1,589)	1:63:A:LYS:HB3	1:63:A:LYS:HG3	1	0.36
(1,589)	1:63:A:LYS:HB3	1:63:A:LYS:HG3	4	0.36
(1,589)	1:63:A:LYS:HB3	1:63:A:LYS:HG3	7	0.36
(1,589)	1:63:A:LYS:HB3	1:63:A:LYS:HG3	15	0.36
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD11	9	0.36
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD12	9	0.36
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD13	9	0.36
(1,543)	1:35:A:ASP:H	1:33:A:SER:HB3	2	0.36
(1,543)	1:35:A:ASP:H	1:33:A:SER:HB3	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,543)	1:35:A:ASP:H	1:33:A:SER:HB3	12	0.36
(1,543)	1:35:A:ASP:H	1:33:A:SER:HB3	15	0.36
(1,484)	1:142:A:VAL:HG11	1:139:A:THR:HA	4	0.36
(1,484)	1:142:A:VAL:HG12	1:139:A:THR:HA	4	0.36
(1,484)	1:142:A:VAL:HG13	1:139:A:THR:HA	4	0.36
(1,385)	1:121:A:LEU:HB3	1:118:A:VAL:HA	19	0.36
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	3	0.36
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	6	0.36
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	10	0.36
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	13	0.36
(1,261)	1:28:A:ARG:HB3	1:29:A:GLY:H	15	0.36
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	9	0.36
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	9	0.36
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	9	0.36
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	16	0.36
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	16	0.36
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	16	0.36
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	2	0.36
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	2	0.36
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	2	0.36
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	7	0.36
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	7	0.36
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	7	0.36
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	8	0.36
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	8	0.36
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	8	0.36
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	11	0.36
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	11	0.36
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	11	0.36
(1,194)	1:123:A:GLN:HG3	1:123:A:GLN:H	6	0.36
(1,154)	1:103:A:GLU:HB3	1:103:A:GLU:HG2	15	0.36
(1,152)	1:104:A:LYS:H	1:103:A:GLU:HG2	8	0.36
(1,95)	1:35:A:ASP:HB3	1:34:A:LEU:HB3	2	0.36
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	6	0.36
(1,49)	1:159:A:THR:H	1:158:A:LYS:HE2	17	0.36
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE1	6	0.35
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE2	6	0.35
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	3	0.35
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	6	0.35
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	1	0.35
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	18	0.35
(1,1725)	1:33:A:SER:H	1:33:A:SER:HB2	2	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1669)	1:93:A:LEU:HB3	1:94:A:ASP:H	14	0.35
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	7	0.35
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	12	0.35
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	14	0.35
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	11	0.35
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	13	0.35
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	13	0.35
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	13	0.35
(1,1548)	1:130:A:GLU:H	1:128:A:TRP:HB3	15	0.35
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	11	0.35
(1,1386)	1:103:A:GLU:H	1:102:A:TYR:HB3	17	0.35
(1,1363)	1:27:A:ASP:H	1:27:A:ASP:HB3	20	0.35
(1,1316)	1:160:A:GLU:H	1:160:A:GLU:HB2	11	0.35
(1,1316)	1:160:A:GLU:H	1:160:A:GLU:HB2	12	0.35
(1,1291)	1:107:A:ASP:HB3	1:108:A:LEU:H	1	0.35
(1,1245)	1:6:A:ARG:HD3	1:7:A:PRO:HD2	1	0.35
(1,1245)	1:6:A:ARG:HD3	1:7:A:PRO:HD2	17	0.35
(1,1206)	1:108:A:LEU:H	1:107:A:ASP:HA	6	0.35
(1,1126)	1:104:A:LYS:HG3	1:104:A:LYS:HA	19	0.35
(1,1106)	1:104:A:LYS:HG3	1:103:A:GLU:HA	11	0.35
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	2	0.35
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	10	0.35
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	15	0.35
(1,1047)	1:77:A:MET:HE1	1:22:A:TYR:HB3	13	0.35
(1,1047)	1:77:A:MET:HE2	1:22:A:TYR:HB3	13	0.35
(1,1047)	1:77:A:MET:HE3	1:22:A:TYR:HB3	13	0.35
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	18	0.35
(1,959)	1:24:A:SER:HB3	1:21:A:PHE:HA	17	0.35
(1,869)	1:13:A:VAL:HG21	1:55:A:LEU:HB2	2	0.35
(1,869)	1:13:A:VAL:HG22	1:55:A:LEU:HB2	2	0.35
(1,869)	1:13:A:VAL:HG23	1:55:A:LEU:HB2	2	0.35
(1,869)	1:13:A:VAL:HG21	1:55:A:LEU:HB2	11	0.35
(1,869)	1:13:A:VAL:HG22	1:55:A:LEU:HB2	11	0.35
(1,869)	1:13:A:VAL:HG23	1:55:A:LEU:HB2	11	0.35
(1,869)	1:13:A:VAL:HG21	1:55:A:LEU:HB2	15	0.35
(1,869)	1:13:A:VAL:HG22	1:55:A:LEU:HB2	15	0.35
(1,869)	1:13:A:VAL:HG23	1:55:A:LEU:HB2	15	0.35
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG11	13	0.35
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG12	13	0.35
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG13	13	0.35
(1,814)	1:38:A:GLU:HA	1:38:A:GLU:HG2	3	0.35
(1,814)	1:38:A:GLU:HA	1:38:A:GLU:HG2	12	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	7	0.35
(1,727)	1:62:A:THR:HG21	1:56:A:CYS:HB2	6	0.35
(1,727)	1:62:A:THR:HG22	1:56:A:CYS:HB2	6	0.35
(1,727)	1:62:A:THR:HG23	1:56:A:CYS:HB2	6	0.35
(1,671)	1:113:A:LEU:HB3	1:142:A:VAL:HG11	6	0.35
(1,671)	1:113:A:LEU:HB3	1:142:A:VAL:HG12	6	0.35
(1,671)	1:113:A:LEU:HB3	1:142:A:VAL:HG13	6	0.35
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG21	5	0.35
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG22	5	0.35
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG23	5	0.35
(1,589)	1:63:A:LYS:HB3	1:63:A:LYS:HG3	5	0.35
(1,588)	1:63:A:LYS:HG3	1:63:A:LYS:HB2	11	0.35
(1,585)	1:101:A:LYS:HG3	1:102:A:TYR:H	5	0.35
(1,582)	1:151:A:LYS:H	1:151:A:LYS:HG3	12	0.35
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD11	16	0.35
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD12	16	0.35
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD13	16	0.35
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD11	20	0.35
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD12	20	0.35
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD13	20	0.35
(1,543)	1:35:A:ASP:H	1:33:A:SER:HB3	14	0.35
(1,419)	1:6:A:ARG:HG3	1:6:A:ARG:H	2	0.35
(1,323)	1:114:A:ARG:HB3	1:115:A:LYS:H	13	0.35
(1,304)	1:147:A:GLU:H	1:147:A:GLU:HB2	5	0.35
(1,264)	1:85:A:LYS:HB3	1:86:A:ILE:H	7	0.35
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	5	0.35
(1,243)	1:81:A:MET:HG3	1:85:A:LYS:HB2	11	0.35
(1,243)	1:81:A:MET:HG2	1:85:A:LYS:HB2	11	0.35
(1,232)	1:91:A:LYS:H	1:91:A:LYS:HB3	17	0.35
(1,194)	1:123:A:GLN:HG3	1:123:A:GLN:H	13	0.35
(1,194)	1:123:A:GLN:HG3	1:123:A:GLN:H	15	0.35
(1,194)	1:123:A:GLN:HG3	1:123:A:GLN:H	18	0.35
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	10	0.35
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	13	0.35
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	3	0.35
(1,142)	1:88:A:GLU:HG3	1:89:A:LYS:H	6	0.35
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	12	0.35
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB1	11	0.35
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB2	11	0.35
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB3	11	0.35
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG11	3	0.34
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG12	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG13	3	0.34
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG11	3	0.34
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG12	3	0.34
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG13	3	0.34
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	16	0.34
(1,1939)	1:55:A:LEU:HD21	1:17:A:PHE:HE1	16	0.34
(1,1939)	1:55:A:LEU:HD21	1:17:A:PHE:HE2	16	0.34
(1,1939)	1:55:A:LEU:HD22	1:17:A:PHE:HE1	16	0.34
(1,1939)	1:55:A:LEU:HD22	1:17:A:PHE:HE2	16	0.34
(1,1939)	1:55:A:LEU:HD23	1:17:A:PHE:HE1	16	0.34
(1,1939)	1:55:A:LEU:HD23	1:17:A:PHE:HE2	16	0.34
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD1	8	0.34
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD2	8	0.34
(1,1879)	1:4:A:GLY:HA3	1:5:A:GLY:H	14	0.34
(1,1879)	1:4:A:GLY:HA3	1:5:A:GLY:H	17	0.34
(1,1836)	1:114:A:ARG:HD3	1:114:A:ARG:H	12	0.34
(1,1836)	1:114:A:ARG:HD3	1:114:A:ARG:H	14	0.34
(1,1777)	1:28:A:ARG:H	1:28:A:ARG:HB2	4	0.34
(1,1756)	1:151:A:LYS:HB3	1:151:A:LYS:H	8	0.34
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	18	0.34
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	2	0.34
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	9	0.34
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	15	0.34
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	5	0.34
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	9	0.34
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	6	0.34
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	18	0.34
(1,1565)	1:117:A:ARG:H	1:116:A:MET:HB3	3	0.34
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	15	0.34
(1,1549)	1:130:A:GLU:H	1:130:A:GLU:HB2	3	0.34
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	14	0.34
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	19	0.34
(1,1529)	1:131:A:GLU:H	1:131:A:GLU:HB2	12	0.34
(1,1522)	1:131:A:GLU:H	1:130:A:GLU:HB3	14	0.34
(1,1492)	1:142:A:VAL:HG11	1:140:A:ASP:H	12	0.34
(1,1492)	1:142:A:VAL:HG12	1:140:A:ASP:H	12	0.34
(1,1492)	1:142:A:VAL:HG13	1:140:A:ASP:H	12	0.34
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	20	0.34
(1,1385)	1:103:A:GLU:H	1:102:A:TYR:HA	5	0.34
(1,1359)	1:63:A:LYS:HB3	1:65:A:ALA:H	13	0.34
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	17	0.34
(1,1316)	1:160:A:GLU:H	1:160:A:GLU:HB2	15	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD11	4	0.34
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD12	4	0.34
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD13	4	0.34
(1,1245)	1:6:A:ARG:HD3	1:7:A:PRO:HD2	9	0.34
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	1	0.34
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	15	0.34
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	20	0.34
(1,1221)	1:65:A:ALA:HA	1:57:A:TYR:HD1	4	0.34
(1,1221)	1:65:A:ALA:HA	1:57:A:TYR:HD2	4	0.34
(1,1221)	1:65:A:ALA:HA	1:57:A:TYR:HD1	12	0.34
(1,1221)	1:65:A:ALA:HA	1:57:A:TYR:HD2	12	0.34
(1,1206)	1:108:A:LEU:H	1:107:A:ASP:HA	4	0.34
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	11	0.34
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	11	0.34
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	11	0.34
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	17	0.34
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	17	0.34
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	17	0.34
(1,1187)	1:64:A:ASP:HA	1:64:A:ASP:HB2	9	0.34
(1,1110)	1:116:A:MET:HA	1:117:A:ARG:HD2	20	0.34
(1,1072)	1:35:A:ASP:HB3	1:35:A:ASP:HA	4	0.34
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE1	6	0.34
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE2	6	0.34
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE3	6	0.34
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE1	19	0.34
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE2	19	0.34
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE3	19	0.34
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	3	0.34
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	8	0.34
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	11	0.34
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	11	0.34
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	11	0.34
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	19	0.34
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	19	0.34
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	19	0.34
(1,787)	1:75:A:ARG:HD3	1:75:A:ARG:HA	3	0.34
(1,671)	1:113:A:LEU:HB3	1:142:A:VAL:HG11	3	0.34
(1,671)	1:113:A:LEU:HB3	1:142:A:VAL:HG12	3	0.34
(1,671)	1:113:A:LEU:HB3	1:142:A:VAL:HG13	3	0.34
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG21	11	0.34
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG22	11	0.34
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG23	11	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	3	0.34
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	19	0.34
(1,642)	1:54:A:ARG:HD3	1:100:A:LEU:HD21	7	0.34
(1,642)	1:54:A:ARG:HD3	1:100:A:LEU:HD22	7	0.34
(1,642)	1:54:A:ARG:HD3	1:100:A:LEU:HD23	7	0.34
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD21	4	0.34
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD22	4	0.34
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD23	4	0.34
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD21	4	0.34
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD22	4	0.34
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD23	4	0.34
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD21	4	0.34
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD22	4	0.34
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD23	4	0.34
(1,582)	1:151:A:LYS:H	1:151:A:LYS:HG3	4	0.34
(1,543)	1:35:A:ASP:H	1:33:A:SER:HB3	3	0.34
(1,543)	1:35:A:ASP:H	1:33:A:SER:HB3	8	0.34
(1,543)	1:35:A:ASP:H	1:33:A:SER:HB3	11	0.34
(1,543)	1:35:A:ASP:H	1:33:A:SER:HB3	13	0.34
(1,543)	1:35:A:ASP:H	1:33:A:SER:HB3	19	0.34
(1,543)	1:35:A:ASP:H	1:33:A:SER:HB3	20	0.34
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	11	0.34
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	3	0.34
(1,323)	1:114:A:ARG:HB3	1:115:A:LYS:H	14	0.34
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	15	0.34
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	15	0.34
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	15	0.34
(1,206)	1:158:A:LYS:HE3	1:158:A:LYS:HB2	3	0.34
(1,194)	1:123:A:GLN:HG3	1:123:A:GLN:H	9	0.34
(1,194)	1:123:A:GLN:HG3	1:123:A:GLN:H	12	0.34
(1,183)	1:101:A:LYS:HB2	1:102:A:TYR:HA	4	0.34
(1,183)	1:101:A:LYS:HB2	1:102:A:TYR:HA	15	0.34
(1,176)	1:137:A:GLU:HB3	1:137:A:GLU:HG2	5	0.34
(1,154)	1:103:A:GLU:HB3	1:103:A:GLU:HG2	7	0.34
(1,152)	1:104:A:LYS:H	1:103:A:GLU:HG2	4	0.34
(1,116)	1:19:A:ASN:H	1:19:A:ASN:HB3	20	0.34
(1,95)	1:35:A:ASP:HB3	1:34:A:LEU:HB3	3	0.34
(1,95)	1:35:A:ASP:HB3	1:34:A:LEU:HB3	12	0.34
(1,87)	1:114:A:ARG:HG2	1:112:A:ASP:HB2	12	0.34
(1,86)	1:28:A:ARG:H	1:27:A:ASP:HB2	7	0.34
(1,27)	1:117:A:ARG:HD3	1:117:A:ARG:HB3	12	0.34
(1,27)	1:117:A:ARG:HD3	1:117:A:ARG:HB3	14	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:117:A:ARG:HD3	1:117:A:ARG:HB3	18	0.34
(1,11)	1:8:A:GLY:HA3	1:15:A:LYS:HE3	2	0.34
(1,5)	1:9:A:ALA:HB1	1:8:A:GLY:HA2	6	0.34
(1,5)	1:9:A:ALA:HB2	1:8:A:GLY:HA2	6	0.34
(1,5)	1:9:A:ALA:HB3	1:8:A:GLY:HA2	6	0.34
(1,5)	1:9:A:ALA:HB1	1:8:A:GLY:HA2	16	0.34
(1,5)	1:9:A:ALA:HB2	1:8:A:GLY:HA2	16	0.34
(1,5)	1:9:A:ALA:HB3	1:8:A:GLY:HA2	16	0.34
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	9	0.33
(1,1878)	1:5:A:GLY:H	1:4:A:GLY:HA2	12	0.33
(1,1725)	1:33:A:SER:H	1:33:A:SER:HB2	9	0.33
(1,1725)	1:33:A:SER:H	1:33:A:SER:HB2	13	0.33
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	7	0.33
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	13	0.33
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	11	0.33
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	11	0.33
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	11	0.33
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	13	0.33
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	13	0.33
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	13	0.33
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	14	0.33
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	16	0.33
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	2	0.33
(1,1586)	1:143:A:ASN:HB3	1:142:A:VAL:H	4	0.33
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	9	0.33
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	10	0.33
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	10	0.33
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	10	0.33
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	16	0.33
(1,1549)	1:130:A:GLU:H	1:130:A:GLU:HB2	2	0.33
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	1	0.33
(1,1385)	1:103:A:GLU:H	1:102:A:TYR:HA	12	0.33
(1,1359)	1:63:A:LYS:HB3	1:65:A:ALA:H	11	0.33
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	6	0.33
(1,1335)	1:30:A:VAL:HA	1:31:A:ASN:H	4	0.33
(1,1319)	1:8:A:GLY:HA3	1:9:A:ALA:H	20	0.33
(1,1316)	1:160:A:GLU:H	1:160:A:GLU:HB2	6	0.33
(1,1291)	1:107:A:ASP:HB3	1:108:A:LEU:H	8	0.33
(1,1223)	1:10:A:ASP:H	1:9:A:ALA:HA	3	0.33
(1,1206)	1:108:A:LEU:H	1:107:A:ASP:HA	20	0.33
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	5	0.33
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	5	0.33
(1,1158)	1:101:A:LYS:HD3	1:101:A:LYS:HA	4	0.33
(1,1158)	1:101:A:LYS:HD3	1:101:A:LYS:HA	7	0.33
(1,1102)	1:158:A:LYS:HG2	1:158:A:LYS:HA	9	0.33
(1,1017)	1:84:A:MET:HE1	1:15:A:LYS:HE2	20	0.33
(1,1017)	1:84:A:MET:HE2	1:15:A:LYS:HE2	20	0.33
(1,1017)	1:84:A:MET:HE3	1:15:A:LYS:HE2	20	0.33
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	1	0.33
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	1	0.33
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	1	0.33
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	6	0.33
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	6	0.33
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	6	0.33
(1,897)	1:52:A:GLU:HA	1:52:A:GLU:HG2	9	0.33
(1,887)	1:65:A:ALA:HB1	1:57:A:TYR:HE1	15	0.33
(1,887)	1:65:A:ALA:HB1	1:57:A:TYR:HE2	15	0.33
(1,887)	1:65:A:ALA:HB2	1:57:A:TYR:HE1	15	0.33
(1,887)	1:65:A:ALA:HB2	1:57:A:TYR:HE2	15	0.33
(1,887)	1:65:A:ALA:HB3	1:57:A:TYR:HE1	15	0.33
(1,887)	1:65:A:ALA:HB3	1:57:A:TYR:HE2	15	0.33
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG11	14	0.33
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG12	14	0.33
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG13	14	0.33
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	16	0.33
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	16	0.33
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	16	0.33
(1,711)	1:139:A:THR:HG21	1:143:A:ASN:HB2	7	0.33
(1,711)	1:139:A:THR:HG22	1:143:A:ASN:HB2	7	0.33
(1,711)	1:139:A:THR:HG23	1:143:A:ASN:HB2	7	0.33
(1,701)	1:71:A:SER:HB3	1:71:A:SER:HA	8	0.33
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	6	0.33
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	7	0.33
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	12	0.33
(1,642)	1:54:A:ARG:HD3	1:100:A:LEU:HD21	19	0.33
(1,642)	1:54:A:ARG:HD3	1:100:A:LEU:HD22	19	0.33
(1,642)	1:54:A:ARG:HD3	1:100:A:LEU:HD23	19	0.33
(1,611)	1:111:A:VAL:HA	1:110:A:SER:HB2	12	0.33
(1,589)	1:63:A:LYS:HB3	1:63:A:LYS:HG3	13	0.33
(1,588)	1:63:A:LYS:HG3	1:63:A:LYS:HB2	16	0.33
(1,557)	1:158:A:LYS:HE3	1:158:A:LYS:HG3	2	0.33
(1,557)	1:158:A:LYS:HE2	1:158:A:LYS:HG3	2	0.33
(1,557)	1:158:A:LYS:HE3	1:158:A:LYS:HG3	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:158:A:LYS:HE2	1:158:A:LYS:HG3	3	0.33
(1,557)	1:158:A:LYS:HE3	1:158:A:LYS:HG3	7	0.33
(1,557)	1:158:A:LYS:HE2	1:158:A:LYS:HG3	7	0.33
(1,557)	1:158:A:LYS:HE3	1:158:A:LYS:HG3	18	0.33
(1,557)	1:158:A:LYS:HE2	1:158:A:LYS:HG3	18	0.33
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	3	0.33
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	3	0.33
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	3	0.33
(1,510)	1:115:A:LYS:H	1:115:A:LYS:HG3	16	0.33
(1,484)	1:142:A:VAL:HG11	1:139:A:THR:HA	19	0.33
(1,484)	1:142:A:VAL:HG12	1:139:A:THR:HA	19	0.33
(1,484)	1:142:A:VAL:HG13	1:139:A:THR:HA	19	0.33
(1,431)	1:141:A:TYR:HB3	1:121:A:LEU:HD21	10	0.33
(1,431)	1:141:A:TYR:HB3	1:121:A:LEU:HD22	10	0.33
(1,431)	1:141:A:TYR:HB3	1:121:A:LEU:HD23	10	0.33
(1,419)	1:6:A:ARG:HG3	1:6:A:ARG:H	19	0.33
(1,385)	1:121:A:LEU:HB3	1:118:A:VAL:HA	14	0.33
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB2	20	0.33
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB3	20	0.33
(1,250)	1:63:A:LYS:HE3	1:63:A:LYS:HB2	8	0.33
(1,250)	1:63:A:LYS:HE3	1:63:A:LYS:HB2	18	0.33
(1,244)	1:85:A:LYS:HB3	1:81:A:MET:HG2	20	0.33
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD11	8	0.33
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD12	8	0.33
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD13	8	0.33
(1,232)	1:91:A:LYS:H	1:91:A:LYS:HB3	1	0.33
(1,196)	1:123:A:GLN:HB3	1:123:A:GLN:HG2	1	0.33
(1,196)	1:123:A:GLN:HB3	1:123:A:GLN:HG2	16	0.33
(1,196)	1:123:A:GLN:HB3	1:123:A:GLN:HG2	19	0.33
(1,194)	1:123:A:GLN:HG3	1:123:A:GLN:H	1	0.33
(1,194)	1:123:A:GLN:HG3	1:123:A:GLN:H	16	0.33
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	7	0.33
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	7	0.33
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	7	0.33
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	2	0.33
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	12	0.33
(1,86)	1:28:A:ARG:H	1:27:A:ASP:HB2	11	0.33
(1,86)	1:28:A:ARG:H	1:27:A:ASP:HB2	19	0.33
(1,63)	1:122:A:LYS:HB3	1:122:A:LYS:HE2	4	0.33
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	2	0.33
(1,27)	1:117:A:ARG:HD3	1:117:A:ARG:HB3	2	0.33
(1,27)	1:117:A:ARG:HD3	1:117:A:ARG:HB3	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD1	9	0.32
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD2	9	0.32
(1,1871)	1:8:A:GLY:H	1:7:A:PRO:HG3	8	0.32
(1,1836)	1:114:A:ARG:HD3	1:114:A:ARG:H	17	0.32
(1,1798)	1:42:A:ILE:HG13	1:43:A:SER:H	6	0.32
(1,1756)	1:151:A:LYS:HB3	1:151:A:LYS:H	9	0.32
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	14	0.32
(1,1725)	1:33:A:SER:H	1:33:A:SER:HB2	7	0.32
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	18	0.32
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	20	0.32
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	13	0.32
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	8	0.32
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	13	0.32
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	15	0.32
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	2	0.32
(1,1565)	1:117:A:ARG:H	1:116:A:MET:HB3	10	0.32
(1,1565)	1:117:A:ARG:H	1:116:A:MET:HB3	17	0.32
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	12	0.32
(1,1387)	1:103:A:GLU:H	1:103:A:GLU:HB2	16	0.32
(1,1363)	1:27:A:ASP:H	1:27:A:ASP:HB3	13	0.32
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	9	0.32
(1,1328)	1:2:A:GLU:HB2	1:2:A:GLU:H	5	0.32
(1,1316)	1:160:A:GLU:H	1:160:A:GLU:HB2	14	0.32
(1,1291)	1:107:A:ASP:HB3	1:108:A:LEU:H	17	0.32
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD11	2	0.32
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD12	2	0.32
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD13	2	0.32
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD11	3	0.32
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD12	3	0.32
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD13	3	0.32
(1,1102)	1:158:A:LYS:HG2	1:158:A:LYS:HA	20	0.32
(1,1058)	1:54:A:ARG:HA	1:54:A:ARG:HD3	7	0.32
(1,1038)	1:121:A:LEU:HD11	1:121:A:LEU:HA	2	0.32
(1,1038)	1:121:A:LEU:HD12	1:121:A:LEU:HA	2	0.32
(1,1038)	1:121:A:LEU:HD13	1:121:A:LEU:HA	2	0.32
(1,1019)	1:84:A:MET:HE1	1:15:A:LYS:HD2	12	0.32
(1,1019)	1:84:A:MET:HE2	1:15:A:LYS:HD2	12	0.32
(1,1019)	1:84:A:MET:HE3	1:15:A:LYS:HD2	12	0.32
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE1	9	0.32
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE2	9	0.32
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE3	9	0.32
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB1	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB2	4	0.32
(1,974)	1:118:A:VAL:HG11	1:119:A:ALA:HB3	4	0.32
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB1	4	0.32
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB2	4	0.32
(1,974)	1:118:A:VAL:HG12	1:119:A:ALA:HB3	4	0.32
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB1	4	0.32
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB2	4	0.32
(1,974)	1:118:A:VAL:HG13	1:119:A:ALA:HB3	4	0.32
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE1	15	0.32
(1,953)	1:58:A:TYR:HA	1:57:A:TYR:HE2	15	0.32
(1,927)	1:23:A:LYS:HA	1:22:A:TYR:HB2	20	0.32
(1,911)	1:9:A:ALA:HB1	1:15:A:LYS:HD2	3	0.32
(1,911)	1:9:A:ALA:HB2	1:15:A:LYS:HD2	3	0.32
(1,911)	1:9:A:ALA:HB3	1:15:A:LYS:HD2	3	0.32
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	7	0.32
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	7	0.32
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	7	0.32
(1,731)	1:148:A:LEU:HD21	1:151:A:LYS:HE2	16	0.32
(1,731)	1:148:A:LEU:HD22	1:151:A:LYS:HE2	16	0.32
(1,731)	1:148:A:LEU:HD23	1:151:A:LYS:HE2	16	0.32
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG21	14	0.32
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG22	14	0.32
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG23	14	0.32
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	15	0.32
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	10	0.32
(1,588)	1:63:A:LYS:HG3	1:63:A:LYS:HB2	6	0.32
(1,583)	1:151:A:LYS:HG2	1:151:A:LYS:H	4	0.32
(1,557)	1:158:A:LYS:HE3	1:158:A:LYS:HG3	12	0.32
(1,557)	1:158:A:LYS:HE2	1:158:A:LYS:HG3	12	0.32
(1,552)	1:31:A:ASN:HD21	1:33:A:SER:HB2	1	0.32
(1,387)	1:86:A:ILE:HG21	1:76:A:PRO:HG3	8	0.32
(1,387)	1:86:A:ILE:HG22	1:76:A:PRO:HG3	8	0.32
(1,387)	1:86:A:ILE:HG23	1:76:A:PRO:HG3	8	0.32
(1,264)	1:85:A:LYS:HB3	1:86:A:ILE:H	4	0.32
(1,263)	1:86:A:ILE:H	1:85:A:LYS:HB2	18	0.32
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	20	0.32
(1,256)	1:86:A:ILE:H	1:81:A:MET:HG2	13	0.32
(1,251)	1:63:A:LYS:HB3	1:63:A:LYS:HE3	17	0.32
(1,225)	1:13:A:VAL:HG11	1:51:A:LYS:HB2	7	0.32
(1,225)	1:13:A:VAL:HG12	1:51:A:LYS:HB2	7	0.32
(1,225)	1:13:A:VAL:HG13	1:51:A:LYS:HB2	7	0.32
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	6	0.32
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	6	0.32
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	19	0.32
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	19	0.32
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	19	0.32
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	20	0.32
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	20	0.32
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	20	0.32
(1,196)	1:123:A:GLN:HB3	1:123:A:GLN:HG2	2	0.32
(1,196)	1:123:A:GLN:HB3	1:123:A:GLN:HG2	4	0.32
(1,196)	1:123:A:GLN:HB3	1:123:A:GLN:HG2	6	0.32
(1,196)	1:123:A:GLN:HB3	1:123:A:GLN:HG2	7	0.32
(1,196)	1:123:A:GLN:HB3	1:123:A:GLN:HG2	9	0.32
(1,196)	1:123:A:GLN:HB3	1:123:A:GLN:HG2	11	0.32
(1,196)	1:123:A:GLN:HB3	1:123:A:GLN:HG2	12	0.32
(1,196)	1:123:A:GLN:HB3	1:123:A:GLN:HG2	13	0.32
(1,196)	1:123:A:GLN:HB3	1:123:A:GLN:HG2	15	0.32
(1,196)	1:123:A:GLN:HB3	1:123:A:GLN:HG2	18	0.32
(1,194)	1:123:A:GLN:HG3	1:123:A:GLN:H	4	0.32
(1,183)	1:101:A:LYS:HB2	1:102:A:TYR:HA	7	0.32
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	4	0.32
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	6	0.32
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	11	0.32
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	17	0.32
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	19	0.32
(1,177)	1:137:A:GLU:HG3	1:137:A:GLU:HB3	20	0.32
(1,176)	1:137:A:GLU:HB3	1:137:A:GLU:HG2	18	0.32
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	1	0.32
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	2	0.32
(1,155)	1:103:A:GLU:HG3	1:103:A:GLU:HB3	18	0.32
(1,154)	1:103:A:GLU:HB3	1:103:A:GLU:HG2	1	0.32
(1,154)	1:103:A:GLU:HB3	1:103:A:GLU:HG2	3	0.32
(1,154)	1:103:A:GLU:HB3	1:103:A:GLU:HG2	6	0.32
(1,154)	1:103:A:GLU:HB3	1:103:A:GLU:HG2	9	0.32
(1,154)	1:103:A:GLU:HB3	1:103:A:GLU:HG2	10	0.32
(1,142)	1:88:A:GLU:HG3	1:89:A:LYS:H	17	0.32
(1,89)	1:47:A:ASP:H	1:47:A:ASP:HB2	1	0.32
(1,46)	1:46:A:LEU:HB2	1:47:A:ASP:HA	3	0.32
(1,27)	1:117:A:ARG:HD3	1:117:A:ARG:HB3	16	0.32
(1,27)	1:117:A:ARG:HD3	1:117:A:ARG:HB3	19	0.32
(1,26)	1:117:A:ARG:HB3	1:117:A:ARG:HD2	20	0.32
(1,9)	1:8:A:GLY:HA2	1:15:A:LYS:HE2	18	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:8:A:GLY:HA3	1:15:A:LYS:HE2	18	0.32
(1,5)	1:9:A:ALA:HB1	1:8:A:GLY:HA2	9	0.32
(1,5)	1:9:A:ALA:HB2	1:8:A:GLY:HA2	9	0.32
(1,5)	1:9:A:ALA:HB3	1:8:A:GLY:HA2	9	0.32
(1,2)	1:8:A:GLY:HA2	1:15:A:LYS:HD2	11	0.32
(1,2)	1:8:A:GLY:HA3	1:15:A:LYS:HD2	11	0.32
(1,1989)	1:156:A:HIS:HB3	1:156:A:HIS:HD2	7	0.31
(1,1989)	1:156:A:HIS:HB3	1:156:A:HIS:HD2	16	0.31
(1,1989)	1:156:A:HIS:HB3	1:156:A:HIS:HD2	18	0.31
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD1	13	0.31
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD2	13	0.31
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD1	14	0.31
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD2	14	0.31
(1,1756)	1:151:A:LYS:HB3	1:151:A:LYS:H	1	0.31
(1,1756)	1:151:A:LYS:HB3	1:151:A:LYS:H	15	0.31
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	5	0.31
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	8	0.31
(1,1725)	1:33:A:SER:H	1:33:A:SER:HB2	6	0.31
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	14	0.31
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	2	0.31
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	10	0.31
(1,1681)	1:64:A:ASP:H	1:63:A:LYS:HB2	4	0.31
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	8	0.31
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	5	0.31
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	8	0.31
(1,1581)	1:126:A:HIS:HB3	1:127:A:SER:H	5	0.31
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	4	0.31
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	10	0.31
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	13	0.31
(1,1529)	1:131:A:GLU:H	1:131:A:GLU:HB2	16	0.31
(1,1423)	1:121:A:LEU:H	1:121:A:LEU:HG	5	0.31
(1,1394)	1:21:A:PHE:H	1:20:A:ARG:HB2	19	0.31
(1,1386)	1:103:A:GLU:H	1:102:A:TYR:HB3	14	0.31
(1,1381)	1:158:A:LYS:H	1:158:A:LYS:HG3	3	0.31
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	9	0.31
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	9	0.31
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	9	0.31
(1,1161)	1:119:A:ALA:HA	1:122:A:LYS:HG2	1	0.31
(1,1161)	1:119:A:ALA:HA	1:122:A:LYS:HG2	15	0.31
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	14	0.31
(1,1125)	1:104:A:LYS:HA	1:104:A:LYS:HG2	11	0.31
(1,1111)	1:117:A:ARG:HD3	1:116:A:MET:HA	19	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1106)	1:104:A:LYS:HG3	1:103:A:GLU:HA	19	0.31
(1,1102)	1:158:A:LYS:HG2	1:158:A:LYS:HA	10	0.31
(1,1088)	1:81:A:MET:HE1	1:81:A:MET:HG2	6	0.31
(1,1088)	1:81:A:MET:HE2	1:81:A:MET:HG2	6	0.31
(1,1088)	1:81:A:MET:HE3	1:81:A:MET:HG2	6	0.31
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE1	17	0.31
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE2	17	0.31
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE3	17	0.31
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB1	18	0.31
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB2	18	0.31
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB3	18	0.31
(1,890)	1:65:A:ALA:HB1	1:64:A:ASP:HB2	11	0.31
(1,890)	1:65:A:ALA:HB2	1:64:A:ASP:HB2	11	0.31
(1,890)	1:65:A:ALA:HB3	1:64:A:ASP:HB2	11	0.31
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	20	0.31
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	20	0.31
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	20	0.31
(1,700)	1:71:A:SER:HA	1:71:A:SER:HB2	2	0.31
(1,700)	1:71:A:SER:HA	1:71:A:SER:HB2	5	0.31
(1,700)	1:71:A:SER:HA	1:71:A:SER:HB2	7	0.31
(1,700)	1:71:A:SER:HA	1:71:A:SER:HB2	11	0.31
(1,700)	1:71:A:SER:HA	1:71:A:SER:HB2	16	0.31
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG21	19	0.31
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG22	19	0.31
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG23	19	0.31
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	11	0.31
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	5	0.31
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	5	0.31
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	5	0.31
(1,642)	1:54:A:ARG:HD3	1:100:A:LEU:HD21	13	0.31
(1,642)	1:54:A:ARG:HD3	1:100:A:LEU:HD22	13	0.31
(1,642)	1:54:A:ARG:HD3	1:100:A:LEU:HD23	13	0.31
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD11	4	0.31
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD12	4	0.31
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD13	4	0.31
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD11	10	0.31
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD12	10	0.31
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD13	10	0.31
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD11	17	0.31
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD12	17	0.31
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD13	17	0.31
(1,550)	1:36:A:THR:HB	1:33:A:SER:HB2	13	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	20	0.31
(1,441)	1:113:A:LEU:HD21	1:146:A:GLN:HG3	5	0.31
(1,441)	1:113:A:LEU:HD22	1:146:A:GLN:HG3	5	0.31
(1,441)	1:113:A:LEU:HD23	1:146:A:GLN:HG3	5	0.31
(1,441)	1:113:A:LEU:HD21	1:146:A:GLN:HG3	9	0.31
(1,441)	1:113:A:LEU:HD22	1:146:A:GLN:HG3	9	0.31
(1,441)	1:113:A:LEU:HD23	1:146:A:GLN:HG3	9	0.31
(1,438)	1:6:A:ARG:HG3	1:6:A:ARG:HB3	12	0.31
(1,435)	1:7:A:PRO:HD2	1:6:A:ARG:HG2	6	0.31
(1,380)	1:81:A:MET:HG3	1:86:A:ILE:HG12	20	0.31
(1,263)	1:86:A:ILE:H	1:85:A:LYS:HB2	3	0.31
(1,251)	1:63:A:LYS:HB3	1:63:A:LYS:HE3	3	0.31
(1,251)	1:63:A:LYS:HB3	1:63:A:LYS:HE3	10	0.31
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	11	0.31
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	11	0.31
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	11	0.31
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD11	1	0.31
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD12	1	0.31
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD13	1	0.31
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	1	0.31
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	1	0.31
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	1	0.31
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	4	0.31
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	4	0.31
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	4	0.31
(1,196)	1:123:A:GLN:HB3	1:123:A:GLN:HG2	14	0.31
(1,194)	1:123:A:GLN:HG3	1:123:A:GLN:H	7	0.31
(1,155)	1:103:A:GLU:HG3	1:103:A:GLU:HB3	11	0.31
(1,155)	1:103:A:GLU:HG3	1:103:A:GLU:HB3	19	0.31
(1,154)	1:103:A:GLU:HB3	1:103:A:GLU:HG2	20	0.31
(1,18)	1:28:A:ARG:HA	1:28:A:ARG:HD2	15	0.31
(1,11)	1:8:A:GLY:HA3	1:15:A:LYS:HE3	13	0.31
(1,11)	1:8:A:GLY:HA3	1:15:A:LYS:HE3	19	0.31
(1,3)	1:15:A:LYS:HD3	1:8:A:GLY:HA2	20	0.31
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG11	7	0.3
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG12	7	0.3
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG13	7	0.3
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG11	7	0.3
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG12	7	0.3
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG13	7	0.3
(1,1972)	1:20:A:ARG:HB3	1:44:A:PHE:HZ	10	0.3
(1,1939)	1:55:A:LEU:HD21	1:17:A:PHE:HE1	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1939)	1:55:A:LEU:HD21	1:17:A:PHE:HE2	5	0.3
(1,1939)	1:55:A:LEU:HD22	1:17:A:PHE:HE1	5	0.3
(1,1939)	1:55:A:LEU:HD22	1:17:A:PHE:HE2	5	0.3
(1,1939)	1:55:A:LEU:HD23	1:17:A:PHE:HE1	5	0.3
(1,1939)	1:55:A:LEU:HD23	1:17:A:PHE:HE2	5	0.3
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	9	0.3
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	17	0.3
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	19	0.3
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	7	0.3
(1,1387)	1:103:A:GLU:H	1:103:A:GLU:HB2	7	0.3
(1,1387)	1:103:A:GLU:H	1:103:A:GLU:HB2	8	0.3
(1,1381)	1:158:A:LYS:H	1:158:A:LYS:HG3	5	0.3
(1,1379)	1:158:A:LYS:H	1:157:A:PRO:HB3	7	0.3
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	14	0.3
(1,1344)	1:104:A:LYS:H	1:103:A:GLU:HA	16	0.3
(1,1161)	1:119:A:ALA:HA	1:122:A:LYS:HG2	11	0.3
(1,1088)	1:81:A:MET:HE1	1:81:A:MET:HG2	7	0.3
(1,1088)	1:81:A:MET:HE2	1:81:A:MET:HG2	7	0.3
(1,1088)	1:81:A:MET:HE3	1:81:A:MET:HG2	7	0.3
(1,1088)	1:81:A:MET:HE1	1:81:A:MET:HG2	17	0.3
(1,1088)	1:81:A:MET:HE2	1:81:A:MET:HG2	17	0.3
(1,1088)	1:81:A:MET:HE3	1:81:A:MET:HG2	17	0.3
(1,997)	1:51:A:LYS:HA	1:51:A:LYS:HG2	8	0.3
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB1	15	0.3
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB2	15	0.3
(1,912)	1:15:A:LYS:HD3	1:9:A:ALA:HB3	15	0.3
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB1	16	0.3
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB2	16	0.3
(1,905)	1:19:A:ASN:HB3	1:83:A:ALA:HB3	16	0.3
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	20	0.3
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	20	0.3
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	20	0.3
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG11	9	0.3
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG12	9	0.3
(1,849)	1:121:A:LEU:HB3	1:118:A:VAL:HG13	9	0.3
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG11	8	0.3
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG12	8	0.3
(1,833)	1:101:A:LYS:H	1:13:A:VAL:HG13	8	0.3
(1,815)	1:38:A:GLU:HG3	1:38:A:GLU:HA	10	0.3
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	10	0.3
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	10	0.3
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,701)	1:71:A:SER:HB3	1:71:A:SER:HA	10	0.3
(1,700)	1:71:A:SER:HA	1:71:A:SER:HB2	1	0.3
(1,700)	1:71:A:SER:HA	1:71:A:SER:HB2	17	0.3
(1,700)	1:71:A:SER:HA	1:71:A:SER:HB2	18	0.3
(1,700)	1:71:A:SER:HA	1:71:A:SER:HB2	20	0.3
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG21	7	0.3
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG22	7	0.3
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG23	7	0.3
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG21	8	0.3
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG22	8	0.3
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG23	8	0.3
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG21	15	0.3
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG22	15	0.3
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG23	15	0.3
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	11	0.3
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	3	0.3
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	3	0.3
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	3	0.3
(1,591)	1:49:A:LYS:HE2	1:49:A:LYS:HG2	18	0.3
(1,591)	1:49:A:LYS:HE3	1:49:A:LYS:HG2	18	0.3
(1,585)	1:101:A:LYS:HG3	1:102:A:TYR:H	17	0.3
(1,584)	1:102:A:TYR:H	1:101:A:LYS:HG2	13	0.3
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD11	6	0.3
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD12	6	0.3
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD13	6	0.3
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD11	11	0.3
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD12	11	0.3
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD13	11	0.3
(1,484)	1:142:A:VAL:HG11	1:139:A:THR:HA	5	0.3
(1,484)	1:142:A:VAL:HG12	1:139:A:THR:HA	5	0.3
(1,484)	1:142:A:VAL:HG13	1:139:A:THR:HA	5	0.3
(1,435)	1:7:A:PRO:HD2	1:6:A:ARG:HG2	4	0.3
(1,418)	1:6:A:ARG:H	1:6:A:ARG:HG2	17	0.3
(1,379)	1:86:A:ILE:HG12	1:81:A:MET:HG2	16	0.3
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG21	14	0.3
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG22	14	0.3
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG23	14	0.3
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	12	0.3
(1,251)	1:63:A:LYS:HB3	1:63:A:LYS:HE3	18	0.3
(1,250)	1:63:A:LYS:HE3	1:63:A:LYS:HB2	3	0.3
(1,250)	1:63:A:LYS:HE3	1:63:A:LYS:HB2	10	0.3
(1,250)	1:63:A:LYS:HE3	1:63:A:LYS:HB2	17	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,248)	1:91:A:LYS:HB3	1:91:A:LYS:HD2	12	0.3
(1,248)	1:91:A:LYS:HB3	1:91:A:LYS:HD3	12	0.3
(1,243)	1:81:A:MET:HG3	1:85:A:LYS:HB2	5	0.3
(1,243)	1:81:A:MET:HG2	1:85:A:LYS:HB2	5	0.3
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD11	13	0.3
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD12	13	0.3
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD13	13	0.3
(1,232)	1:91:A:LYS:H	1:91:A:LYS:HB3	6	0.3
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	10	0.3
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	10	0.3
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	10	0.3
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	12	0.3
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	12	0.3
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	12	0.3
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD21	14	0.3
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD22	14	0.3
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD23	14	0.3
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD21	19	0.3
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD22	19	0.3
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD23	19	0.3
(1,194)	1:123:A:GLN:HG3	1:123:A:GLN:H	19	0.3
(1,174)	1:137:A:GLU:H	1:137:A:GLU:HG2	19	0.3
(1,155)	1:103:A:GLU:HG3	1:103:A:GLU:HB3	16	0.3
(1,154)	1:103:A:GLU:HB3	1:103:A:GLU:HG2	4	0.3
(1,95)	1:35:A:ASP:HB3	1:34:A:LEU:HB3	5	0.3
(1,95)	1:35:A:ASP:HB3	1:34:A:LEU:HB3	11	0.3
(1,89)	1:47:A:ASP:H	1:47:A:ASP:HB2	19	0.3
(1,89)	1:47:A:ASP:H	1:47:A:ASP:HB2	20	0.3
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE2	16	0.3
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE3	16	0.3
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE2	18	0.3
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE3	18	0.3
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB1	8	0.3
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB2	8	0.3
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB3	8	0.3
(1,1989)	1:156:A:HIS:HB3	1:156:A:HIS:HD2	5	0.29
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE1	8	0.29
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE2	8	0.29
(1,1915)	1:140:A:ASP:HB3	1:141:A:TYR:HD1	11	0.29
(1,1915)	1:140:A:ASP:HB3	1:141:A:TYR:HD2	11	0.29
(1,1879)	1:4:A:GLY:HA3	1:5:A:GLY:H	10	0.29
(1,1756)	1:151:A:LYS:HB3	1:151:A:LYS:H	2	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1756)	1:151:A:LYS:HB3	1:151:A:LYS:H	11	0.29
(1,1756)	1:151:A:LYS:HB3	1:151:A:LYS:H	20	0.29
(1,1725)	1:33:A:SER:H	1:33:A:SER:HB2	12	0.29
(1,1703)	1:152:A:TYR:H	1:151:A:LYS:HB2	6	0.29
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	9	0.29
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	4	0.29
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	4	0.29
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	4	0.29
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	9	0.29
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	18	0.29
(1,1628)	1:148:A:LEU:H	1:147:A:GLU:HG2	14	0.29
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	3	0.29
(1,1548)	1:130:A:GLU:H	1:128:A:TRP:HB3	5	0.29
(1,1548)	1:130:A:GLU:H	1:128:A:TRP:HB3	8	0.29
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	16	0.29
(1,1386)	1:103:A:GLU:H	1:102:A:TYR:HB3	13	0.29
(1,1385)	1:103:A:GLU:H	1:102:A:TYR:HA	2	0.29
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	6	0.29
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	8	0.29
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	15	0.29
(1,1357)	1:64:A:ASP:HB3	1:65:A:ALA:H	13	0.29
(1,1291)	1:107:A:ASP:HB3	1:108:A:LEU:H	5	0.29
(1,1227)	1:26:A:ILE:HD11	1:23:A:LYS:HA	4	0.29
(1,1227)	1:26:A:ILE:HD12	1:23:A:LYS:HA	4	0.29
(1,1227)	1:26:A:ILE:HD13	1:23:A:LYS:HA	4	0.29
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	6	0.29
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	6	0.29
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	6	0.29
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	2	0.29
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	20	0.29
(1,1088)	1:81:A:MET:HE1	1:81:A:MET:HG2	1	0.29
(1,1088)	1:81:A:MET:HE2	1:81:A:MET:HG2	1	0.29
(1,1088)	1:81:A:MET:HE3	1:81:A:MET:HG2	1	0.29
(1,1088)	1:81:A:MET:HE1	1:81:A:MET:HG2	8	0.29
(1,1088)	1:81:A:MET:HE2	1:81:A:MET:HG2	8	0.29
(1,1088)	1:81:A:MET:HE3	1:81:A:MET:HG2	8	0.29
(1,1088)	1:81:A:MET:HE1	1:81:A:MET:HG2	11	0.29
(1,1088)	1:81:A:MET:HE2	1:81:A:MET:HG2	11	0.29
(1,1088)	1:81:A:MET:HE3	1:81:A:MET:HG2	11	0.29
(1,1081)	1:42:A:ILE:HG12	1:42:A:ILE:HG21	10	0.29
(1,1081)	1:42:A:ILE:HG12	1:42:A:ILE:HG22	10	0.29
(1,1081)	1:42:A:ILE:HG12	1:42:A:ILE:HG23	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE1	7	0.29
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE2	7	0.29
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE3	7	0.29
(1,1017)	1:84:A:MET:HE1	1:15:A:LYS:HE2	5	0.29
(1,1017)	1:84:A:MET:HE2	1:15:A:LYS:HE2	5	0.29
(1,1017)	1:84:A:MET:HE3	1:15:A:LYS:HE2	5	0.29
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	15	0.29
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	20	0.29
(1,990)	1:37:A:ILE:HG21	1:77:A:MET:HB3	3	0.29
(1,990)	1:37:A:ILE:HG22	1:77:A:MET:HB3	3	0.29
(1,990)	1:37:A:ILE:HG23	1:77:A:MET:HB3	3	0.29
(1,963)	1:110:A:SER:HB3	1:110:A:SER:HA	20	0.29
(1,911)	1:9:A:ALA:HB1	1:15:A:LYS:HD2	17	0.29
(1,911)	1:9:A:ALA:HB2	1:15:A:LYS:HD2	17	0.29
(1,911)	1:9:A:ALA:HB3	1:15:A:LYS:HD2	17	0.29
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG11	11	0.29
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG12	11	0.29
(1,844)	1:122:A:LYS:HE2	1:118:A:VAL:HG13	11	0.29
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD2	20	0.29
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD2	20	0.29
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD2	20	0.29
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD3	20	0.29
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD3	20	0.29
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD3	20	0.29
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	15	0.29
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	19	0.29
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	19	0.29
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	19	0.29
(1,791)	1:95:A:SER:HA	1:91:A:LYS:HG3	19	0.29
(1,755)	1:127:A:SER:HB3	1:127:A:SER:HA	1	0.29
(1,755)	1:127:A:SER:HB3	1:127:A:SER:HA	2	0.29
(1,755)	1:127:A:SER:HB3	1:127:A:SER:HA	4	0.29
(1,755)	1:127:A:SER:HB3	1:127:A:SER:HA	6	0.29
(1,755)	1:127:A:SER:HB3	1:127:A:SER:HA	7	0.29
(1,755)	1:127:A:SER:HB3	1:127:A:SER:HA	9	0.29
(1,755)	1:127:A:SER:HB3	1:127:A:SER:HA	11	0.29
(1,755)	1:127:A:SER:HB3	1:127:A:SER:HA	15	0.29
(1,755)	1:127:A:SER:HB3	1:127:A:SER:HA	16	0.29
(1,755)	1:127:A:SER:HB3	1:127:A:SER:HA	19	0.29
(1,754)	1:127:A:SER:HA	1:127:A:SER:HB2	3	0.29
(1,754)	1:127:A:SER:HA	1:127:A:SER:HB2	12	0.29
(1,700)	1:71:A:SER:HA	1:71:A:SER:HB2	14	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,700)	1:71:A:SER:HA	1:71:A:SER:HB2	19	0.29
(1,687)	1:17:A:PHE:HA	1:20:A:ARG:HB2	1	0.29
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG21	1	0.29
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG22	1	0.29
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG23	1	0.29
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG21	3	0.29
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG22	3	0.29
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG23	3	0.29
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	14	0.29
(1,658)	1:8:A:GLY:HA3	1:7:A:PRO:HA	16	0.29
(1,655)	1:161:A:LEU:HA	1:161:A:LEU:HD11	3	0.29
(1,655)	1:161:A:LEU:HA	1:161:A:LEU:HD12	3	0.29
(1,655)	1:161:A:LEU:HA	1:161:A:LEU:HD13	3	0.29
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	17	0.29
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	17	0.29
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	17	0.29
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD21	3	0.29
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD22	3	0.29
(1,641)	1:73:A:VAL:HG11	1:59:A:LEU:HD23	3	0.29
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD21	3	0.29
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD22	3	0.29
(1,641)	1:73:A:VAL:HG12	1:59:A:LEU:HD23	3	0.29
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD21	3	0.29
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD22	3	0.29
(1,641)	1:73:A:VAL:HG13	1:59:A:LEU:HD23	3	0.29
(1,636)	1:26:A:ILE:HA	1:26:A:ILE:HG12	4	0.29
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD11	13	0.29
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD12	13	0.29
(1,570)	1:34:A:LEU:HB2	1:34:A:LEU:HD13	13	0.29
(1,545)	1:33:A:SER:HB3	1:34:A:LEU:H	2	0.29
(1,545)	1:33:A:SER:HB3	1:34:A:LEU:H	16	0.29
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	1	0.29
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	10	0.29
(1,333)	1:54:A:ARG:HB2	1:100:A:LEU:HD21	8	0.29
(1,333)	1:54:A:ARG:HB2	1:100:A:LEU:HD22	8	0.29
(1,333)	1:54:A:ARG:HB2	1:100:A:LEU:HD23	8	0.29
(1,324)	1:142:A:VAL:HG21	1:114:A:ARG:HB2	9	0.29
(1,324)	1:142:A:VAL:HG22	1:114:A:ARG:HB2	9	0.29
(1,324)	1:142:A:VAL:HG23	1:114:A:ARG:HB2	9	0.29
(1,324)	1:142:A:VAL:HG21	1:114:A:ARG:HB2	19	0.29
(1,324)	1:142:A:VAL:HG22	1:114:A:ARG:HB2	19	0.29
(1,324)	1:142:A:VAL:HG23	1:114:A:ARG:HB2	19	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,323)	1:114:A:ARG:HB3	1:115:A:LYS:H	7	0.29
(1,323)	1:114:A:ARG:HB3	1:115:A:LYS:H	9	0.29
(1,323)	1:114:A:ARG:HB3	1:115:A:LYS:H	10	0.29
(1,312)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	10	0.29
(1,280)	1:104:A:LYS:H	1:103:A:GLU:HB3	15	0.29
(1,264)	1:85:A:LYS:HB3	1:86:A:ILE:H	12	0.29
(1,251)	1:63:A:LYS:HB3	1:63:A:LYS:HE3	8	0.29
(1,232)	1:91:A:LYS:H	1:91:A:LYS:HB3	8	0.29
(1,155)	1:103:A:GLU:HG3	1:103:A:GLU:HB3	17	0.29
(1,142)	1:88:A:GLU:HG3	1:89:A:LYS:H	13	0.29
(1,95)	1:35:A:ASP:HB3	1:34:A:LEU:HB3	8	0.29
(1,84)	1:47:A:ASP:HB3	1:48:A:THR:HG21	1	0.29
(1,84)	1:47:A:ASP:HB3	1:48:A:THR:HG22	1	0.29
(1,84)	1:47:A:ASP:HB3	1:48:A:THR:HG23	1	0.29
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE2	8	0.29
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE3	8	0.29
(1,9)	1:8:A:GLY:HA2	1:15:A:LYS:HE2	14	0.29
(1,9)	1:8:A:GLY:HA3	1:15:A:LYS:HE2	14	0.29
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB1	18	0.29
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB2	18	0.29
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB3	18	0.29
(1,5)	1:9:A:ALA:HB1	1:8:A:GLY:HA2	13	0.29
(1,5)	1:9:A:ALA:HB2	1:8:A:GLY:HA2	13	0.29
(1,5)	1:9:A:ALA:HB3	1:8:A:GLY:HA2	13	0.29
(1,1951)	1:44:A:PHE:HE1	1:24:A:SER:HB3	12	0.28
(1,1951)	1:44:A:PHE:HE2	1:24:A:SER:HB3	12	0.28
(1,1771)	1:35:A:ASP:H	1:34:A:LEU:HB3	4	0.28
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	17	0.28
(1,1725)	1:33:A:SER:H	1:33:A:SER:HB2	1	0.28
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	12	0.28
(1,1682)	1:63:A:LYS:HB3	1:64:A:ASP:H	17	0.28
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	12	0.28
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	15	0.28
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	19	0.28
(1,1623)	1:77:A:MET:H	1:77:A:MET:HG2	3	0.28
(1,1581)	1:126:A:HIS:HB3	1:127:A:SER:H	7	0.28
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	3	0.28
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	12	0.28
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	18	0.28
(1,1529)	1:131:A:GLU:H	1:131:A:GLU:HB2	10	0.28
(1,1462)	1:107:A:ASP:HB3	1:109:A:ALA:H	7	0.28
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	1	0.28
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	8	0.28
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	15	0.28
(1,1379)	1:158:A:LYS:H	1:157:A:PRO:HB3	10	0.28
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	12	0.28
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	20	0.28
(1,1319)	1:8:A:GLY:HA3	1:9:A:ALA:H	18	0.28
(1,1161)	1:119:A:ALA:HA	1:122:A:LYS:HG2	19	0.28
(1,1147)	1:83:A:ALA:HA	1:86:A:ILE:HG12	13	0.28
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	1	0.28
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	12	0.28
(1,1102)	1:158:A:LYS:HG2	1:158:A:LYS:HA	11	0.28
(1,1088)	1:81:A:MET:HE1	1:81:A:MET:HG2	18	0.28
(1,1088)	1:81:A:MET:HE2	1:81:A:MET:HG2	18	0.28
(1,1088)	1:81:A:MET:HE3	1:81:A:MET:HG2	18	0.28
(1,1088)	1:81:A:MET:HE1	1:81:A:MET:HG2	19	0.28
(1,1088)	1:81:A:MET:HE2	1:81:A:MET:HG2	19	0.28
(1,1088)	1:81:A:MET:HE3	1:81:A:MET:HG2	19	0.28
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE1	7	0.28
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE2	7	0.28
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE3	7	0.28
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE1	8	0.28
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE2	8	0.28
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE3	8	0.28
(1,1059)	1:54:A:ARG:HA	1:57:A:TYR:HB2	4	0.28
(1,1047)	1:77:A:MET:HE1	1:22:A:TYR:HB3	11	0.28
(1,1047)	1:77:A:MET:HE2	1:22:A:TYR:HB3	11	0.28
(1,1047)	1:77:A:MET:HE3	1:22:A:TYR:HB3	11	0.28
(1,1047)	1:77:A:MET:HE1	1:22:A:TYR:HB3	14	0.28
(1,1047)	1:77:A:MET:HE2	1:22:A:TYR:HB3	14	0.28
(1,1047)	1:77:A:MET:HE3	1:22:A:TYR:HB3	14	0.28
(1,1017)	1:84:A:MET:HE1	1:15:A:LYS:HE2	8	0.28
(1,1017)	1:84:A:MET:HE2	1:15:A:LYS:HE2	8	0.28
(1,1017)	1:84:A:MET:HE3	1:15:A:LYS:HE2	8	0.28
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	7	0.28
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	19	0.28
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	9	0.28
(1,963)	1:110:A:SER:HB3	1:110:A:SER:HA	6	0.28
(1,963)	1:110:A:SER:HB3	1:110:A:SER:HA	17	0.28
(1,963)	1:110:A:SER:HB3	1:110:A:SER:HA	18	0.28
(1,959)	1:24:A:SER:HB3	1:21:A:PHE:HA	1	0.28
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	15	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	15	0.28
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	15	0.28
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	20	0.28
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	20	0.28
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	20	0.28
(1,927)	1:23:A:LYS:HA	1:22:A:TYR:HB2	6	0.28
(1,754)	1:127:A:SER:HA	1:127:A:SER:HB2	5	0.28
(1,754)	1:127:A:SER:HA	1:127:A:SER:HB2	8	0.28
(1,754)	1:127:A:SER:HA	1:127:A:SER:HB2	10	0.28
(1,754)	1:127:A:SER:HA	1:127:A:SER:HB2	13	0.28
(1,754)	1:127:A:SER:HA	1:127:A:SER:HB2	14	0.28
(1,754)	1:127:A:SER:HA	1:127:A:SER:HB2	17	0.28
(1,754)	1:127:A:SER:HA	1:127:A:SER:HB2	18	0.28
(1,754)	1:127:A:SER:HA	1:127:A:SER:HB2	20	0.28
(1,731)	1:148:A:LEU:HD21	1:151:A:LYS:HE2	18	0.28
(1,731)	1:148:A:LEU:HD22	1:151:A:LYS:HE2	18	0.28
(1,731)	1:148:A:LEU:HD23	1:151:A:LYS:HE2	18	0.28
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	20	0.28
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	20	0.28
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	20	0.28
(1,700)	1:71:A:SER:HA	1:71:A:SER:HB2	4	0.28
(1,687)	1:17:A:PHE:HA	1:20:A:ARG:HB2	16	0.28
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG21	9	0.28
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG22	9	0.28
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG23	9	0.28
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG21	16	0.28
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG22	16	0.28
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG23	16	0.28
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	5	0.28
(1,552)	1:31:A:ASN:HD21	1:33:A:SER:HB2	8	0.28
(1,545)	1:33:A:SER:HB3	1:34:A:LEU:H	10	0.28
(1,532)	1:92:A:LYS:HB3	1:92:A:LYS:HD3	19	0.28
(1,504)	1:54:A:ARG:H	1:54:A:ARG:HG3	7	0.28
(1,497)	1:93:A:LEU:HD11	1:90:A:LEU:HA	4	0.28
(1,497)	1:93:A:LEU:HD12	1:90:A:LEU:HA	4	0.28
(1,497)	1:93:A:LEU:HD13	1:90:A:LEU:HA	4	0.28
(1,336)	1:42:A:ILE:H	1:42:A:ILE:HG13	16	0.28
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	19	0.28
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG21	7	0.28
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG22	7	0.28
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG23	7	0.28
(1,312)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,311)	1:91:A:LYS:HD3	1:95:A:SER:HA	5	0.28
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	2	0.28
(1,264)	1:85:A:LYS:HB3	1:86:A:ILE:H	6	0.28
(1,264)	1:85:A:LYS:HB3	1:86:A:ILE:H	8	0.28
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	13	0.28
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	13	0.28
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	13	0.28
(1,183)	1:101:A:LYS:HB2	1:102:A:TYR:HA	6	0.28
(1,154)	1:103:A:GLU:HB3	1:103:A:GLU:HG2	8	0.28
(1,145)	1:85:A:LYS:HA	1:88:A:GLU:HG2	2	0.28
(1,30)	1:6:A:ARG:HA	1:6:A:ARG:HD2	8	0.28
(1,30)	1:6:A:ARG:HA	1:6:A:ARG:HD3	8	0.28
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB1	16	0.28
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB2	16	0.28
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB3	16	0.28
(1,9)	1:8:A:GLY:HA2	1:15:A:LYS:HE2	3	0.28
(1,9)	1:8:A:GLY:HA3	1:15:A:LYS:HE2	3	0.28
(1,5)	1:9:A:ALA:HB1	1:8:A:GLY:HA2	8	0.28
(1,5)	1:9:A:ALA:HB2	1:8:A:GLY:HA2	8	0.28
(1,5)	1:9:A:ALA:HB3	1:8:A:GLY:HA2	8	0.28
(1,5)	1:9:A:ALA:HB1	1:8:A:GLY:HA2	12	0.28
(1,5)	1:9:A:ALA:HB2	1:8:A:GLY:HA2	12	0.28
(1,5)	1:9:A:ALA:HB3	1:8:A:GLY:HA2	12	0.28
(1,2013)	1:151:A:LYS:HE3	1:152:A:TYR:HE1	18	0.27
(1,2013)	1:151:A:LYS:HE3	1:152:A:TYR:HE2	18	0.27
(1,2008)	1:64:A:ASP:HB3	1:57:A:TYR:HE1	2	0.27
(1,2008)	1:64:A:ASP:HB3	1:57:A:TYR:HE2	2	0.27
(1,1989)	1:156:A:HIS:HB3	1:156:A:HIS:HD2	1	0.27
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	8	0.27
(1,1836)	1:114:A:ARG:HD3	1:114:A:ARG:H	3	0.27
(1,1798)	1:42:A:ILE:HG13	1:43:A:SER:H	4	0.27
(1,1765)	1:101:A:LYS:HB3	1:100:A:LEU:H	2	0.27
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	19	0.27
(1,1703)	1:152:A:TYR:H	1:151:A:LYS:HB2	7	0.27
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	16	0.27
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	20	0.27
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	8	0.27
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	12	0.27
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	18	0.27
(1,1613)	1:40:A:GLU:H	1:39:A:LYS:HB3	9	0.27
(1,1581)	1:126:A:HIS:HB3	1:127:A:SER:H	4	0.27
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	2	0.27
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	5	0.27
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	8	0.27
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	20	0.27
(1,1529)	1:131:A:GLU:H	1:131:A:GLU:HB2	11	0.27
(1,1522)	1:131:A:GLU:H	1:130:A:GLU:HB3	15	0.27
(1,1387)	1:103:A:GLU:H	1:103:A:GLU:HB2	6	0.27
(1,1385)	1:103:A:GLU:H	1:102:A:TYR:HA	10	0.27
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	14	0.27
(1,1310)	1:107:A:ASP:HB3	1:107:A:ASP:H	19	0.27
(1,1308)	1:67:A:THR:HG21	1:66:A:ALA:H	5	0.27
(1,1308)	1:67:A:THR:HG22	1:66:A:ALA:H	5	0.27
(1,1308)	1:67:A:THR:HG23	1:66:A:ALA:H	5	0.27
(1,1291)	1:107:A:ASP:HB3	1:108:A:LEU:H	16	0.27
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	8	0.27
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	8	0.27
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	8	0.27
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	4	0.27
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	6	0.27
(1,1126)	1:104:A:LYS:HG3	1:104:A:LYS:HA	10	0.27
(1,1106)	1:104:A:LYS:HG3	1:103:A:GLU:HA	9	0.27
(1,1104)	1:103:A:GLU:HG3	1:103:A:GLU:HA	10	0.27
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE1	5	0.27
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE2	5	0.27
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE3	5	0.27
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE1	14	0.27
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE2	14	0.27
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE3	14	0.27
(1,1088)	1:81:A:MET:HE1	1:81:A:MET:HG2	20	0.27
(1,1088)	1:81:A:MET:HE2	1:81:A:MET:HG2	20	0.27
(1,1088)	1:81:A:MET:HE3	1:81:A:MET:HG2	20	0.27
(1,1047)	1:77:A:MET:HE1	1:22:A:TYR:HB3	10	0.27
(1,1047)	1:77:A:MET:HE2	1:22:A:TYR:HB3	10	0.27
(1,1047)	1:77:A:MET:HE3	1:22:A:TYR:HB3	10	0.27
(1,1047)	1:77:A:MET:HE1	1:22:A:TYR:HB3	18	0.27
(1,1047)	1:77:A:MET:HE2	1:22:A:TYR:HB3	18	0.27
(1,1047)	1:77:A:MET:HE3	1:22:A:TYR:HB3	18	0.27
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	8	0.27
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	11	0.27
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	18	0.27
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	12	0.27
(1,995)	1:63:A:LYS:HA	1:63:A:LYS:HG2	14	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:110:A:SER:HB3	1:110:A:SER:HA	2	0.27
(1,963)	1:110:A:SER:HB3	1:110:A:SER:HA	4	0.27
(1,963)	1:110:A:SER:HB3	1:110:A:SER:HA	8	0.27
(1,963)	1:110:A:SER:HB3	1:110:A:SER:HA	14	0.27
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	12	0.27
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	12	0.27
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	12	0.27
(1,936)	1:9:A:ALA:HB1	1:10:A:ASP:HB3	10	0.27
(1,936)	1:9:A:ALA:HB2	1:10:A:ASP:HB3	10	0.27
(1,936)	1:9:A:ALA:HB3	1:10:A:ASP:HB3	10	0.27
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	13	0.27
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	13	0.27
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	13	0.27
(1,815)	1:38:A:GLU:HG3	1:38:A:GLU:HA	6	0.27
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	14	0.27
(1,700)	1:71:A:SER:HA	1:71:A:SER:HB2	15	0.27
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	17	0.27
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	18	0.27
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	18	0.27
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	18	0.27
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	20	0.27
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	20	0.27
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	20	0.27
(1,605)	1:107:A:ASP:HB3	1:110:A:SER:HB3	6	0.27
(1,573)	1:106:A:LEU:HD21	1:108:A:LEU:HA	4	0.27
(1,573)	1:106:A:LEU:HD22	1:108:A:LEU:HA	4	0.27
(1,573)	1:106:A:LEU:HD23	1:108:A:LEU:HA	4	0.27
(1,550)	1:36:A:THR:HB	1:33:A:SER:HB2	1	0.27
(1,550)	1:36:A:THR:HB	1:33:A:SER:HB2	7	0.27
(1,550)	1:36:A:THR:HB	1:33:A:SER:HB2	12	0.27
(1,545)	1:33:A:SER:HB3	1:34:A:LEU:H	1	0.27
(1,545)	1:33:A:SER:HB3	1:34:A:LEU:H	12	0.27
(1,545)	1:33:A:SER:HB3	1:34:A:LEU:H	17	0.27
(1,439)	1:147:A:GLU:HG2	1:144:A:LEU:HG	1	0.27
(1,387)	1:86:A:ILE:HG21	1:76:A:PRO:HG3	4	0.27
(1,387)	1:86:A:ILE:HG22	1:76:A:PRO:HG3	4	0.27
(1,387)	1:86:A:ILE:HG23	1:76:A:PRO:HG3	4	0.27
(1,353)	1:139:A:THR:HB	1:137:A:GLU:HG2	9	0.27
(1,347)	1:54:A:ARG:HB2	1:55:A:LEU:HA	11	0.27
(1,336)	1:42:A:ILE:H	1:42:A:ILE:HG13	4	0.27
(1,336)	1:42:A:ILE:H	1:42:A:ILE:HG13	6	0.27
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	16	0.27
(1,323)	1:114:A:ARG:HB3	1:115:A:LYS:H	3	0.27
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	20	0.27
(1,299)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	3	0.27
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB2	16	0.27
(1,285)	1:160:A:GLU:HB3	1:161:A:LEU:HB3	16	0.27
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD21	9	0.27
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD22	9	0.27
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD23	9	0.27
(1,205)	1:158:A:LYS:HB2	1:158:A:LYS:HE2	11	0.27
(1,183)	1:101:A:LYS:HB2	1:102:A:TYR:HA	13	0.27
(1,174)	1:137:A:GLU:H	1:137:A:GLU:HG2	7	0.27
(1,163)	1:2:A:GLU:HA	1:2:A:GLU:HG2	7	0.27
(1,151)	1:103:A:GLU:H	1:103:A:GLU:HG2	12	0.27
(1,151)	1:103:A:GLU:H	1:103:A:GLU:HG3	12	0.27
(1,95)	1:35:A:ASP:HB3	1:34:A:LEU:HB3	14	0.27
(1,28)	1:117:A:ARG:HG3	1:117:A:ARG:HD2	3	0.27
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB1	18	0.27
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB2	18	0.27
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB3	18	0.27
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	15	0.26
(1,1878)	1:5:A:GLY:H	1:4:A:GLY:HA2	5	0.26
(1,1878)	1:5:A:GLY:H	1:4:A:GLY:HA2	8	0.26
(1,1806)	1:24:A:SER:H	1:23:A:LYS:HB2	13	0.26
(1,1798)	1:42:A:ILE:HG13	1:43:A:SER:H	16	0.26
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	16	0.26
(1,1677)	1:79:A:VAL:H	1:80:A:HIS:H	10	0.26
(1,1677)	1:79:A:VAL:H	1:80:A:HIS:H	14	0.26
(1,1677)	1:79:A:VAL:H	1:80:A:HIS:H	15	0.26
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	4	0.26
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	14	0.26
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	19	0.26
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	20	0.26
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	7	0.26
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	1	0.26
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	20	0.26
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	4	0.26
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	4	0.26
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	4	0.26
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	15	0.26
(1,1522)	1:131:A:GLU:H	1:130:A:GLU:HB3	2	0.26
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB2	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB3	2	0.26
(1,1423)	1:121:A:LEU:H	1:121:A:LEU:HG	17	0.26
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	15	0.26
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	19	0.26
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	1	0.26
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	16	0.26
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	17	0.26
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	18	0.26
(1,1328)	1:2:A:GLU:HB2	1:2:A:GLU:H	19	0.26
(1,1310)	1:107:A:ASP:HB3	1:107:A:ASP:H	3	0.26
(1,1245)	1:6:A:ARG:HD3	1:7:A:PRO:HD2	14	0.26
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	4	0.26
(1,1161)	1:119:A:ALA:HA	1:122:A:LYS:HG2	4	0.26
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	1	0.26
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	2	0.26
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	4	0.26
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	6	0.26
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	8	0.26
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	9	0.26
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	10	0.26
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	11	0.26
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	12	0.26
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	17	0.26
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	18	0.26
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	19	0.26
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	20	0.26
(1,1126)	1:104:A:LYS:HG3	1:104:A:LYS:HA	7	0.26
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	10	0.26
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE1	2	0.26
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE2	2	0.26
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE3	2	0.26
(1,1088)	1:81:A:MET:HE1	1:81:A:MET:HG2	13	0.26
(1,1088)	1:81:A:MET:HE2	1:81:A:MET:HG2	13	0.26
(1,1088)	1:81:A:MET:HE3	1:81:A:MET:HG2	13	0.26
(1,1088)	1:81:A:MET:HE1	1:81:A:MET:HG2	15	0.26
(1,1088)	1:81:A:MET:HE2	1:81:A:MET:HG2	15	0.26
(1,1088)	1:81:A:MET:HE3	1:81:A:MET:HG2	15	0.26
(1,1058)	1:54:A:ARG:HA	1:54:A:ARG:HD3	12	0.26
(1,1058)	1:54:A:ARG:HA	1:54:A:ARG:HD3	18	0.26
(1,1017)	1:84:A:MET:HE1	1:15:A:LYS:HE2	11	0.26
(1,1017)	1:84:A:MET:HE2	1:15:A:LYS:HE2	11	0.26
(1,1017)	1:84:A:MET:HE3	1:15:A:LYS:HE2	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	1	0.26
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	6	0.26
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	16	0.26
(1,963)	1:110:A:SER:HB3	1:110:A:SER:HA	5	0.26
(1,921)	1:89:A:LYS:HA	1:89:A:LYS:HB2	10	0.26
(1,921)	1:89:A:LYS:HA	1:89:A:LYS:HB2	17	0.26
(1,921)	1:89:A:LYS:HA	1:89:A:LYS:HB2	20	0.26
(1,887)	1:65:A:ALA:HB1	1:57:A:TYR:HE1	10	0.26
(1,887)	1:65:A:ALA:HB1	1:57:A:TYR:HE2	10	0.26
(1,887)	1:65:A:ALA:HB2	1:57:A:TYR:HE1	10	0.26
(1,887)	1:65:A:ALA:HB2	1:57:A:TYR:HE2	10	0.26
(1,887)	1:65:A:ALA:HB3	1:57:A:TYR:HE1	10	0.26
(1,887)	1:65:A:ALA:HB3	1:57:A:TYR:HE2	10	0.26
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB1	3	0.26
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB2	3	0.26
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB3	3	0.26
(1,750)	1:159:A:THR:HA	1:159:A:THR:HB	5	0.26
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	11	0.26
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	11	0.26
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	11	0.26
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	15	0.26
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	2	0.26
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	2	0.26
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	2	0.26
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	4	0.26
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	4	0.26
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	4	0.26
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	6	0.26
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	6	0.26
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	6	0.26
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	9	0.26
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	9	0.26
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	9	0.26
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	16	0.26
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	16	0.26
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	16	0.26
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	19	0.26
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	19	0.26
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	19	0.26
(1,611)	1:111:A:VAL:HA	1:110:A:SER:HB2	1	0.26
(1,602)	1:55:A:LEU:HD11	1:100:A:LEU:HG	5	0.26
(1,602)	1:55:A:LEU:HD12	1:100:A:LEU:HG	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,602)	1:55:A:LEU:HD13	1:100:A:LEU:HG	5	0.26
(1,584)	1:102:A:TYR:H	1:101:A:LYS:HG2	11	0.26
(1,566)	1:46:A:LEU:HD11	1:43:A:SER:HB3	8	0.26
(1,566)	1:46:A:LEU:HD12	1:43:A:SER:HB3	8	0.26
(1,566)	1:46:A:LEU:HD13	1:43:A:SER:HB3	8	0.26
(1,552)	1:31:A:ASN:HD21	1:33:A:SER:HB2	12	0.26
(1,550)	1:36:A:THR:HB	1:33:A:SER:HB2	9	0.26
(1,545)	1:33:A:SER:HB3	1:34:A:LEU:H	7	0.26
(1,545)	1:33:A:SER:HB3	1:34:A:LEU:H	18	0.26
(1,543)	1:35:A:ASP:H	1:33:A:SER:HB3	5	0.26
(1,532)	1:92:A:LYS:HB3	1:92:A:LYS:HD3	8	0.26
(1,504)	1:54:A:ARG:H	1:54:A:ARG:HG3	18	0.26
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	20	0.26
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG21	1	0.26
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG22	1	0.26
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG23	1	0.26
(1,313)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	5	0.26
(1,274)	1:73:A:VAL:HA	1:76:A:PRO:HB2	15	0.26
(1,259)	1:81:A:MET:HG3	1:81:A:MET:HA	3	0.26
(1,251)	1:63:A:LYS:HB3	1:63:A:LYS:HE3	5	0.26
(1,250)	1:63:A:LYS:HE3	1:63:A:LYS:HB2	5	0.26
(1,243)	1:81:A:MET:HG3	1:85:A:LYS:HB2	15	0.26
(1,243)	1:81:A:MET:HG2	1:85:A:LYS:HB2	15	0.26
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	2	0.26
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	2	0.26
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	2	0.26
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD21	15	0.26
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD22	15	0.26
(1,212)	1:68:A:LYS:HB2	1:70:A:LEU:HD23	15	0.26
(1,203)	1:158:A:LYS:HB3	1:158:A:LYS:HE2	19	0.26
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	13	0.26
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	13	0.26
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	13	0.26
(1,178)	1:136:A:ALA:HB1	1:137:A:GLU:HG2	11	0.26
(1,178)	1:136:A:ALA:HB2	1:137:A:GLU:HG2	11	0.26
(1,178)	1:136:A:ALA:HB3	1:137:A:GLU:HG2	11	0.26
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	10	0.26
(1,105)	1:31:A:ASN:HB3	1:32:A:PHE:H	16	0.26
(1,95)	1:35:A:ASP:HB3	1:34:A:LEU:HB3	19	0.26
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE2	17	0.26
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE3	17	0.26
(1,54)	1:151:A:LYS:HE2	1:151:A:LYS:HG3	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:151:A:LYS:HE3	1:151:A:LYS:HG3	7	0.26
(1,29)	1:117:A:ARG:HD3	1:117:A:ARG:HG3	1	0.26
(1,9)	1:8:A:GLY:HA2	1:15:A:LYS:HE2	1	0.26
(1,9)	1:8:A:GLY:HA3	1:15:A:LYS:HE2	1	0.26
(1,2)	1:8:A:GLY:HA2	1:15:A:LYS:HD2	6	0.26
(1,2)	1:8:A:GLY:HA3	1:15:A:LYS:HD2	6	0.26
(1,2008)	1:64:A:ASP:HB3	1:57:A:TYR:HE1	11	0.25
(1,2008)	1:64:A:ASP:HB3	1:57:A:TYR:HE2	11	0.25
(1,1987)	1:157:A:PRO:HD2	1:156:A:HIS:HD2	12	0.25
(1,1907)	1:64:A:ASP:HB3	1:57:A:TYR:HD1	2	0.25
(1,1907)	1:64:A:ASP:HB3	1:57:A:TYR:HD2	2	0.25
(1,1876)	1:49:A:LYS:HB3	1:50:A:GLY:H	9	0.25
(1,1838)	1:114:A:ARG:HB3	1:114:A:ARG:H	9	0.25
(1,1798)	1:42:A:ILE:HG13	1:43:A:SER:H	3	0.25
(1,1798)	1:42:A:ILE:HG13	1:43:A:SER:H	13	0.25
(1,1771)	1:35:A:ASP:H	1:34:A:LEU:HB3	2	0.25
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	13	0.25
(1,1725)	1:33:A:SER:H	1:33:A:SER:HB2	4	0.25
(1,1703)	1:152:A:TYR:H	1:151:A:LYS:HB2	13	0.25
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	3	0.25
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	18	0.25
(1,1656)	1:122:A:LYS:H	1:122:A:LYS:HG2	8	0.25
(1,1656)	1:122:A:LYS:H	1:122:A:LYS:HG2	19	0.25
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	1	0.25
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	17	0.25
(1,1613)	1:40:A:GLU:H	1:39:A:LYS:HB3	5	0.25
(1,1586)	1:143:A:ASN:HB3	1:142:A:VAL:H	18	0.25
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	6	0.25
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	13	0.25
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	17	0.25
(1,1423)	1:121:A:LEU:H	1:121:A:LEU:HG	15	0.25
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	5	0.25
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	9	0.25
(1,1387)	1:103:A:GLU:H	1:103:A:GLU:HB2	19	0.25
(1,1385)	1:103:A:GLU:H	1:102:A:TYR:HA	7	0.25
(1,1385)	1:103:A:GLU:H	1:102:A:TYR:HA	20	0.25
(1,1379)	1:158:A:LYS:H	1:157:A:PRO:HB3	20	0.25
(1,1370)	1:112:A:ASP:HB3	1:112:A:ASP:H	13	0.25
(1,1356)	1:65:A:ALA:H	1:64:A:ASP:HB2	11	0.25
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	18	0.25
(1,1278)	1:127:A:SER:HB3	1:128:A:TRP:HE1	14	0.25
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1232)	1:26:A:ILE:HD11	1:27:A:ASP:H	4	0.25
(1,1232)	1:26:A:ILE:HD12	1:27:A:ASP:H	4	0.25
(1,1232)	1:26:A:ILE:HD13	1:27:A:ASP:H	4	0.25
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	3	0.25
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	5	0.25
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	13	0.25
(1,1125)	1:104:A:LYS:HA	1:104:A:LYS:HG2	13	0.25
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	2	0.25
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	5	0.25
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE1	9	0.25
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE2	9	0.25
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE3	9	0.25
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE1	12	0.25
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE2	12	0.25
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE3	12	0.25
(1,1058)	1:54:A:ARG:HA	1:54:A:ARG:HD3	11	0.25
(1,1052)	1:92:A:LYS:HA	1:92:A:LYS:HB2	3	0.25
(1,1052)	1:92:A:LYS:HA	1:92:A:LYS:HB2	9	0.25
(1,1052)	1:92:A:LYS:HA	1:92:A:LYS:HB2	12	0.25
(1,1052)	1:92:A:LYS:HA	1:92:A:LYS:HB2	20	0.25
(1,1017)	1:84:A:MET:HE1	1:15:A:LYS:HE2	19	0.25
(1,1017)	1:84:A:MET:HE2	1:15:A:LYS:HE2	19	0.25
(1,1017)	1:84:A:MET:HE3	1:15:A:LYS:HE2	19	0.25
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	3	0.25
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	10	0.25
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	17	0.25
(1,963)	1:110:A:SER:HB3	1:110:A:SER:HA	10	0.25
(1,963)	1:110:A:SER:HB3	1:110:A:SER:HA	13	0.25
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	10	0.25
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	10	0.25
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	10	0.25
(1,943)	1:79:A:VAL:HG21	1:81:A:MET:H	3	0.25
(1,943)	1:79:A:VAL:HG22	1:81:A:MET:H	3	0.25
(1,943)	1:79:A:VAL:HG23	1:81:A:MET:H	3	0.25
(1,927)	1:23:A:LYS:HA	1:22:A:TYR:HB2	10	0.25
(1,921)	1:89:A:LYS:HA	1:89:A:LYS:HB2	8	0.25
(1,921)	1:89:A:LYS:HA	1:89:A:LYS:HB2	19	0.25
(1,911)	1:9:A:ALA:HB1	1:15:A:LYS:HD2	4	0.25
(1,911)	1:9:A:ALA:HB2	1:15:A:LYS:HD2	4	0.25
(1,911)	1:9:A:ALA:HB3	1:15:A:LYS:HD2	4	0.25
(1,887)	1:65:A:ALA:HB1	1:57:A:TYR:HE1	14	0.25
(1,887)	1:65:A:ALA:HB1	1:57:A:TYR:HE2	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,887)	1:65:A:ALA:HB2	1:57:A:TYR:HE1	14	0.25
(1,887)	1:65:A:ALA:HB2	1:57:A:TYR:HE2	14	0.25
(1,887)	1:65:A:ALA:HB3	1:57:A:TYR:HE1	14	0.25
(1,887)	1:65:A:ALA:HB3	1:57:A:TYR:HE2	14	0.25
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	6	0.25
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD11	7	0.25
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD12	7	0.25
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD13	7	0.25
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD11	7	0.25
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD12	7	0.25
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD13	7	0.25
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD11	7	0.25
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD12	7	0.25
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD13	7	0.25
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD11	11	0.25
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD12	11	0.25
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD13	11	0.25
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD11	11	0.25
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD12	11	0.25
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD13	11	0.25
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD11	11	0.25
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD12	11	0.25
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD13	11	0.25
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB1	15	0.25
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB2	15	0.25
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB3	15	0.25
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	8	0.25
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	8	0.25
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	8	0.25
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	17	0.25
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	17	0.25
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	17	0.25
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	19	0.25
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	19	0.25
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	19	0.25
(1,698)	1:71:A:SER:HB2	1:75:A:ARG:HD2	18	0.25
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG21	20	0.25
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG22	20	0.25
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG23	20	0.25
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	8	0.25
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	14	0.25
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	1	0.25
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	1	0.25
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	7	0.25
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	7	0.25
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	7	0.25
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	8	0.25
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	8	0.25
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	8	0.25
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	12	0.25
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	12	0.25
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	12	0.25
(1,582)	1:151:A:LYS:H	1:151:A:LYS:HG3	7	0.25
(1,568)	1:34:A:LEU:HD11	1:75:A:ARG:HD2	6	0.25
(1,568)	1:34:A:LEU:HD12	1:75:A:ARG:HD2	6	0.25
(1,568)	1:34:A:LEU:HD13	1:75:A:ARG:HD2	6	0.25
(1,552)	1:31:A:ASN:HD21	1:33:A:SER:HB2	7	0.25
(1,550)	1:36:A:THR:HB	1:33:A:SER:HB2	6	0.25
(1,550)	1:36:A:THR:HB	1:33:A:SER:HB2	16	0.25
(1,550)	1:36:A:THR:HB	1:33:A:SER:HB2	18	0.25
(1,545)	1:33:A:SER:HB3	1:34:A:LEU:H	9	0.25
(1,545)	1:33:A:SER:HB3	1:34:A:LEU:H	13	0.25
(1,531)	1:92:A:LYS:HD3	1:92:A:LYS:HB2	7	0.25
(1,504)	1:54:A:ARG:H	1:54:A:ARG:HG3	17	0.25
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	15	0.25
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	17	0.25
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG21	16	0.25
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG22	16	0.25
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG23	16	0.25
(1,324)	1:142:A:VAL:HG21	1:114:A:ARG:HB2	12	0.25
(1,324)	1:142:A:VAL:HG22	1:114:A:ARG:HB2	12	0.25
(1,324)	1:142:A:VAL:HG23	1:114:A:ARG:HB2	12	0.25
(1,312)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	11	0.25
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	16	0.25
(1,299)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	4	0.25
(1,252)	1:151:A:LYS:HB3	1:152:A:TYR:HD1	2	0.25
(1,252)	1:151:A:LYS:HB3	1:152:A:TYR:HD2	2	0.25
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD11	10	0.25
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD12	10	0.25
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD13	10	0.25
(1,199)	1:111:A:VAL:HB	1:111:A:VAL:H	17	0.25
(1,171)	1:137:A:GLU:HG3	1:140:A:ASP:H	18	0.25
(1,163)	1:2:A:GLU:HA	1:2:A:GLU:HG2	17	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,153)	1:103:A:GLU:HG3	1:104:A:LYS:H	19	0.25
(1,135)	1:74:A:THR:HG21	1:38:A:GLU:HG2	3	0.25
(1,135)	1:74:A:THR:HG22	1:38:A:GLU:HG2	3	0.25
(1,135)	1:74:A:THR:HG23	1:38:A:GLU:HG2	3	0.25
(1,95)	1:35:A:ASP:HB3	1:34:A:LEU:HB3	13	0.25
(1,86)	1:28:A:ARG:H	1:27:A:ASP:HB2	4	0.25
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE2	11	0.25
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE3	11	0.25
(1,29)	1:117:A:ARG:HD3	1:117:A:ARG:HG3	4	0.25
(1,29)	1:117:A:ARG:HD3	1:117:A:ARG:HG3	10	0.25
(1,28)	1:117:A:ARG:HG3	1:117:A:ARG:HD2	6	0.25
(1,28)	1:117:A:ARG:HG3	1:117:A:ARG:HD2	11	0.25
(1,28)	1:117:A:ARG:HG3	1:117:A:ARG:HD2	15	0.25
(1,28)	1:117:A:ARG:HG3	1:117:A:ARG:HD2	16	0.25
(1,28)	1:117:A:ARG:HG3	1:117:A:ARG:HD2	17	0.25
(1,19)	1:28:A:ARG:HD3	1:28:A:ARG:HA	19	0.25
(1,17)	1:20:A:ARG:HB3	1:20:A:ARG:HD2	14	0.25
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB1	4	0.25
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB2	4	0.25
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB3	4	0.25
(1,2)	1:8:A:GLY:HA2	1:15:A:LYS:HD2	13	0.25
(1,2)	1:8:A:GLY:HA3	1:15:A:LYS:HD2	13	0.25
(1,2013)	1:151:A:LYS:HE3	1:152:A:TYR:HE1	19	0.24
(1,2013)	1:151:A:LYS:HE3	1:152:A:TYR:HE2	19	0.24
(1,1989)	1:156:A:HIS:HB3	1:156:A:HIS:HD2	3	0.24
(1,1989)	1:156:A:HIS:HB3	1:156:A:HIS:HD2	8	0.24
(1,1989)	1:156:A:HIS:HB3	1:156:A:HIS:HD2	19	0.24
(1,1879)	1:4:A:GLY:HA3	1:5:A:GLY:H	4	0.24
(1,1771)	1:35:A:ASP:H	1:34:A:LEU:HB3	1	0.24
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	4	0.24
(1,1703)	1:152:A:TYR:H	1:151:A:LYS:HB2	12	0.24
(1,1699)	1:23:A:LYS:H	1:23:A:LYS:HB2	4	0.24
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	3	0.24
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	8	0.24
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	19	0.24
(1,1692)	1:64:A:ASP:H	1:64:A:ASP:HB2	11	0.24
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	17	0.24
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	20	0.24
(1,1656)	1:122:A:LYS:H	1:122:A:LYS:HG2	13	0.24
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	11	0.24
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	6	0.24
(1,1548)	1:130:A:GLU:H	1:128:A:TRP:HB3	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	9	0.24
(1,1423)	1:121:A:LEU:H	1:121:A:LEU:HG	8	0.24
(1,1423)	1:121:A:LEU:H	1:121:A:LEU:HG	18	0.24
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	6	0.24
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	13	0.24
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	20	0.24
(1,1387)	1:103:A:GLU:H	1:103:A:GLU:HB2	4	0.24
(1,1385)	1:103:A:GLU:H	1:102:A:TYR:HA	11	0.24
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	14	0.24
(1,1206)	1:108:A:LEU:H	1:107:A:ASP:HA	14	0.24
(1,1161)	1:119:A:ALA:HA	1:122:A:LYS:HG2	2	0.24
(1,1142)	1:143:A:ASN:HA	1:143:A:ASN:HB2	15	0.24
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	14	0.24
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	18	0.24
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	20	0.24
(1,1102)	1:158:A:LYS:HG2	1:158:A:LYS:HA	13	0.24
(1,1088)	1:81:A:MET:HE1	1:81:A:MET:HG2	4	0.24
(1,1088)	1:81:A:MET:HE2	1:81:A:MET:HG2	4	0.24
(1,1088)	1:81:A:MET:HE3	1:81:A:MET:HG2	4	0.24
(1,1056)	1:116:A:MET:HG3	1:113:A:LEU:HA	17	0.24
(1,1052)	1:92:A:LYS:HA	1:92:A:LYS:HB2	6	0.24
(1,927)	1:23:A:LYS:HA	1:22:A:TYR:HB2	5	0.24
(1,927)	1:23:A:LYS:HA	1:22:A:TYR:HB2	8	0.24
(1,921)	1:89:A:LYS:HA	1:89:A:LYS:HB2	9	0.24
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	4	0.24
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	4	0.24
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	4	0.24
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	18	0.24
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	18	0.24
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	18	0.24
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	20	0.24
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	20	0.24
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	20	0.24
(1,790)	1:95:A:SER:HA	1:91:A:LYS:HA	2	0.24
(1,790)	1:95:A:SER:HA	1:91:A:LYS:HA	4	0.24
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD11	18	0.24
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD12	18	0.24
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD13	18	0.24
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD11	18	0.24
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD12	18	0.24
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD13	18	0.24
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD11	18	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD12	18	0.24
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD13	18	0.24
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	3	0.24
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	3	0.24
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	3	0.24
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	7	0.24
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	7	0.24
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	7	0.24
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	10	0.24
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	10	0.24
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	10	0.24
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	15	0.24
(1,687)	1:17:A:PHE:HA	1:20:A:ARG:HB2	4	0.24
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG21	6	0.24
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG22	6	0.24
(1,667)	1:30:A:VAL:HG21	1:36:A:THR:HG23	6	0.24
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG21	6	0.24
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG22	6	0.24
(1,667)	1:30:A:VAL:HG22	1:36:A:THR:HG23	6	0.24
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG21	6	0.24
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG22	6	0.24
(1,667)	1:30:A:VAL:HG23	1:36:A:THR:HG23	6	0.24
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	2	0.24
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	13	0.24
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	10	0.24
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	10	0.24
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	10	0.24
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	11	0.24
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	11	0.24
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	11	0.24
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	13	0.24
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	13	0.24
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	13	0.24
(1,611)	1:111:A:VAL:HA	1:110:A:SER:HB2	3	0.24
(1,584)	1:102:A:TYR:H	1:101:A:LYS:HG2	15	0.24
(1,573)	1:106:A:LEU:HD21	1:108:A:LEU:HA	3	0.24
(1,573)	1:106:A:LEU:HD22	1:108:A:LEU:HA	3	0.24
(1,573)	1:106:A:LEU:HD23	1:108:A:LEU:HA	3	0.24
(1,550)	1:36:A:THR:HB	1:33:A:SER:HB2	2	0.24
(1,550)	1:36:A:THR:HB	1:33:A:SER:HB2	17	0.24
(1,510)	1:115:A:LYS:H	1:115:A:LYS:HG3	6	0.24
(1,510)	1:115:A:LYS:H	1:115:A:LYS:HG3	19	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,508)	1:92:A:LYS:H	1:92:A:LYS:HG2	2	0.24
(1,508)	1:92:A:LYS:H	1:92:A:LYS:HG3	2	0.24
(1,504)	1:54:A:ARG:H	1:54:A:ARG:HG3	8	0.24
(1,504)	1:54:A:ARG:H	1:54:A:ARG:HG3	9	0.24
(1,504)	1:54:A:ARG:H	1:54:A:ARG:HG3	13	0.24
(1,504)	1:54:A:ARG:H	1:54:A:ARG:HG3	19	0.24
(1,419)	1:6:A:ARG:HG3	1:6:A:ARG:H	11	0.24
(1,385)	1:121:A:LEU:HB3	1:118:A:VAL:HA	8	0.24
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	2	0.24
(1,336)	1:42:A:ILE:H	1:42:A:ILE:HG13	3	0.24
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	1	0.24
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	3	0.24
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	4	0.24
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	12	0.24
(1,324)	1:142:A:VAL:HG21	1:114:A:ARG:HB2	13	0.24
(1,324)	1:142:A:VAL:HG22	1:114:A:ARG:HB2	13	0.24
(1,324)	1:142:A:VAL:HG23	1:114:A:ARG:HB2	13	0.24
(1,323)	1:114:A:ARG:HB3	1:115:A:LYS:H	5	0.24
(1,312)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	15	0.24
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	19	0.24
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	14	0.24
(1,154)	1:103:A:GLU:HB3	1:103:A:GLU:HG2	14	0.24
(1,153)	1:103:A:GLU:HG3	1:104:A:LYS:H	17	0.24
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE2	1	0.24
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE3	1	0.24
(1,54)	1:151:A:LYS:HE2	1:151:A:LYS:HG3	6	0.24
(1,54)	1:151:A:LYS:HE3	1:151:A:LYS:HG3	6	0.24
(1,29)	1:117:A:ARG:HD3	1:117:A:ARG:HG3	5	0.24
(1,28)	1:117:A:ARG:HG3	1:117:A:ARG:HD2	19	0.24
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	17	0.24
(1,1989)	1:156:A:HIS:HB3	1:156:A:HIS:HD2	9	0.23
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD1	18	0.23
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD2	18	0.23
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE1	19	0.23
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE2	19	0.23
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE1	20	0.23
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE2	20	0.23
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	1	0.23
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	9	0.23
(1,1838)	1:114:A:ARG:HB3	1:114:A:ARG:H	1	0.23
(1,1825)	1:45:A:CYS:HB3	1:45:A:CYS:H	3	0.23
(1,1798)	1:42:A:ILE:HG13	1:43:A:SER:H	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1798)	1:42:A:ILE:HG13	1:43:A:SER:H	19	0.23
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	1	0.23
(1,1703)	1:152:A:TYR:H	1:151:A:LYS:HB2	5	0.23
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	1	0.23
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	2	0.23
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	19	0.23
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	1	0.23
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	13	0.23
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	10	0.23
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	13	0.23
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	16	0.23
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	2	0.23
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	4	0.23
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	17	0.23
(1,1586)	1:143:A:ASN:HB3	1:142:A:VAL:H	12	0.23
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	10	0.23
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	18	0.23
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	1	0.23
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	1	0.23
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	1	0.23
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	7	0.23
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	7	0.23
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	7	0.23
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	12	0.23
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	12	0.23
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	12	0.23
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	19	0.23
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	19	0.23
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	19	0.23
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	6	0.23
(1,1522)	1:131:A:GLU:H	1:130:A:GLU:HB3	3	0.23
(1,1473)	1:101:A:LYS:HB2	1:102:A:TYR:H	5	0.23
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	6	0.23
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	10	0.23
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	14	0.23
(1,1387)	1:103:A:GLU:H	1:103:A:GLU:HB2	11	0.23
(1,1385)	1:103:A:GLU:H	1:102:A:TYR:HA	8	0.23
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	3	0.23
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	5	0.23
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	10	0.23
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD11	15	0.23
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD12	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1194)	1:121:A:LEU:HB2	1:124:A:ILE:HD13	15	0.23
(1,1165)	1:117:A:ARG:HD3	1:117:A:ARG:HA	19	0.23
(1,1161)	1:119:A:ALA:HA	1:122:A:LYS:HG2	17	0.23
(1,1158)	1:101:A:LYS:HD3	1:101:A:LYS:HA	6	0.23
(1,1158)	1:101:A:LYS:HD3	1:101:A:LYS:HA	17	0.23
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	11	0.23
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	15	0.23
(1,1126)	1:104:A:LYS:HG3	1:104:A:LYS:HA	5	0.23
(1,1125)	1:104:A:LYS:HA	1:104:A:LYS:HG2	1	0.23
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	17	0.23
(1,1102)	1:158:A:LYS:HG2	1:158:A:LYS:HA	19	0.23
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE1	16	0.23
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE2	16	0.23
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE3	16	0.23
(1,1059)	1:54:A:ARG:HA	1:57:A:TYR:HB2	1	0.23
(1,1053)	1:92:A:LYS:HB3	1:92:A:LYS:HA	2	0.23
(1,1052)	1:92:A:LYS:HA	1:92:A:LYS:HB2	1	0.23
(1,1052)	1:92:A:LYS:HA	1:92:A:LYS:HB2	10	0.23
(1,1052)	1:92:A:LYS:HA	1:92:A:LYS:HB2	14	0.23
(1,1052)	1:92:A:LYS:HA	1:92:A:LYS:HB2	15	0.23
(1,1052)	1:92:A:LYS:HA	1:92:A:LYS:HB2	16	0.23
(1,1046)	1:18:A:LEU:HA	1:77:A:MET:HE1	3	0.23
(1,1046)	1:18:A:LEU:HA	1:77:A:MET:HE2	3	0.23
(1,1046)	1:18:A:LEU:HA	1:77:A:MET:HE3	3	0.23
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE1	4	0.23
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE2	4	0.23
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE3	4	0.23
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE1	6	0.23
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE2	6	0.23
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE3	6	0.23
(1,948)	1:79:A:VAL:HG21	1:81:A:MET:HB2	14	0.23
(1,948)	1:79:A:VAL:HG22	1:81:A:MET:HB2	14	0.23
(1,948)	1:79:A:VAL:HG23	1:81:A:MET:HB2	14	0.23
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	9	0.23
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	2	0.23
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	2	0.23
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	2	0.23
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	5	0.23
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	5	0.23
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	5	0.23
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	6	0.23
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	6	0.23
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	14	0.23
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	14	0.23
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	14	0.23
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	10	0.23
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	10	0.23
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	10	0.23
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	14	0.23
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	14	0.23
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	14	0.23
(1,787)	1:75:A:ARG:HD3	1:75:A:ARG:HA	20	0.23
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	4	0.23
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	4	0.23
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	4	0.23
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	5	0.23
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	5	0.23
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	5	0.23
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	13	0.23
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	13	0.23
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	13	0.23
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	16	0.23
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	16	0.23
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	16	0.23
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	4	0.23
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	15	0.23
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	15	0.23
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	15	0.23
(1,550)	1:36:A:THR:HB	1:33:A:SER:HB2	10	0.23
(1,535)	1:86:A:ILE:HA	1:89:A:LYS:HG2	10	0.23
(1,385)	1:121:A:LEU:HB3	1:118:A:VAL:HA	3	0.23
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	11	0.23
(1,353)	1:139:A:THR:HB	1:137:A:GLU:HG2	15	0.23
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	20	0.23
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	9	0.23
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	15	0.23
(1,262)	1:84:A:MET:H	1:85:A:LYS:HB2	3	0.23
(1,262)	1:84:A:MET:H	1:85:A:LYS:HB3	3	0.23
(1,251)	1:63:A:LYS:HB3	1:63:A:LYS:HE3	12	0.23
(1,245)	1:81:A:MET:HG3	1:85:A:LYS:HB3	12	0.23
(1,237)	1:148:A:LEU:HA	1:151:A:LYS:HB3	8	0.23
(1,217)	1:136:A:ALA:HB1	1:137:A:GLU:HB2	3	0.23
(1,217)	1:136:A:ALA:HB2	1:137:A:GLU:HB2	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,217)	1:136:A:ALA:HB3	1:137:A:GLU:HB2	3	0.23
(1,204)	1:158:A:LYS:HE3	1:158:A:LYS:HB3	11	0.23
(1,174)	1:137:A:GLU:H	1:137:A:GLU:HG2	5	0.23
(1,174)	1:137:A:GLU:H	1:137:A:GLU:HG2	18	0.23
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	4	0.23
(1,163)	1:2:A:GLU:HA	1:2:A:GLU:HG2	9	0.23
(1,147)	1:88:A:GLU:HG2	1:88:A:GLU:H	19	0.23
(1,145)	1:85:A:LYS:HA	1:88:A:GLU:HG2	15	0.23
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	11	0.23
(1,48)	1:86:A:ILE:HG21	1:89:A:LYS:HE3	10	0.23
(1,48)	1:86:A:ILE:HG22	1:89:A:LYS:HE3	10	0.23
(1,48)	1:86:A:ILE:HG23	1:89:A:LYS:HE3	10	0.23
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB1	4	0.23
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB2	4	0.23
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB3	4	0.23
(1,1989)	1:156:A:HIS:HB3	1:156:A:HIS:HD2	6	0.22
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	13	0.22
(1,1951)	1:44:A:PHE:HE1	1:24:A:SER:HB3	13	0.22
(1,1951)	1:44:A:PHE:HE2	1:24:A:SER:HB3	13	0.22
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE1	16	0.22
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE2	16	0.22
(1,1929)	1:83:A:ALA:HB1	1:22:A:TYR:HD1	3	0.22
(1,1929)	1:83:A:ALA:HB1	1:22:A:TYR:HD2	3	0.22
(1,1929)	1:83:A:ALA:HB2	1:22:A:TYR:HD1	3	0.22
(1,1929)	1:83:A:ALA:HB2	1:22:A:TYR:HD2	3	0.22
(1,1929)	1:83:A:ALA:HB3	1:22:A:TYR:HD1	3	0.22
(1,1929)	1:83:A:ALA:HB3	1:22:A:TYR:HD2	3	0.22
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	19	0.22
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	20	0.22
(1,1871)	1:8:A:GLY:H	1:7:A:PRO:HG3	4	0.22
(1,1835)	1:114:A:ARG:H	1:114:A:ARG:HD2	8	0.22
(1,1835)	1:114:A:ARG:H	1:114:A:ARG:HD2	15	0.22
(1,1825)	1:45:A:CYS:HB3	1:45:A:CYS:H	12	0.22
(1,1825)	1:45:A:CYS:HB3	1:45:A:CYS:H	15	0.22
(1,1825)	1:45:A:CYS:HB3	1:45:A:CYS:H	18	0.22
(1,1798)	1:42:A:ILE:HG13	1:43:A:SER:H	15	0.22
(1,1798)	1:42:A:ILE:HG13	1:43:A:SER:H	20	0.22
(1,1771)	1:35:A:ASP:H	1:34:A:LEU:HB3	5	0.22
(1,1771)	1:35:A:ASP:H	1:34:A:LEU:HB3	12	0.22
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	16	0.22
(1,1711)	1:143:A:ASN:H	1:146:A:GLN:HE22	12	0.22
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	6	0.22
(1,1677)	1:79:A:VAL:H	1:80:A:HIS:H	3	0.22
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	1	0.22
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	4	0.22
(1,1656)	1:122:A:LYS:H	1:122:A:LYS:HG2	20	0.22
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	3	0.22
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	4	0.22
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	16	0.22
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	16	0.22
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	16	0.22
(1,1548)	1:130:A:GLU:H	1:128:A:TRP:HB3	14	0.22
(1,1544)	1:119:A:ALA:H	1:118:A:VAL:HB	11	0.22
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB2	11	0.22
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB3	11	0.22
(1,1462)	1:107:A:ASP:HB3	1:109:A:ALA:H	15	0.22
(1,1423)	1:121:A:LEU:H	1:121:A:LEU:HG	9	0.22
(1,1423)	1:121:A:LEU:H	1:121:A:LEU:HG	14	0.22
(1,1423)	1:121:A:LEU:H	1:121:A:LEU:HG	20	0.22
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	2	0.22
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	18	0.22
(1,1402)	1:56:A:CYS:HB3	1:57:A:TYR:H	5	0.22
(1,1387)	1:103:A:GLU:H	1:103:A:GLU:HB2	9	0.22
(1,1385)	1:103:A:GLU:H	1:102:A:TYR:HA	4	0.22
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	2	0.22
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	12	0.22
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	2	0.22
(1,1235)	1:61:A:ALA:HA	1:42:A:ILE:HG13	10	0.22
(1,1230)	1:26:A:ILE:HD11	1:25:A:LEU:HB3	3	0.22
(1,1230)	1:26:A:ILE:HD12	1:25:A:LEU:HB3	3	0.22
(1,1230)	1:26:A:ILE:HD13	1:25:A:LEU:HB3	3	0.22
(1,1161)	1:119:A:ALA:HA	1:122:A:LYS:HG2	10	0.22
(1,1157)	1:101:A:LYS:HA	1:101:A:LYS:HD2	13	0.22
(1,1142)	1:143:A:ASN:HA	1:143:A:ASN:HB2	7	0.22
(1,1139)	1:145:A:ILE:HB	1:145:A:ILE:HD11	14	0.22
(1,1139)	1:145:A:ILE:HB	1:145:A:ILE:HD12	14	0.22
(1,1139)	1:145:A:ILE:HB	1:145:A:ILE:HD13	14	0.22
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	7	0.22
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	11	0.22
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	12	0.22
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	15	0.22
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	19	0.22
(1,1102)	1:158:A:LYS:HG2	1:158:A:LYS:HA	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE1	10	0.22
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE2	10	0.22
(1,1089)	1:81:A:MET:HG3	1:81:A:MET:HE3	10	0.22
(1,1052)	1:92:A:LYS:HA	1:92:A:LYS:HB2	4	0.22
(1,1052)	1:92:A:LYS:HA	1:92:A:LYS:HB2	5	0.22
(1,1052)	1:92:A:LYS:HA	1:92:A:LYS:HB2	8	0.22
(1,1052)	1:92:A:LYS:HA	1:92:A:LYS:HB2	13	0.22
(1,1052)	1:92:A:LYS:HA	1:92:A:LYS:HB2	18	0.22
(1,1052)	1:92:A:LYS:HA	1:92:A:LYS:HB2	19	0.22
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	19	0.22
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	19	0.22
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	19	0.22
(1,1001)	1:142:A:VAL:HG11	1:114:A:ARG:HA	10	0.22
(1,1001)	1:142:A:VAL:HG12	1:114:A:ARG:HA	10	0.22
(1,1001)	1:142:A:VAL:HG13	1:114:A:ARG:HA	10	0.22
(1,907)	1:18:A:LEU:HB3	1:83:A:ALA:HB1	14	0.22
(1,907)	1:18:A:LEU:HB3	1:83:A:ALA:HB2	14	0.22
(1,907)	1:18:A:LEU:HB3	1:83:A:ALA:HB3	14	0.22
(1,906)	1:82:A:PRO:HB3	1:83:A:ALA:HB1	13	0.22
(1,906)	1:82:A:PRO:HB3	1:83:A:ALA:HB2	13	0.22
(1,906)	1:82:A:PRO:HB3	1:83:A:ALA:HB3	13	0.22
(1,869)	1:13:A:VAL:HG21	1:55:A:LEU:HB2	7	0.22
(1,869)	1:13:A:VAL:HG22	1:55:A:LEU:HB2	7	0.22
(1,869)	1:13:A:VAL:HG23	1:55:A:LEU:HB2	7	0.22
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG11	2	0.22
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG12	2	0.22
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG13	2	0.22
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	13	0.22
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	13	0.22
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	13	0.22
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	3	0.22
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	3	0.22
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	3	0.22
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	8	0.22
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	8	0.22
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	8	0.22
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	10	0.22
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	10	0.22
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	10	0.22
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	15	0.22
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	15	0.22
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,797)	1:138:A:LYS:HA	1:138:A:LYS:HG2	5	0.22
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD11	19	0.22
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD12	19	0.22
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD13	19	0.22
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD11	19	0.22
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD12	19	0.22
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD13	19	0.22
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD11	19	0.22
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD12	19	0.22
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD13	19	0.22
(1,765)	1:155:A:THR:H	1:155:A:THR:HG21	2	0.22
(1,765)	1:155:A:THR:H	1:155:A:THR:HG22	2	0.22
(1,765)	1:155:A:THR:H	1:155:A:THR:HG23	2	0.22
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	6	0.22
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	6	0.22
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	6	0.22
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	12	0.22
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	12	0.22
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	12	0.22
(1,716)	1:148:A:LEU:HD21	1:147:A:GLU:HG2	7	0.22
(1,716)	1:148:A:LEU:HD22	1:147:A:GLU:HG2	7	0.22
(1,716)	1:148:A:LEU:HD23	1:147:A:GLU:HG2	7	0.22
(1,711)	1:139:A:THR:HG21	1:143:A:ASN:HB2	19	0.22
(1,711)	1:139:A:THR:HG22	1:143:A:ASN:HB2	19	0.22
(1,711)	1:139:A:THR:HG23	1:143:A:ASN:HB2	19	0.22
(1,585)	1:101:A:LYS:HG3	1:102:A:TYR:H	1	0.22
(1,568)	1:34:A:LEU:HD11	1:75:A:ARG:HD2	14	0.22
(1,568)	1:34:A:LEU:HD12	1:75:A:ARG:HD2	14	0.22
(1,568)	1:34:A:LEU:HD13	1:75:A:ARG:HD2	14	0.22
(1,545)	1:33:A:SER:HB3	1:34:A:LEU:H	6	0.22
(1,537)	1:70:A:LEU:HD21	1:68:A:LYS:HG2	17	0.22
(1,537)	1:70:A:LEU:HD22	1:68:A:LYS:HG2	17	0.22
(1,537)	1:70:A:LEU:HD23	1:68:A:LYS:HG2	17	0.22
(1,537)	1:70:A:LEU:HD21	1:68:A:LYS:HG3	17	0.22
(1,537)	1:70:A:LEU:HD22	1:68:A:LYS:HG3	17	0.22
(1,537)	1:70:A:LEU:HD23	1:68:A:LYS:HG3	17	0.22
(1,529)	1:92:A:LYS:H	1:92:A:LYS:HD2	11	0.22
(1,529)	1:92:A:LYS:H	1:92:A:LYS:HD3	11	0.22
(1,504)	1:54:A:ARG:H	1:54:A:ARG:HG3	5	0.22
(1,489)	1:108:A:LEU:HD11	1:146:A:GLN:HG2	12	0.22
(1,489)	1:108:A:LEU:HD12	1:146:A:GLN:HG2	12	0.22
(1,489)	1:108:A:LEU:HD13	1:146:A:GLN:HG2	12	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:7:A:PRO:HD2	1:6:A:ARG:HG2	7	0.22
(1,385)	1:121:A:LEU:HB3	1:118:A:VAL:HA	16	0.22
(1,341)	1:104:A:LYS:H	1:104:A:LYS:HD2	18	0.22
(1,341)	1:104:A:LYS:H	1:104:A:LYS:HD3	18	0.22
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD2	20	0.22
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD3	20	0.22
(1,336)	1:42:A:ILE:H	1:42:A:ILE:HG13	19	0.22
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	10	0.22
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	13	0.22
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	3	0.22
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	4	0.22
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	5	0.22
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	10	0.22
(1,323)	1:114:A:ARG:HB3	1:115:A:LYS:H	15	0.22
(1,312)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	14	0.22
(1,300)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	15	0.22
(1,297)	1:99:A:GLU:HG3	1:99:A:GLU:HB2	5	0.22
(1,297)	1:99:A:GLU:HG3	1:99:A:GLU:HB2	9	0.22
(1,287)	1:161:A:LEU:H	1:160:A:GLU:HB2	5	0.22
(1,264)	1:85:A:LYS:HB3	1:86:A:ILE:H	1	0.22
(1,256)	1:86:A:ILE:H	1:81:A:MET:HG2	1	0.22
(1,251)	1:63:A:LYS:HB3	1:63:A:LYS:HE3	11	0.22
(1,251)	1:63:A:LYS:HB3	1:63:A:LYS:HE3	14	0.22
(1,196)	1:123:A:GLN:HB3	1:123:A:GLN:HG2	8	0.22
(1,171)	1:137:A:GLU:HG3	1:140:A:ASP:H	5	0.22
(1,165)	1:147:A:GLU:HG2	1:147:A:GLU:HA	9	0.22
(1,152)	1:104:A:LYS:H	1:103:A:GLU:HG2	9	0.22
(1,122)	1:94:A:ASP:HB3	1:97:A:ILE:HB	9	0.22
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG21	2	0.22
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG22	2	0.22
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG23	2	0.22
(1,105)	1:31:A:ASN:HB3	1:32:A:PHE:H	10	0.22
(1,86)	1:28:A:ARG:H	1:27:A:ASP:HB2	2	0.22
(1,86)	1:28:A:ARG:H	1:27:A:ASP:HB2	6	0.22
(1,86)	1:28:A:ARG:H	1:27:A:ASP:HB2	14	0.22
(1,61)	1:122:A:LYS:HE3	1:141:A:TYR:HE1	16	0.22
(1,61)	1:122:A:LYS:HE3	1:141:A:TYR:HE2	16	0.22
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE2	19	0.22
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE3	19	0.22
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	8	0.22
(1,46)	1:46:A:LEU:HB2	1:47:A:ASP:HA	10	0.22
(1,26)	1:117:A:ARG:HB3	1:117:A:ARG:HD2	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:114:A:ARG:HB3	1:114:A:ARG:HD3	13	0.22
(1,22)	1:114:A:ARG:HB3	1:114:A:ARG:HD2	13	0.22
(1,1968)	1:44:A:PHE:HZ	1:20:A:ARG:HE	12	0.21
(1,1899)	1:69:A:ILE:HG12	1:60:A:GLY:H	14	0.21
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	6	0.21
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	12	0.21
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	14	0.21
(1,1876)	1:49:A:LYS:HB3	1:50:A:GLY:H	5	0.21
(1,1871)	1:8:A:GLY:H	1:7:A:PRO:HG3	16	0.21
(1,1838)	1:114:A:ARG:HB3	1:114:A:ARG:H	8	0.21
(1,1835)	1:114:A:ARG:H	1:114:A:ARG:HD2	5	0.21
(1,1825)	1:45:A:CYS:HB3	1:45:A:CYS:H	2	0.21
(1,1825)	1:45:A:CYS:HB3	1:45:A:CYS:H	4	0.21
(1,1825)	1:45:A:CYS:HB3	1:45:A:CYS:H	7	0.21
(1,1825)	1:45:A:CYS:HB3	1:45:A:CYS:H	13	0.21
(1,1825)	1:45:A:CYS:HB3	1:45:A:CYS:H	17	0.21
(1,1825)	1:45:A:CYS:HB3	1:45:A:CYS:H	20	0.21
(1,1798)	1:42:A:ILE:HG13	1:43:A:SER:H	7	0.21
(1,1771)	1:35:A:ASP:H	1:34:A:LEU:HB3	7	0.21
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	5	0.21
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	8	0.21
(1,1725)	1:33:A:SER:H	1:33:A:SER:HB2	16	0.21
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	18	0.21
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	16	0.21
(1,1645)	1:86:A:ILE:HG21	1:87:A:CYS:H	3	0.21
(1,1645)	1:86:A:ILE:HG22	1:87:A:CYS:H	3	0.21
(1,1645)	1:86:A:ILE:HG23	1:87:A:CYS:H	3	0.21
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	2	0.21
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	12	0.21
(1,1613)	1:40:A:GLU:H	1:39:A:LYS:HB3	18	0.21
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	15	0.21
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	15	0.21
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	15	0.21
(1,1566)	1:117:A:ARG:H	1:117:A:ARG:HG3	16	0.21
(1,1527)	1:116:A:MET:H	1:115:A:LYS:HB2	5	0.21
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	14	0.21
(1,1423)	1:121:A:LEU:H	1:121:A:LEU:HG	12	0.21
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	4	0.21
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	7	0.21
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	12	0.21
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	13	0.21
(1,1359)	1:63:A:LYS:HB3	1:65:A:ALA:H	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	1	0.21
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	11	0.21
(1,1275)	1:2:A:GLU:H	1:3:A:ALA:H	1	0.21
(1,1275)	1:2:A:GLU:H	1:3:A:ALA:H	15	0.21
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	14	0.21
(1,1161)	1:119:A:ALA:HA	1:122:A:LYS:HG2	3	0.21
(1,1142)	1:143:A:ASN:HA	1:143:A:ASN:HB2	14	0.21
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	3	0.21
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	8	0.21
(1,1106)	1:104:A:LYS:HG3	1:103:A:GLU:HA	12	0.21
(1,1104)	1:103:A:GLU:HG3	1:103:A:GLU:HA	17	0.21
(1,1102)	1:158:A:LYS:HG2	1:158:A:LYS:HA	8	0.21
(1,994)	1:63:A:LYS:HB3	1:63:A:LYS:HA	4	0.21
(1,993)	1:63:A:LYS:HA	1:63:A:LYS:HB2	2	0.21
(1,952)	1:126:A:HIS:HB3	1:126:A:HIS:HA	1	0.21
(1,952)	1:126:A:HIS:HB3	1:126:A:HIS:HA	8	0.21
(1,952)	1:126:A:HIS:HB3	1:126:A:HIS:HA	10	0.21
(1,952)	1:126:A:HIS:HB3	1:126:A:HIS:HA	13	0.21
(1,952)	1:126:A:HIS:HB3	1:126:A:HIS:HA	14	0.21
(1,952)	1:126:A:HIS:HB3	1:126:A:HIS:HA	16	0.21
(1,952)	1:126:A:HIS:HB3	1:126:A:HIS:HA	18	0.21
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	3	0.21
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	7	0.21
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	17	0.21
(1,927)	1:23:A:LYS:HA	1:22:A:TYR:HB2	7	0.21
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD2	9	0.21
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD2	9	0.21
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD2	9	0.21
(1,835)	1:13:A:VAL:HG11	1:51:A:LYS:HD3	9	0.21
(1,835)	1:13:A:VAL:HG12	1:51:A:LYS:HD3	9	0.21
(1,835)	1:13:A:VAL:HG13	1:51:A:LYS:HD3	9	0.21
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	3	0.21
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	9	0.21
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	9	0.21
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	9	0.21
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	13	0.21
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	13	0.21
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	13	0.21
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	16	0.21
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	16	0.21
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	16	0.21
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	19	0.21
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	19	0.21
(1,797)	1:138:A:LYS:HA	1:138:A:LYS:HG2	1	0.21
(1,797)	1:138:A:LYS:HA	1:138:A:LYS:HG2	10	0.21
(1,797)	1:138:A:LYS:HA	1:138:A:LYS:HG2	14	0.21
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD11	5	0.21
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD12	5	0.21
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD13	5	0.21
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD11	5	0.21
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD12	5	0.21
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD13	5	0.21
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD11	5	0.21
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD12	5	0.21
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD13	5	0.21
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD11	6	0.21
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD12	6	0.21
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD13	6	0.21
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD11	6	0.21
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD12	6	0.21
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD13	6	0.21
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD11	6	0.21
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD12	6	0.21
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD13	6	0.21
(1,762)	1:105:A:THR:H	1:105:A:THR:HG21	10	0.21
(1,762)	1:105:A:THR:H	1:105:A:THR:HG22	10	0.21
(1,762)	1:105:A:THR:H	1:105:A:THR:HG23	10	0.21
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB1	20	0.21
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB2	20	0.21
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB3	20	0.21
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	1	0.21
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	1	0.21
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	1	0.21
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	9	0.21
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	9	0.21
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	9	0.21
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	11	0.21
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	11	0.21
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	11	0.21
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	14	0.21
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	14	0.21
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	14	0.21
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	18	0.21
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	18	0.21
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	9	0.21
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG21	6	0.21
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG22	6	0.21
(1,665)	1:31:A:ASN:HB2	1:36:A:THR:HG23	6	0.21
(1,649)	1:118:A:VAL:HG21	1:118:A:VAL:HA	14	0.21
(1,649)	1:118:A:VAL:HG22	1:118:A:VAL:HA	14	0.21
(1,649)	1:118:A:VAL:HG23	1:118:A:VAL:HA	14	0.21
(1,611)	1:111:A:VAL:HA	1:110:A:SER:HB2	19	0.21
(1,592)	1:49:A:LYS:HG3	1:49:A:LYS:HE2	19	0.21
(1,592)	1:49:A:LYS:HG3	1:49:A:LYS:HE3	19	0.21
(1,591)	1:49:A:LYS:HE2	1:49:A:LYS:HG2	20	0.21
(1,591)	1:49:A:LYS:HE3	1:49:A:LYS:HG2	20	0.21
(1,583)	1:151:A:LYS:HG2	1:151:A:LYS:H	13	0.21
(1,568)	1:34:A:LEU:HD11	1:75:A:ARG:HD2	12	0.21
(1,568)	1:34:A:LEU:HD12	1:75:A:ARG:HD2	12	0.21
(1,568)	1:34:A:LEU:HD13	1:75:A:ARG:HD2	12	0.21
(1,568)	1:34:A:LEU:HD11	1:75:A:ARG:HD2	15	0.21
(1,568)	1:34:A:LEU:HD12	1:75:A:ARG:HD2	15	0.21
(1,568)	1:34:A:LEU:HD13	1:75:A:ARG:HD2	15	0.21
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD11	2	0.21
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD12	2	0.21
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD13	2	0.21
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD11	5	0.21
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD12	5	0.21
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD13	5	0.21
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD11	12	0.21
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD12	12	0.21
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD13	12	0.21
(1,566)	1:46:A:LEU:HD11	1:43:A:SER:HB3	6	0.21
(1,566)	1:46:A:LEU:HD12	1:43:A:SER:HB3	6	0.21
(1,566)	1:46:A:LEU:HD13	1:43:A:SER:HB3	6	0.21
(1,552)	1:31:A:ASN:HD21	1:33:A:SER:HB2	20	0.21
(1,550)	1:36:A:THR:HB	1:33:A:SER:HB2	4	0.21
(1,504)	1:54:A:ARG:H	1:54:A:ARG:HG3	16	0.21
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	2	0.21
(1,395)	1:118:A:VAL:HA	1:122:A:LYS:HG2	14	0.21
(1,387)	1:86:A:ILE:HG21	1:76:A:PRO:HG3	19	0.21
(1,387)	1:86:A:ILE:HG22	1:76:A:PRO:HG3	19	0.21
(1,387)	1:86:A:ILE:HG23	1:76:A:PRO:HG3	19	0.21
(1,385)	1:121:A:LEU:HB3	1:118:A:VAL:HA	17	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD2	8	0.21
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD3	8	0.21
(1,336)	1:42:A:ILE:H	1:42:A:ILE:HG13	5	0.21
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	5	0.21
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	1	0.21
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	7	0.21
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	8	0.21
(1,300)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	1	0.21
(1,297)	1:99:A:GLU:HG3	1:99:A:GLU:HB2	7	0.21
(1,297)	1:99:A:GLU:HG3	1:99:A:GLU:HB2	20	0.21
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	18	0.21
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	18	0.21
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	18	0.21
(1,163)	1:2:A:GLU:HA	1:2:A:GLU:HG2	4	0.21
(1,163)	1:2:A:GLU:HA	1:2:A:GLU:HG2	18	0.21
(1,86)	1:28:A:ARG:H	1:27:A:ASP:HB2	3	0.21
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE2	10	0.21
(1,55)	1:151:A:LYS:HG2	1:151:A:LYS:HE3	10	0.21
(1,46)	1:46:A:LEU:HB2	1:47:A:ASP:HA	19	0.21
(1,19)	1:28:A:ARG:HD3	1:28:A:ARG:HA	7	0.21
(1,17)	1:20:A:ARG:HB3	1:20:A:ARG:HD2	18	0.21
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG11	13	0.2
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG12	13	0.2
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG13	13	0.2
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG11	13	0.2
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG12	13	0.2
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG13	13	0.2
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE1	12	0.2
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE2	12	0.2
(1,1935)	1:58:A:TYR:H	1:58:A:TYR:HD1	5	0.2
(1,1935)	1:58:A:TYR:H	1:58:A:TYR:HD2	5	0.2
(1,1901)	1:103:A:GLU:H	1:102:A:TYR:HD1	3	0.2
(1,1901)	1:103:A:GLU:H	1:102:A:TYR:HD2	3	0.2
(1,1876)	1:49:A:LYS:HB3	1:50:A:GLY:H	1	0.2
(1,1835)	1:114:A:ARG:H	1:114:A:ARG:HD2	3	0.2
(1,1835)	1:114:A:ARG:H	1:114:A:ARG:HD2	4	0.2
(1,1835)	1:114:A:ARG:H	1:114:A:ARG:HD2	10	0.2
(1,1825)	1:45:A:CYS:HB3	1:45:A:CYS:H	11	0.2
(1,1825)	1:45:A:CYS:HB3	1:45:A:CYS:H	14	0.2
(1,1815)	1:33:A:SER:HB2	1:31:A:ASN:HD22	8	0.2
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	10	0.2
(1,1756)	1:151:A:LYS:HB3	1:151:A:LYS:H	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1703)	1:152:A:TYR:H	1:151:A:LYS:HB2	3	0.2
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	2	0.2
(1,1669)	1:93:A:LEU:HB3	1:94:A:ASP:H	20	0.2
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	11	0.2
(1,1656)	1:122:A:LYS:H	1:122:A:LYS:HG2	16	0.2
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	5	0.2
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	11	0.2
(1,1613)	1:40:A:GLU:H	1:39:A:LYS:HB3	14	0.2
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	7	0.2
(1,1581)	1:126:A:HIS:HB3	1:127:A:SER:H	2	0.2
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	9	0.2
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	9	0.2
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	9	0.2
(1,1548)	1:130:A:GLU:H	1:128:A:TRP:HB3	6	0.2
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	4	0.2
(1,1527)	1:116:A:MET:H	1:115:A:LYS:HB2	1	0.2
(1,1527)	1:116:A:MET:H	1:115:A:LYS:HB2	10	0.2
(1,1527)	1:116:A:MET:H	1:115:A:LYS:HB2	18	0.2
(1,1499)	1:90:A:LEU:H	1:86:A:ILE:HA	4	0.2
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	5	0.2
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	10	0.2
(1,1450)	1:96:A:GLN:H	1:94:A:ASP:HB2	3	0.2
(1,1438)	1:96:A:GLN:H	1:94:A:ASP:HA	5	0.2
(1,1423)	1:121:A:LEU:H	1:121:A:LEU:HG	11	0.2
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	13	0.2
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	11	0.2
(1,1386)	1:103:A:GLU:H	1:102:A:TYR:HB3	6	0.2
(1,1385)	1:103:A:GLU:H	1:102:A:TYR:HA	15	0.2
(1,1318)	1:9:A:ALA:H	1:8:A:GLY:HA2	14	0.2
(1,1291)	1:107:A:ASP:HB3	1:108:A:LEU:H	7	0.2
(1,1291)	1:107:A:ASP:HB3	1:108:A:LEU:H	15	0.2
(1,1275)	1:2:A:GLU:H	1:3:A:ALA:H	3	0.2
(1,1164)	1:117:A:ARG:HA	1:117:A:ARG:HD2	15	0.2
(1,1126)	1:104:A:LYS:HG3	1:104:A:LYS:HA	2	0.2
(1,1125)	1:104:A:LYS:HA	1:104:A:LYS:HG2	16	0.2
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	9	0.2
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	9	0.2
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	9	0.2
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	9	0.2
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	9	0.2
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	9	0.2
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	9	0.2
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	9	0.2
(1,1102)	1:158:A:LYS:HG2	1:158:A:LYS:HA	6	0.2
(1,1102)	1:158:A:LYS:HG2	1:158:A:LYS:HA	14	0.2
(1,1102)	1:158:A:LYS:HG2	1:158:A:LYS:HA	16	0.2
(1,1101)	1:158:A:LYS:HA	1:158:A:LYS:HG3	1	0.2
(1,1101)	1:158:A:LYS:HA	1:158:A:LYS:HG3	14	0.2
(1,1097)	1:68:A:LYS:HA	1:68:A:LYS:HG2	17	0.2
(1,1029)	1:116:A:MET:HE1	1:116:A:MET:HB3	6	0.2
(1,1029)	1:116:A:MET:HE2	1:116:A:MET:HB3	6	0.2
(1,1029)	1:116:A:MET:HE3	1:116:A:MET:HB3	6	0.2
(1,1019)	1:84:A:MET:HE1	1:15:A:LYS:HD2	16	0.2
(1,1019)	1:84:A:MET:HE2	1:15:A:LYS:HD2	16	0.2
(1,1019)	1:84:A:MET:HE3	1:15:A:LYS:HD2	16	0.2
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	9	0.2
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	9	0.2
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	9	0.2
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	20	0.2
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	20	0.2
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	20	0.2
(1,952)	1:126:A:HIS:HB3	1:126:A:HIS:HA	6	0.2
(1,952)	1:126:A:HIS:HB3	1:126:A:HIS:HA	9	0.2
(1,952)	1:126:A:HIS:HB3	1:126:A:HIS:HA	15	0.2
(1,952)	1:126:A:HIS:HB3	1:126:A:HIS:HA	20	0.2
(1,942)	1:79:A:VAL:HG21	1:80:A:HIS:H	14	0.2
(1,942)	1:79:A:VAL:HG22	1:80:A:HIS:H	14	0.2
(1,942)	1:79:A:VAL:HG23	1:80:A:HIS:H	14	0.2
(1,942)	1:79:A:VAL:HG21	1:80:A:HIS:H	15	0.2
(1,942)	1:79:A:VAL:HG22	1:80:A:HIS:H	15	0.2
(1,942)	1:79:A:VAL:HG23	1:80:A:HIS:H	15	0.2
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	2	0.2
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	6	0.2
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	12	0.2
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	14	0.2
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	19	0.2
(1,927)	1:23:A:LYS:HA	1:22:A:TYR:HB2	19	0.2
(1,910)	1:108:A:LEU:H	1:153:A:ALA:HB1	1	0.2
(1,910)	1:108:A:LEU:H	1:153:A:ALA:HB2	1	0.2
(1,910)	1:108:A:LEU:H	1:153:A:ALA:HB3	1	0.2
(1,869)	1:13:A:VAL:HG21	1:55:A:LEU:HB2	17	0.2
(1,869)	1:13:A:VAL:HG22	1:55:A:LEU:HB2	17	0.2
(1,869)	1:13:A:VAL:HG23	1:55:A:LEU:HB2	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	1	0.2
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	15	0.2
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	15	0.2
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	15	0.2
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	4	0.2
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	4	0.2
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	4	0.2
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	6	0.2
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	6	0.2
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	6	0.2
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	7	0.2
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	7	0.2
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	7	0.2
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	8	0.2
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	8	0.2
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	8	0.2
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	11	0.2
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	11	0.2
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	11	0.2
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	13	0.2
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	13	0.2
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	13	0.2
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	16	0.2
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	16	0.2
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	16	0.2
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	17	0.2
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	17	0.2
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	17	0.2
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	18	0.2
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	18	0.2
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	18	0.2
(1,797)	1:138:A:LYS:HA	1:138:A:LYS:HG2	11	0.2
(1,797)	1:138:A:LYS:HA	1:138:A:LYS:HG2	13	0.2
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD11	14	0.2
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD12	14	0.2
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD13	14	0.2
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD11	14	0.2
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD12	14	0.2
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD13	14	0.2
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD11	14	0.2
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD12	14	0.2
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD13	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD11	15	0.2
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD12	15	0.2
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD13	15	0.2
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD11	15	0.2
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD12	15	0.2
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD13	15	0.2
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD11	15	0.2
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD12	15	0.2
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD13	15	0.2
(1,763)	1:155:A:THR:HG21	1:156:A:HIS:HB2	18	0.2
(1,763)	1:155:A:THR:HG22	1:156:A:HIS:HB2	18	0.2
(1,763)	1:155:A:THR:HG23	1:156:A:HIS:HB2	18	0.2
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	15	0.2
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	15	0.2
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	15	0.2
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	3	0.2
(1,690)	1:46:A:LEU:HG	1:43:A:SER:HB3	18	0.2
(1,677)	1:59:A:LEU:HB3	1:56:A:CYS:HA	19	0.2
(1,657)	1:7:A:PRO:HA	1:8:A:GLY:HA2	16	0.2
(1,591)	1:49:A:LYS:HE2	1:49:A:LYS:HG2	1	0.2
(1,591)	1:49:A:LYS:HE3	1:49:A:LYS:HG2	1	0.2
(1,584)	1:102:A:TYR:H	1:101:A:LYS:HG2	17	0.2
(1,568)	1:34:A:LEU:HD11	1:75:A:ARG:HD2	18	0.2
(1,568)	1:34:A:LEU:HD12	1:75:A:ARG:HD2	18	0.2
(1,568)	1:34:A:LEU:HD13	1:75:A:ARG:HD2	18	0.2
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD11	7	0.2
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD12	7	0.2
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD13	7	0.2
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD11	14	0.2
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD12	14	0.2
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD13	14	0.2
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD11	15	0.2
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD12	15	0.2
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD13	15	0.2
(1,529)	1:92:A:LYS:H	1:92:A:LYS:HD2	2	0.2
(1,529)	1:92:A:LYS:H	1:92:A:LYS:HD3	2	0.2
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	19	0.2
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	19	0.2
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	19	0.2
(1,439)	1:147:A:GLU:HG2	1:144:A:LEU:HG	11	0.2
(1,419)	1:6:A:ARG:HG3	1:6:A:ARG:H	16	0.2
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	7	0.2
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	9	0.2
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	10	0.2
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	16	0.2
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	17	0.2
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	20	0.2
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD2	3	0.2
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD3	3	0.2
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	7	0.2
(1,322)	1:115:A:LYS:H	1:114:A:ARG:HB2	14	0.2
(1,313)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	14	0.2
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	9	0.2
(1,298)	1:99:A:GLU:HB3	1:99:A:GLU:HG3	17	0.2
(1,297)	1:99:A:GLU:HG3	1:99:A:GLU:HB2	3	0.2
(1,297)	1:99:A:GLU:HG3	1:99:A:GLU:HB2	13	0.2
(1,280)	1:104:A:LYS:H	1:103:A:GLU:HB3	19	0.2
(1,264)	1:85:A:LYS:HB3	1:86:A:ILE:H	13	0.2
(1,194)	1:123:A:GLN:HG3	1:123:A:GLN:H	10	0.2
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	20	0.2
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	20	0.2
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	20	0.2
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	19	0.2
(1,163)	1:2:A:GLU:HA	1:2:A:GLU:HG2	19	0.2
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD11	1	0.2
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD12	1	0.2
(1,139)	1:38:A:GLU:HG3	1:42:A:ILE:HD13	1	0.2
(1,86)	1:28:A:ARG:H	1:27:A:ASP:HB2	12	0.2
(1,86)	1:28:A:ARG:H	1:27:A:ASP:HB2	18	0.2
(1,61)	1:122:A:LYS:HE3	1:141:A:TYR:HE1	11	0.2
(1,61)	1:122:A:LYS:HE3	1:141:A:TYR:HE2	11	0.2
(1,49)	1:159:A:THR:H	1:158:A:LYS:HE2	5	0.2
(1,46)	1:46:A:LEU:HB2	1:47:A:ASP:HA	1	0.2
(1,19)	1:28:A:ARG:HD3	1:28:A:ARG:HA	11	0.2
(1,17)	1:20:A:ARG:HB3	1:20:A:ARG:HD2	17	0.2
(1,17)	1:20:A:ARG:HB3	1:20:A:ARG:HD2	19	0.2
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB1	17	0.2
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB2	17	0.2
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB3	17	0.2
(1,2)	1:8:A:GLY:HA2	1:15:A:LYS:HD2	12	0.2
(1,2)	1:8:A:GLY:HA3	1:15:A:LYS:HD2	12	0.2
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG11	5	0.19
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG12	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG13	5	0.19
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG11	5	0.19
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG12	5	0.19
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG13	5	0.19
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	2	0.19
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	2	0.19
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	11	0.19
(1,1836)	1:114:A:ARG:HD3	1:114:A:ARG:H	13	0.19
(1,1835)	1:114:A:ARG:H	1:114:A:ARG:HD2	1	0.19
(1,1835)	1:114:A:ARG:H	1:114:A:ARG:HD2	18	0.19
(1,1798)	1:42:A:ILE:HG13	1:43:A:SER:H	9	0.19
(1,1756)	1:151:A:LYS:HB3	1:151:A:LYS:H	16	0.19
(1,1734)	1:159:A:THR:H	1:159:A:THR:HB	10	0.19
(1,1725)	1:33:A:SER:H	1:33:A:SER:HB2	17	0.19
(1,1725)	1:33:A:SER:H	1:33:A:SER:HB2	18	0.19
(1,1703)	1:152:A:TYR:H	1:151:A:LYS:HB2	4	0.19
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	4	0.19
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	10	0.19
(1,1656)	1:122:A:LYS:H	1:122:A:LYS:HG2	10	0.19
(1,1656)	1:122:A:LYS:H	1:122:A:LYS:HG2	17	0.19
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	4	0.19
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	10	0.19
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	4	0.19
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	14	0.19
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	15	0.19
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	6	0.19
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	6	0.19
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	6	0.19
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	6	0.19
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	14	0.19
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	14	0.19
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	14	0.19
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	17	0.19
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	17	0.19
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	17	0.19
(1,1565)	1:117:A:ARG:H	1:116:A:MET:HB3	18	0.19
(1,1548)	1:130:A:GLU:H	1:128:A:TRP:HB3	12	0.19
(1,1529)	1:131:A:GLU:H	1:131:A:GLU:HB2	8	0.19
(1,1527)	1:116:A:MET:H	1:115:A:LYS:HB2	14	0.19
(1,1511)	1:25:A:LEU:H	1:25:A:LEU:HG	3	0.19
(1,1499)	1:90:A:LEU:H	1:86:A:ILE:HA	2	0.19
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	8	0.19
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	11	0.19
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	13	0.19
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	18	0.19
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	20	0.19
(1,1423)	1:121:A:LEU:H	1:121:A:LEU:HG	7	0.19
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	9	0.19
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	5	0.19
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	16	0.19
(1,1386)	1:103:A:GLU:H	1:102:A:TYR:HB3	15	0.19
(1,1385)	1:103:A:GLU:H	1:102:A:TYR:HA	6	0.19
(1,1381)	1:158:A:LYS:H	1:158:A:LYS:HG3	19	0.19
(1,1359)	1:63:A:LYS:HB3	1:65:A:ALA:H	7	0.19
(1,1359)	1:63:A:LYS:HB3	1:65:A:ALA:H	20	0.19
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	8	0.19
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	16	0.19
(1,1326)	1:1:A:GLN:HA	1:2:A:GLU:H	18	0.19
(1,1291)	1:107:A:ASP:HB3	1:108:A:LEU:H	11	0.19
(1,1275)	1:2:A:GLU:H	1:3:A:ALA:H	2	0.19
(1,1275)	1:2:A:GLU:H	1:3:A:ALA:H	13	0.19
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	10	0.19
(1,1157)	1:101:A:LYS:HA	1:101:A:LYS:HD2	9	0.19
(1,1143)	1:143:A:ASN:HB3	1:143:A:ASN:HA	16	0.19
(1,1125)	1:104:A:LYS:HA	1:104:A:LYS:HG2	8	0.19
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	2	0.19
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	2	0.19
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	2	0.19
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	1	0.19
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	6	0.19
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	9	0.19
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	13	0.19
(1,1109)	1:116:A:MET:HA	1:116:A:MET:HG2	16	0.19
(1,1105)	1:103:A:GLU:HA	1:104:A:LYS:HG2	10	0.19
(1,1101)	1:158:A:LYS:HA	1:158:A:LYS:HG3	16	0.19
(1,1063)	1:30:A:VAL:HG11	1:25:A:LEU:HA	14	0.19
(1,1063)	1:30:A:VAL:HG12	1:25:A:LEU:HA	14	0.19
(1,1063)	1:30:A:VAL:HG13	1:25:A:LEU:HA	14	0.19
(1,1017)	1:84:A:MET:HE1	1:15:A:LYS:HE2	13	0.19
(1,1017)	1:84:A:MET:HE2	1:15:A:LYS:HE2	13	0.19
(1,1017)	1:84:A:MET:HE3	1:15:A:LYS:HE2	13	0.19
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	14	0.19
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	14	0.19
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	18	0.19
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	18	0.19
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	18	0.19
(1,959)	1:24:A:SER:HB3	1:21:A:PHE:HA	15	0.19
(1,952)	1:126:A:HIS:HB3	1:126:A:HIS:HA	19	0.19
(1,942)	1:79:A:VAL:HG21	1:80:A:HIS:H	10	0.19
(1,942)	1:79:A:VAL:HG22	1:80:A:HIS:H	10	0.19
(1,942)	1:79:A:VAL:HG23	1:80:A:HIS:H	10	0.19
(1,929)	1:23:A:LYS:HB3	1:23:A:LYS:HA	8	0.19
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	9	0.19
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	11	0.19
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	16	0.19
(1,927)	1:23:A:LYS:HA	1:22:A:TYR:HB2	17	0.19
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG11	1	0.19
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG12	1	0.19
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG13	1	0.19
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	1	0.19
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	1	0.19
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	1	0.19
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	11	0.19
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	11	0.19
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	11	0.19
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	12	0.19
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	12	0.19
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	12	0.19
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	1	0.19
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	1	0.19
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	1	0.19
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	5	0.19
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	5	0.19
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	5	0.19
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	12	0.19
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	12	0.19
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	12	0.19
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	19	0.19
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	19	0.19
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	19	0.19
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	20	0.19
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	20	0.19
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	20	0.19
(1,797)	1:138:A:LYS:HA	1:138:A:LYS:HG2	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	2	0.19
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	2	0.19
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	2	0.19
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD21	20	0.19
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD22	20	0.19
(1,733)	1:148:A:LEU:HB2	1:148:A:LEU:HD23	20	0.19
(1,711)	1:139:A:THR:HG21	1:143:A:ASN:HB2	10	0.19
(1,711)	1:139:A:THR:HG22	1:143:A:ASN:HB2	10	0.19
(1,711)	1:139:A:THR:HG23	1:143:A:ASN:HB2	10	0.19
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD11	9	0.19
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD12	9	0.19
(1,569)	1:75:A:ARG:HD3	1:34:A:LEU:HD13	9	0.19
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD11	1	0.19
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD12	1	0.19
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD13	1	0.19
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD11	18	0.19
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD12	18	0.19
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD13	18	0.19
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD11	19	0.19
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD12	19	0.19
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD13	19	0.19
(1,566)	1:46:A:LEU:HD11	1:43:A:SER:HB3	2	0.19
(1,566)	1:46:A:LEU:HD12	1:43:A:SER:HB3	2	0.19
(1,566)	1:46:A:LEU:HD13	1:43:A:SER:HB3	2	0.19
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	8	0.19
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	8	0.19
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	8	0.19
(1,514)	1:115:A:LYS:H	1:115:A:LYS:HG2	20	0.19
(1,445)	1:90:A:LEU:HD11	1:73:A:VAL:H	4	0.19
(1,445)	1:90:A:LEU:HD12	1:73:A:VAL:H	4	0.19
(1,445)	1:90:A:LEU:HD13	1:73:A:VAL:H	4	0.19
(1,441)	1:113:A:LEU:HD21	1:146:A:GLN:HG3	10	0.19
(1,441)	1:113:A:LEU:HD22	1:146:A:GLN:HG3	10	0.19
(1,441)	1:113:A:LEU:HD23	1:146:A:GLN:HG3	10	0.19
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	19	0.19
(1,401)	1:69:A:ILE:HG12	1:69:A:ILE:HA	3	0.19
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	12	0.19
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	15	0.19
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	19	0.19
(1,339)	1:23:A:LYS:H	1:23:A:LYS:HD2	5	0.19
(1,339)	1:23:A:LYS:H	1:23:A:LYS:HD3	5	0.19
(1,336)	1:42:A:ILE:H	1:42:A:ILE:HG13	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	6	0.19
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	8	0.19
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	12	0.19
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	18	0.19
(1,323)	1:114:A:ARG:HB3	1:115:A:LYS:H	6	0.19
(1,312)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	1	0.19
(1,300)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	7	0.19
(1,298)	1:99:A:GLU:HB3	1:99:A:GLU:HG3	11	0.19
(1,298)	1:99:A:GLU:HB3	1:99:A:GLU:HG3	16	0.19
(1,298)	1:99:A:GLU:HB3	1:99:A:GLU:HG3	18	0.19
(1,297)	1:99:A:GLU:HG3	1:99:A:GLU:HB2	19	0.19
(1,251)	1:63:A:LYS:HB3	1:63:A:LYS:HE3	9	0.19
(1,251)	1:63:A:LYS:HB3	1:63:A:LYS:HE3	13	0.19
(1,242)	1:9:A:ALA:HB1	1:7:A:PRO:HB3	12	0.19
(1,242)	1:9:A:ALA:HB2	1:7:A:PRO:HB3	12	0.19
(1,242)	1:9:A:ALA:HB3	1:7:A:PRO:HB3	12	0.19
(1,163)	1:2:A:GLU:HA	1:2:A:GLU:HG2	8	0.19
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	15	0.19
(1,26)	1:117:A:ARG:HB3	1:117:A:ARG:HD2	9	0.19
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB1	13	0.19
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB2	13	0.19
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB3	13	0.19
(1,2013)	1:151:A:LYS:HE3	1:152:A:TYR:HE1	11	0.18
(1,2013)	1:151:A:LYS:HE3	1:152:A:TYR:HE2	11	0.18
(1,2007)	1:57:A:TYR:HE1	1:64:A:ASP:HB2	5	0.18
(1,2007)	1:57:A:TYR:HE2	1:64:A:ASP:HB2	5	0.18
(1,1972)	1:20:A:ARG:HB3	1:44:A:PHE:HZ	2	0.18
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE1	7	0.18
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE2	7	0.18
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	13	0.18
(1,1887)	1:126:A:HIS:H	1:129:A:GLY:H	19	0.18
(1,1887)	1:126:A:HIS:H	1:129:A:GLY:H	20	0.18
(1,1879)	1:4:A:GLY:HA3	1:5:A:GLY:H	18	0.18
(1,1872)	1:8:A:GLY:H	1:8:A:GLY:HA2	7	0.18
(1,1872)	1:8:A:GLY:H	1:8:A:GLY:HA2	16	0.18
(1,1838)	1:114:A:ARG:HB3	1:114:A:ARG:H	18	0.18
(1,1836)	1:114:A:ARG:HD3	1:114:A:ARG:H	16	0.18
(1,1835)	1:114:A:ARG:H	1:114:A:ARG:HD2	7	0.18
(1,1816)	1:96:A:GLN:HB3	1:96:A:GLN:HE21	18	0.18
(1,1798)	1:42:A:ILE:HG13	1:43:A:SER:H	5	0.18
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	11	0.18
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	13	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	17	0.18
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	19	0.18
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	20	0.18
(1,1731)	1:146:A:GLN:H	1:146:A:GLN:HB3	12	0.18
(1,1703)	1:152:A:TYR:H	1:151:A:LYS:HB2	10	0.18
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	17	0.18
(1,1664)	1:36:A:THR:H	1:35:A:ASP:HB2	10	0.18
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	17	0.18
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	2	0.18
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	5	0.18
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	7	0.18
(1,1613)	1:40:A:GLU:H	1:39:A:LYS:HB3	19	0.18
(1,1604)	1:54:A:ARG:HB3	1:54:A:ARG:H	3	0.18
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	15	0.18
(1,1548)	1:130:A:GLU:H	1:128:A:TRP:HB3	13	0.18
(1,1522)	1:131:A:GLU:H	1:130:A:GLU:HB3	17	0.18
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	3	0.18
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	4	0.18
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	7	0.18
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	15	0.18
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	17	0.18
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	19	0.18
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	11	0.18
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	5	0.18
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	6	0.18
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	15	0.18
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	2	0.18
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	6	0.18
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	9	0.18
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	17	0.18
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	18	0.18
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD11	13	0.18
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD12	13	0.18
(1,1271)	1:128:A:TRP:HE1	1:106:A:LEU:HD13	13	0.18
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	9	0.18
(1,1203)	1:42:A:ILE:HB	1:42:A:ILE:HD11	10	0.18
(1,1203)	1:42:A:ILE:HB	1:42:A:ILE:HD12	10	0.18
(1,1203)	1:42:A:ILE:HB	1:42:A:ILE:HD13	10	0.18
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	1	0.18
(1,1161)	1:119:A:ALA:HA	1:122:A:LYS:HG2	13	0.18
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD11	18	0.18
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD12	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD13	18	0.18
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	17	0.18
(1,1103)	1:103:A:GLU:HA	1:103:A:GLU:HG2	12	0.18
(1,1101)	1:158:A:LYS:HA	1:158:A:LYS:HG3	6	0.18
(1,1101)	1:158:A:LYS:HA	1:158:A:LYS:HG3	20	0.18
(1,1058)	1:54:A:ARG:HA	1:54:A:ARG:HD3	20	0.18
(1,996)	1:63:A:LYS:HG3	1:63:A:LYS:HA	13	0.18
(1,951)	1:126:A:HIS:HA	1:126:A:HIS:HB2	3	0.18
(1,951)	1:126:A:HIS:HA	1:126:A:HIS:HB2	5	0.18
(1,929)	1:23:A:LYS:HB3	1:23:A:LYS:HA	1	0.18
(1,897)	1:52:A:GLU:HA	1:52:A:GLU:HG2	19	0.18
(1,805)	1:111:A:VAL:HG11	1:111:A:VAL:HA	7	0.18
(1,805)	1:111:A:VAL:HG12	1:111:A:VAL:HA	7	0.18
(1,805)	1:111:A:VAL:HG13	1:111:A:VAL:HA	7	0.18
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	2	0.18
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	2	0.18
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	2	0.18
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	3	0.18
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	3	0.18
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	3	0.18
(1,804)	1:79:A:VAL:HG11	1:79:A:VAL:HA	9	0.18
(1,804)	1:79:A:VAL:HG12	1:79:A:VAL:HA	9	0.18
(1,804)	1:79:A:VAL:HG13	1:79:A:VAL:HA	9	0.18
(1,797)	1:138:A:LYS:HA	1:138:A:LYS:HG2	20	0.18
(1,782)	1:155:A:THR:HA	1:156:A:HIS:H	8	0.18
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD11	8	0.18
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD12	8	0.18
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD13	8	0.18
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD11	8	0.18
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD12	8	0.18
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD13	8	0.18
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD11	8	0.18
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD12	8	0.18
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD13	8	0.18
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	2	0.18
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	16	0.18
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	16	0.18
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	16	0.18
(1,711)	1:139:A:THR:HG21	1:143:A:ASN:HB2	12	0.18
(1,711)	1:139:A:THR:HG22	1:143:A:ASN:HB2	12	0.18
(1,711)	1:139:A:THR:HG23	1:143:A:ASN:HB2	12	0.18
(1,711)	1:139:A:THR:HG21	1:143:A:ASN:HB2	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,711)	1:139:A:THR:HG22	1:143:A:ASN:HB2	14	0.18
(1,711)	1:139:A:THR:HG23	1:143:A:ASN:HB2	14	0.18
(1,699)	1:75:A:ARG:HB2	1:71:A:SER:HB2	14	0.18
(1,699)	1:75:A:ARG:HB2	1:71:A:SER:HB3	14	0.18
(1,655)	1:161:A:LEU:HA	1:161:A:LEU:HD11	12	0.18
(1,655)	1:161:A:LEU:HA	1:161:A:LEU:HD12	12	0.18
(1,655)	1:161:A:LEU:HA	1:161:A:LEU:HD13	12	0.18
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD11	3	0.18
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD12	3	0.18
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD13	3	0.18
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD11	8	0.18
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD12	8	0.18
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD13	8	0.18
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD11	20	0.18
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD12	20	0.18
(1,567)	1:34:A:LEU:HA	1:34:A:LEU:HD13	20	0.18
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD21	5	0.18
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD22	5	0.18
(1,528)	1:92:A:LYS:HD3	1:93:A:LEU:HD23	5	0.18
(1,385)	1:121:A:LEU:HB3	1:118:A:VAL:HA	11	0.18
(1,385)	1:121:A:LEU:HB3	1:118:A:VAL:HA	18	0.18
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	1	0.18
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	3	0.18
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	8	0.18
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD2	12	0.18
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD3	12	0.18
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD2	4	0.18
(1,337)	1:39:A:LYS:HB3	1:39:A:LYS:HD3	4	0.18
(1,326)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	13	0.18
(1,323)	1:114:A:ARG:HB3	1:115:A:LYS:H	19	0.18
(1,312)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	5	0.18
(1,297)	1:99:A:GLU:HG3	1:99:A:GLU:HB2	15	0.18
(1,274)	1:73:A:VAL:HA	1:76:A:PRO:HB2	14	0.18
(1,256)	1:86:A:ILE:H	1:81:A:MET:HG2	8	0.18
(1,220)	1:131:A:GLU:HG3	1:131:A:GLU:HB3	8	0.18
(1,209)	1:67:A:THR:HG21	1:68:A:LYS:HB3	15	0.18
(1,209)	1:67:A:THR:HG22	1:68:A:LYS:HB3	15	0.18
(1,209)	1:67:A:THR:HG23	1:68:A:LYS:HB3	15	0.18
(1,185)	1:146:A:GLN:HG3	1:145:A:ILE:HG21	12	0.18
(1,185)	1:146:A:GLN:HG3	1:145:A:ILE:HG22	12	0.18
(1,185)	1:146:A:GLN:HG3	1:145:A:ILE:HG23	12	0.18
(1,178)	1:136:A:ALA:HB1	1:137:A:GLU:HG2	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,178)	1:136:A:ALA:HB2	1:137:A:GLU:HG2	6	0.18
(1,178)	1:136:A:ALA:HB3	1:137:A:GLU:HG2	6	0.18
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	11	0.18
(1,152)	1:104:A:LYS:H	1:103:A:GLU:HG2	11	0.18
(1,98)	1:121:A:LEU:HD11	1:141:A:TYR:HB2	6	0.18
(1,98)	1:121:A:LEU:HD12	1:141:A:TYR:HB2	6	0.18
(1,98)	1:121:A:LEU:HD13	1:141:A:TYR:HB2	6	0.18
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	13	0.18
(1,46)	1:46:A:LEU:HB2	1:47:A:ASP:HA	2	0.18
(1,46)	1:46:A:LEU:HB2	1:47:A:ASP:HA	17	0.18
(1,17)	1:20:A:ARG:HB3	1:20:A:ARG:HD2	3	0.18
(1,17)	1:20:A:ARG:HB3	1:20:A:ARG:HD2	9	0.18
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB1	9	0.18
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB2	9	0.18
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB3	9	0.18
(1,5)	1:9:A:ALA:HB1	1:8:A:GLY:HA2	2	0.18
(1,5)	1:9:A:ALA:HB2	1:8:A:GLY:HA2	2	0.18
(1,5)	1:9:A:ALA:HB3	1:8:A:GLY:HA2	2	0.18
(1,2012)	1:152:A:TYR:HE1	1:151:A:LYS:HE2	1	0.17
(1,2012)	1:152:A:TYR:HE2	1:151:A:LYS:HE2	1	0.17
(1,1964)	1:21:A:PHE:HD1	1:44:A:PHE:HZ	16	0.17
(1,1964)	1:21:A:PHE:HD2	1:44:A:PHE:HZ	16	0.17
(1,1907)	1:64:A:ASP:HB3	1:57:A:TYR:HD1	1	0.17
(1,1907)	1:64:A:ASP:HB3	1:57:A:TYR:HD2	1	0.17
(1,1901)	1:103:A:GLU:H	1:102:A:TYR:HD1	17	0.17
(1,1901)	1:103:A:GLU:H	1:102:A:TYR:HD2	17	0.17
(1,1901)	1:103:A:GLU:H	1:102:A:TYR:HD1	19	0.17
(1,1901)	1:103:A:GLU:H	1:102:A:TYR:HD2	19	0.17
(1,1839)	1:114:A:ARG:H	1:114:A:ARG:HG3	20	0.17
(1,1825)	1:45:A:CYS:HB3	1:45:A:CYS:H	5	0.17
(1,1802)	1:24:A:SER:H	1:25:A:LEU:HG	17	0.17
(1,1771)	1:35:A:ASP:H	1:34:A:LEU:HB3	20	0.17
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	9	0.17
(1,1693)	1:64:A:ASP:HB3	1:64:A:ASP:H	18	0.17
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	14	0.17
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	14	0.17
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	14	0.17
(1,1669)	1:93:A:LEU:HB3	1:94:A:ASP:H	2	0.17
(1,1669)	1:93:A:LEU:HB3	1:94:A:ASP:H	16	0.17
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	12	0.17
(1,1656)	1:122:A:LYS:H	1:122:A:LYS:HG2	5	0.17
(1,1656)	1:122:A:LYS:H	1:122:A:LYS:HG2	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1656)	1:122:A:LYS:H	1:122:A:LYS:HG2	18	0.17
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	1	0.17
(1,1602)	1:54:A:ARG:HD2	1:54:A:ARG:H	15	0.17
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	5	0.17
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	5	0.17
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	5	0.17
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	20	0.17
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	20	0.17
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	20	0.17
(1,1567)	1:117:A:ARG:H	1:117:A:ARG:HB2	15	0.17
(1,1565)	1:117:A:ARG:H	1:116:A:MET:HB3	14	0.17
(1,1511)	1:25:A:LEU:H	1:25:A:LEU:HG	2	0.17
(1,1511)	1:25:A:LEU:H	1:25:A:LEU:HG	13	0.17
(1,1511)	1:25:A:LEU:H	1:25:A:LEU:HG	19	0.17
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB2	1	0.17
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB3	1	0.17
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB2	4	0.17
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB3	4	0.17
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB2	5	0.17
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB3	5	0.17
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB2	7	0.17
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB3	7	0.17
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB2	16	0.17
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB3	16	0.17
(1,1472)	1:102:A:TYR:HB2	1:102:A:TYR:H	16	0.17
(1,1462)	1:107:A:ASP:HB3	1:109:A:ALA:H	11	0.17
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	4	0.17
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	18	0.17
(1,1387)	1:103:A:GLU:H	1:103:A:GLU:HB2	10	0.17
(1,1386)	1:103:A:GLU:H	1:102:A:TYR:HB3	1	0.17
(1,1385)	1:103:A:GLU:H	1:102:A:TYR:HA	13	0.17
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	3	0.17
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	7	0.17
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	8	0.17
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	12	0.17
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	20	0.17
(1,1329)	1:121:A:LEU:H	1:118:A:VAL:H	5	0.17
(1,1328)	1:2:A:GLU:HB2	1:2:A:GLU:H	7	0.17
(1,1318)	1:9:A:ALA:H	1:8:A:GLY:HA2	17	0.17
(1,1128)	1:103:A:GLU:HB3	1:103:A:GLU:HA	12	0.17
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	14	0.17
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	14	0.17
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	14	0.17
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	14	0.17
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	14	0.17
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	14	0.17
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	14	0.17
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	14	0.17
(1,1103)	1:103:A:GLU:HA	1:103:A:GLU:HG2	6	0.17
(1,1086)	1:28:A:ARG:HA	1:28:A:ARG:HE	20	0.17
(1,1059)	1:54:A:ARG:HA	1:57:A:TYR:HB2	10	0.17
(1,1056)	1:116:A:MET:HG3	1:113:A:LEU:HA	7	0.17
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE1	3	0.17
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE2	3	0.17
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE3	3	0.17
(1,1019)	1:84:A:MET:HE1	1:15:A:LYS:HD2	20	0.17
(1,1019)	1:84:A:MET:HE2	1:15:A:LYS:HD2	20	0.17
(1,1019)	1:84:A:MET:HE3	1:15:A:LYS:HD2	20	0.17
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE1	1	0.17
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE2	1	0.17
(1,1018)	1:15:A:LYS:HE3	1:84:A:MET:HE3	1	0.17
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	1	0.17
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	1	0.17
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	1	0.17
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	15	0.17
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	15	0.17
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	15	0.17
(1,951)	1:126:A:HIS:HA	1:126:A:HIS:HB2	4	0.17
(1,951)	1:126:A:HIS:HA	1:126:A:HIS:HB2	11	0.17
(1,951)	1:126:A:HIS:HA	1:126:A:HIS:HB2	12	0.17
(1,951)	1:126:A:HIS:HA	1:126:A:HIS:HB2	17	0.17
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	18	0.17
(1,904)	1:83:A:ALA:HB1	1:19:A:ASN:HD22	1	0.17
(1,904)	1:83:A:ALA:HB2	1:19:A:ASN:HD22	1	0.17
(1,904)	1:83:A:ALA:HB3	1:19:A:ASN:HD22	1	0.17
(1,816)	1:74:A:THR:HG21	1:38:A:GLU:HA	3	0.17
(1,816)	1:74:A:THR:HG22	1:38:A:GLU:HA	3	0.17
(1,816)	1:74:A:THR:HG23	1:38:A:GLU:HA	3	0.17
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	4	0.17
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	7	0.17
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	7	0.17
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	7	0.17
(1,797)	1:138:A:LYS:HA	1:138:A:LYS:HG2	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD11	3	0.17
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD12	3	0.17
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD13	3	0.17
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD11	3	0.17
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD12	3	0.17
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD13	3	0.17
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD11	3	0.17
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD12	3	0.17
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD13	3	0.17
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB1	6	0.17
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB2	6	0.17
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB3	6	0.17
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	16	0.17
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB2	13	0.17
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB3	13	0.17
(1,552)	1:31:A:ASN:HD21	1:33:A:SER:HB2	3	0.17
(1,552)	1:31:A:ASN:HD21	1:33:A:SER:HB2	14	0.17
(1,529)	1:92:A:LYS:H	1:92:A:LYS:HD2	17	0.17
(1,529)	1:92:A:LYS:H	1:92:A:LYS:HD3	17	0.17
(1,419)	1:6:A:ARG:HG3	1:6:A:ARG:H	13	0.17
(1,409)	1:161:A:LEU:H	1:161:A:LEU:HG	13	0.17
(1,387)	1:86:A:ILE:HG21	1:76:A:PRO:HG3	10	0.17
(1,387)	1:86:A:ILE:HG22	1:76:A:PRO:HG3	10	0.17
(1,387)	1:86:A:ILE:HG23	1:76:A:PRO:HG3	10	0.17
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	4	0.17
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	6	0.17
(1,374)	1:81:A:MET:HA	1:82:A:PRO:HG2	3	0.17
(1,374)	1:81:A:MET:HA	1:82:A:PRO:HG3	3	0.17
(1,353)	1:139:A:THR:HB	1:137:A:GLU:HG2	2	0.17
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD2	2	0.17
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD3	2	0.17
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD2	19	0.17
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD3	19	0.17
(1,336)	1:42:A:ILE:H	1:42:A:ILE:HG13	9	0.17
(1,336)	1:42:A:ILE:H	1:42:A:ILE:HG13	15	0.17
(1,336)	1:42:A:ILE:H	1:42:A:ILE:HG13	20	0.17
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	2	0.17
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	16	0.17
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG21	8	0.17
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG22	8	0.17
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG23	8	0.17
(1,312)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,269)	1:128:A:TRP:HZ3	1:145:A:ILE:HG12	14	0.17
(1,260)	1:86:A:ILE:HA	1:89:A:LYS:HB2	12	0.17
(1,260)	1:86:A:ILE:HA	1:89:A:LYS:HB3	12	0.17
(1,237)	1:148:A:LEU:HA	1:151:A:LYS:HB3	11	0.17
(1,219)	1:131:A:GLU:HB3	1:131:A:GLU:HG2	1	0.17
(1,219)	1:131:A:GLU:HB3	1:131:A:GLU:HG2	6	0.17
(1,209)	1:67:A:THR:HG21	1:68:A:LYS:HB3	7	0.17
(1,209)	1:67:A:THR:HG22	1:68:A:LYS:HB3	7	0.17
(1,209)	1:67:A:THR:HG23	1:68:A:LYS:HB3	7	0.17
(1,168)	1:17:A:PHE:H	1:16:A:GLU:HG2	20	0.17
(1,163)	1:2:A:GLU:HA	1:2:A:GLU:HG2	10	0.17
(1,163)	1:2:A:GLU:HA	1:2:A:GLU:HG2	14	0.17
(1,161)	1:3:A:ALA:HB1	1:2:A:GLU:HG2	6	0.17
(1,161)	1:3:A:ALA:HB2	1:2:A:GLU:HG2	6	0.17
(1,161)	1:3:A:ALA:HB3	1:2:A:GLU:HG2	6	0.17
(1,161)	1:3:A:ALA:HB1	1:2:A:GLU:HG3	6	0.17
(1,161)	1:3:A:ALA:HB2	1:2:A:GLU:HG3	6	0.17
(1,161)	1:3:A:ALA:HB3	1:2:A:GLU:HG3	6	0.17
(1,105)	1:31:A:ASN:HB3	1:32:A:PHE:H	1	0.17
(1,93)	1:64:A:ASP:HB3	1:57:A:TYR:HD1	2	0.17
(1,93)	1:64:A:ASP:HB3	1:57:A:TYR:HD2	2	0.17
(1,92)	1:64:A:ASP:HB3	1:57:A:TYR:HE1	4	0.17
(1,92)	1:64:A:ASP:HB3	1:57:A:TYR:HE2	4	0.17
(1,78)	1:121:A:LEU:HB2	1:141:A:TYR:HB3	2	0.17
(1,46)	1:46:A:LEU:HB2	1:47:A:ASP:HA	11	0.17
(1,46)	1:46:A:LEU:HB2	1:47:A:ASP:HA	15	0.17
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB1	5	0.17
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB2	5	0.17
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB3	5	0.17
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB1	12	0.17
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB2	12	0.17
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB3	12	0.17
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB1	13	0.17
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB2	13	0.17
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB3	13	0.17
(1,1988)	1:156:A:HIS:H	1:156:A:HIS:HD2	9	0.16
(1,1972)	1:20:A:ARG:HB3	1:44:A:PHE:HZ	5	0.16
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD1	6	0.16
(1,1948)	1:25:A:LEU:HB2	1:32:A:PHE:HD2	6	0.16
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD1	6	0.16
(1,1904)	1:101:A:LYS:HB2	1:102:A:TYR:HD2	6	0.16
(1,1902)	1:102:A:TYR:H	1:102:A:TYR:HD1	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1902)	1:102:A:TYR:H	1:102:A:TYR:HD2	5	0.16
(1,1899)	1:69:A:ILE:HG12	1:60:A:GLY:H	15	0.16
(1,1887)	1:126:A:HIS:H	1:129:A:GLY:H	1	0.16
(1,1872)	1:8:A:GLY:H	1:8:A:GLY:HA2	6	0.16
(1,1872)	1:8:A:GLY:H	1:8:A:GLY:HA2	9	0.16
(1,1838)	1:114:A:ARG:HB3	1:114:A:ARG:H	4	0.16
(1,1824)	1:31:A:ASN:HD21	1:32:A:PHE:HA	13	0.16
(1,1802)	1:24:A:SER:H	1:25:A:LEU:HG	8	0.16
(1,1787)	1:73:A:VAL:H	1:71:A:SER:HA	9	0.16
(1,1787)	1:73:A:VAL:H	1:71:A:SER:HA	11	0.16
(1,1725)	1:33:A:SER:H	1:33:A:SER:HB2	10	0.16
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	11	0.16
(1,1710)	1:31:A:ASN:HB2	1:33:A:SER:H	19	0.16
(1,1709)	1:115:A:LYS:H	1:112:A:ASP:H	4	0.16
(1,1666)	1:30:A:VAL:HB	1:28:A:ARG:HE	12	0.16
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	18	0.16
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	8	0.16
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	8	0.16
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	8	0.16
(1,1564)	1:117:A:ARG:H	1:120:A:GLU:HB3	1	0.16
(1,1553)	1:93:A:LEU:H	1:92:A:LYS:HB2	13	0.16
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	19	0.16
(1,1511)	1:25:A:LEU:H	1:25:A:LEU:HG	7	0.16
(1,1511)	1:25:A:LEU:H	1:25:A:LEU:HG	11	0.16
(1,1423)	1:121:A:LEU:H	1:121:A:LEU:HG	16	0.16
(1,1387)	1:103:A:GLU:H	1:103:A:GLU:HB2	14	0.16
(1,1385)	1:103:A:GLU:H	1:102:A:TYR:HA	9	0.16
(1,1368)	1:113:A:LEU:H	1:112:A:ASP:H	16	0.16
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	20	0.16
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	5	0.16
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	15	0.16
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	16	0.16
(1,1326)	1:1:A:GLN:HA	1:2:A:GLU:H	10	0.16
(1,1308)	1:67:A:THR:HG21	1:66:A:ALA:H	20	0.16
(1,1308)	1:67:A:THR:HG22	1:66:A:ALA:H	20	0.16
(1,1308)	1:67:A:THR:HG23	1:66:A:ALA:H	20	0.16
(1,1231)	1:26:A:ILE:HD11	1:26:A:ILE:HG21	4	0.16
(1,1231)	1:26:A:ILE:HD11	1:26:A:ILE:HG22	4	0.16
(1,1231)	1:26:A:ILE:HD11	1:26:A:ILE:HG23	4	0.16
(1,1231)	1:26:A:ILE:HD12	1:26:A:ILE:HG21	4	0.16
(1,1231)	1:26:A:ILE:HD12	1:26:A:ILE:HG22	4	0.16
(1,1231)	1:26:A:ILE:HD12	1:26:A:ILE:HG23	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1231)	1:26:A:ILE:HD13	1:26:A:ILE:HG21	4	0.16
(1,1231)	1:26:A:ILE:HD13	1:26:A:ILE:HG22	4	0.16
(1,1231)	1:26:A:ILE:HD13	1:26:A:ILE:HG23	4	0.16
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	3	0.16
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	4	0.16
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	8	0.16
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	11	0.16
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	18	0.16
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	20	0.16
(1,1161)	1:119:A:ALA:HA	1:122:A:LYS:HG2	7	0.16
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD11	7	0.16
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD12	7	0.16
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD13	7	0.16
(1,1128)	1:103:A:GLU:HB3	1:103:A:GLU:HA	2	0.16
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	10	0.16
(1,1125)	1:104:A:LYS:HA	1:104:A:LYS:HG2	19	0.16
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	16	0.16
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	16	0.16
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	16	0.16
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE1	18	0.16
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE2	18	0.16
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE3	18	0.16
(1,1056)	1:116:A:MET:HG3	1:113:A:LEU:HA	5	0.16
(1,1050)	1:143:A:ASN:H	1:140:A:ASP:HA	15	0.16
(1,1047)	1:77:A:MET:HE1	1:22:A:TYR:HB3	8	0.16
(1,1047)	1:77:A:MET:HE2	1:22:A:TYR:HB3	8	0.16
(1,1047)	1:77:A:MET:HE3	1:22:A:TYR:HB3	8	0.16
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE1	10	0.16
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE2	10	0.16
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE3	10	0.16
(1,1019)	1:84:A:MET:HE1	1:15:A:LYS:HD2	5	0.16
(1,1019)	1:84:A:MET:HE2	1:15:A:LYS:HD2	5	0.16
(1,1019)	1:84:A:MET:HE3	1:15:A:LYS:HD2	5	0.16
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	6	0.16
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	6	0.16
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	6	0.16
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	7	0.16
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	7	0.16
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	7	0.16
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	11	0.16
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	11	0.16
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	12	0.16
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	12	0.16
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	12	0.16
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	13	0.16
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	13	0.16
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	13	0.16
(1,993)	1:63:A:LYS:HA	1:63:A:LYS:HB2	5	0.16
(1,979)	1:119:A:ALA:HB1	1:122:A:LYS:HD2	10	0.16
(1,979)	1:119:A:ALA:HB2	1:122:A:LYS:HD2	10	0.16
(1,979)	1:119:A:ALA:HB3	1:122:A:LYS:HD2	10	0.16
(1,964)	1:69:A:ILE:HA	1:70:A:LEU:HA	16	0.16
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	14	0.16
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	14	0.16
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	14	0.16
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	10	0.16
(1,927)	1:23:A:LYS:HA	1:22:A:TYR:HB2	3	0.16
(1,897)	1:52:A:GLU:HA	1:52:A:GLU:HG2	1	0.16
(1,806)	1:41:A:LEU:HD21	1:44:A:PHE:HB2	17	0.16
(1,806)	1:41:A:LEU:HD22	1:44:A:PHE:HB2	17	0.16
(1,806)	1:41:A:LEU:HD23	1:44:A:PHE:HB2	17	0.16
(1,797)	1:138:A:LYS:HA	1:138:A:LYS:HG2	4	0.16
(1,797)	1:138:A:LYS:HA	1:138:A:LYS:HG2	6	0.16
(1,787)	1:75:A:ARG:HD3	1:75:A:ARG:HA	12	0.16
(1,782)	1:155:A:THR:HA	1:156:A:HIS:H	12	0.16
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD11	10	0.16
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD12	10	0.16
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD13	10	0.16
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD11	10	0.16
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD12	10	0.16
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD13	10	0.16
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD11	10	0.16
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD12	10	0.16
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD13	10	0.16
(1,765)	1:155:A:THR:H	1:155:A:THR:HG21	15	0.16
(1,765)	1:155:A:THR:H	1:155:A:THR:HG22	15	0.16
(1,765)	1:155:A:THR:H	1:155:A:THR:HG23	15	0.16
(1,762)	1:105:A:THR:H	1:105:A:THR:HG21	16	0.16
(1,762)	1:105:A:THR:H	1:105:A:THR:HG22	16	0.16
(1,762)	1:105:A:THR:H	1:105:A:THR:HG23	16	0.16
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	20	0.16
(1,727)	1:62:A:THR:HG21	1:56:A:CYS:HB2	20	0.16
(1,727)	1:62:A:THR:HG22	1:56:A:CYS:HB2	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,727)	1:62:A:THR:HG23	1:56:A:CYS:HB2	20	0.16
(1,711)	1:139:A:THR:HG21	1:143:A:ASN:HB2	5	0.16
(1,711)	1:139:A:THR:HG22	1:143:A:ASN:HB2	5	0.16
(1,711)	1:139:A:THR:HG23	1:143:A:ASN:HB2	5	0.16
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB2	4	0.16
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB3	4	0.16
(1,603)	1:111:A:VAL:H	1:110:A:SER:HB3	19	0.16
(1,552)	1:31:A:ASN:HD21	1:33:A:SER:HB2	19	0.16
(1,484)	1:142:A:VAL:HG11	1:139:A:THR:HA	10	0.16
(1,484)	1:142:A:VAL:HG12	1:139:A:THR:HA	10	0.16
(1,484)	1:142:A:VAL:HG13	1:139:A:THR:HA	10	0.16
(1,419)	1:6:A:ARG:HG3	1:6:A:ARG:H	4	0.16
(1,415)	1:113:A:LEU:H	1:113:A:LEU:HG	4	0.16
(1,390)	1:117:A:ARG:HG3	1:117:A:ARG:HA	9	0.16
(1,385)	1:121:A:LEU:HB3	1:118:A:VAL:HA	7	0.16
(1,385)	1:121:A:LEU:HB3	1:118:A:VAL:HA	12	0.16
(1,382)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	18	0.16
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	11	0.16
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	2	0.16
(1,327)	1:114:A:ARG:HB3	1:114:A:ARG:HG3	11	0.16
(1,323)	1:114:A:ARG:HB3	1:115:A:LYS:H	4	0.16
(1,313)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	10	0.16
(1,313)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	20	0.16
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	16	0.16
(1,244)	1:85:A:LYS:HB3	1:81:A:MET:HG2	16	0.16
(1,237)	1:148:A:LEU:HA	1:151:A:LYS:HB3	1	0.16
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	11	0.16
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	11	0.16
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	11	0.16
(1,220)	1:131:A:GLU:HG3	1:131:A:GLU:HB3	4	0.16
(1,220)	1:131:A:GLU:HG3	1:131:A:GLU:HB3	10	0.16
(1,220)	1:131:A:GLU:HG3	1:131:A:GLU:HB3	15	0.16
(1,220)	1:131:A:GLU:HG3	1:131:A:GLU:HB3	16	0.16
(1,220)	1:131:A:GLU:HG3	1:131:A:GLU:HB3	17	0.16
(1,219)	1:131:A:GLU:HB3	1:131:A:GLU:HG2	14	0.16
(1,213)	1:159:A:THR:H	1:158:A:LYS:HB2	5	0.16
(1,188)	1:96:A:GLN:HA	1:96:A:GLN:HG2	1	0.16
(1,178)	1:136:A:ALA:HB1	1:137:A:GLU:HG2	18	0.16
(1,178)	1:136:A:ALA:HB2	1:137:A:GLU:HG2	18	0.16
(1,178)	1:136:A:ALA:HB3	1:137:A:GLU:HG2	18	0.16
(1,153)	1:103:A:GLU:HG3	1:104:A:LYS:H	6	0.16
(1,136)	1:38:A:GLU:HG3	1:74:A:THR:HG21	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,136)	1:38:A:GLU:HG3	1:74:A:THR:HG22	8	0.16
(1,136)	1:38:A:GLU:HG3	1:74:A:THR:HG23	8	0.16
(1,98)	1:121:A:LEU:HD11	1:141:A:TYR:HB2	9	0.16
(1,98)	1:121:A:LEU:HD12	1:141:A:TYR:HB2	9	0.16
(1,98)	1:121:A:LEU:HD13	1:141:A:TYR:HB2	9	0.16
(1,48)	1:86:A:ILE:HG21	1:89:A:LYS:HE3	7	0.16
(1,48)	1:86:A:ILE:HG22	1:89:A:LYS:HE3	7	0.16
(1,48)	1:86:A:ILE:HG23	1:89:A:LYS:HE3	7	0.16
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG11	16	0.15
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG12	16	0.15
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG13	16	0.15
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG11	16	0.15
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG12	16	0.15
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG13	16	0.15
(1,1988)	1:156:A:HIS:H	1:156:A:HIS:HD2	6	0.15
(1,1964)	1:21:A:PHE:HD1	1:44:A:PHE:HZ	4	0.15
(1,1964)	1:21:A:PHE:HD2	1:44:A:PHE:HZ	4	0.15
(1,1937)	1:58:A:TYR:HD1	1:97:A:ILE:HG13	16	0.15
(1,1937)	1:58:A:TYR:HD2	1:97:A:ILE:HG13	16	0.15
(1,1901)	1:103:A:GLU:H	1:102:A:TYR:HD1	14	0.15
(1,1901)	1:103:A:GLU:H	1:102:A:TYR:HD2	14	0.15
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	10	0.15
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	16	0.15
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	18	0.15
(1,1887)	1:126:A:HIS:H	1:129:A:GLY:H	7	0.15
(1,1887)	1:126:A:HIS:H	1:129:A:GLY:H	13	0.15
(1,1872)	1:8:A:GLY:H	1:8:A:GLY:HA2	12	0.15
(1,1870)	1:29:A:GLY:H	1:26:A:ILE:HG21	4	0.15
(1,1870)	1:29:A:GLY:H	1:26:A:ILE:HG22	4	0.15
(1,1870)	1:29:A:GLY:H	1:26:A:ILE:HG23	4	0.15
(1,1806)	1:24:A:SER:H	1:23:A:LYS:HB2	18	0.15
(1,1802)	1:24:A:SER:H	1:25:A:LEU:HG	14	0.15
(1,1787)	1:73:A:VAL:H	1:71:A:SER:HA	3	0.15
(1,1787)	1:73:A:VAL:H	1:71:A:SER:HA	7	0.15
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	7	0.15
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	12	0.15
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	14	0.15
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	18	0.15
(1,1715)	1:143:A:ASN:H	1:143:A:ASN:HB2	16	0.15
(1,1669)	1:93:A:LEU:HB3	1:94:A:ASP:H	9	0.15
(1,1666)	1:30:A:VAL:HB	1:28:A:ARG:HE	9	0.15
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1656)	1:122:A:LYS:H	1:122:A:LYS:HG2	1	0.15
(1,1633)	1:87:A:CYS:H	1:87:A:CYS:HB3	10	0.15
(1,1633)	1:87:A:CYS:H	1:87:A:CYS:HB3	14	0.15
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	10	0.15
(1,1586)	1:143:A:ASN:HB3	1:142:A:VAL:H	20	0.15
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	18	0.15
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	18	0.15
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	18	0.15
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	2	0.15
(1,1446)	1:96:A:GLN:HG3	1:96:A:GLN:H	10	0.15
(1,1423)	1:121:A:LEU:H	1:121:A:LEU:HG	1	0.15
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	17	0.15
(1,1358)	1:65:A:ALA:H	1:63:A:LYS:HB2	4	0.15
(1,1336)	1:31:A:ASN:HB2	1:31:A:ASN:H	4	0.15
(1,1329)	1:121:A:LEU:H	1:118:A:VAL:H	17	0.15
(1,1311)	1:107:A:ASP:H	1:107:A:ASP:HB2	6	0.15
(1,1248)	1:6:A:ARG:HB3	1:7:A:PRO:HD2	1	0.15
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	10	0.15
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	16	0.15
(1,1235)	1:61:A:ALA:HA	1:42:A:ILE:HG13	14	0.15
(1,1205)	1:39:A:LYS:HA	1:42:A:ILE:HD11	10	0.15
(1,1205)	1:39:A:LYS:HA	1:42:A:ILE:HD12	10	0.15
(1,1205)	1:39:A:LYS:HA	1:42:A:ILE:HD13	10	0.15
(1,1173)	1:97:A:ILE:HD11	1:94:A:ASP:H	5	0.15
(1,1173)	1:97:A:ILE:HD12	1:94:A:ASP:H	5	0.15
(1,1173)	1:97:A:ILE:HD13	1:94:A:ASP:H	5	0.15
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	9	0.15
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	10	0.15
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	12	0.15
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	13	0.15
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	16	0.15
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	17	0.15
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	19	0.15
(1,1161)	1:119:A:ALA:HA	1:122:A:LYS:HG2	12	0.15
(1,1134)	1:83:A:ALA:HA	1:86:A:ILE:H	3	0.15
(1,1126)	1:104:A:LYS:HG3	1:104:A:LYS:HA	11	0.15
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	5	0.15
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	5	0.15
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	5	0.15
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	5	0.15
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	5	0.15
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	5	0.15
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	5	0.15
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	5	0.15
(1,1103)	1:103:A:GLU:HA	1:103:A:GLU:HG2	19	0.15
(1,1101)	1:158:A:LYS:HA	1:158:A:LYS:HG3	18	0.15
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE1	3	0.15
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE2	3	0.15
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE3	3	0.15
(1,1019)	1:84:A:MET:HE1	1:15:A:LYS:HD2	15	0.15
(1,1019)	1:84:A:MET:HE2	1:15:A:LYS:HD2	15	0.15
(1,1019)	1:84:A:MET:HE3	1:15:A:LYS:HD2	15	0.15
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD2	12	0.15
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD3	12	0.15
(1,927)	1:23:A:LYS:HA	1:22:A:TYR:HB2	15	0.15
(1,904)	1:83:A:ALA:HB1	1:19:A:ASN:HD22	14	0.15
(1,904)	1:83:A:ALA:HB2	1:19:A:ASN:HD22	14	0.15
(1,904)	1:83:A:ALA:HB3	1:19:A:ASN:HD22	14	0.15
(1,897)	1:52:A:GLU:HA	1:52:A:GLU:HG2	15	0.15
(1,897)	1:52:A:GLU:HA	1:52:A:GLU:HG2	16	0.15
(1,856)	1:59:A:LEU:HB3	1:61:A:ALA:HB1	11	0.15
(1,856)	1:59:A:LEU:HB3	1:61:A:ALA:HB2	11	0.15
(1,856)	1:59:A:LEU:HB3	1:61:A:ALA:HB3	11	0.15
(1,856)	1:59:A:LEU:HB3	1:61:A:ALA:HB1	16	0.15
(1,856)	1:59:A:LEU:HB3	1:61:A:ALA:HB2	16	0.15
(1,856)	1:59:A:LEU:HB3	1:61:A:ALA:HB3	16	0.15
(1,797)	1:138:A:LYS:HA	1:138:A:LYS:HG2	19	0.15
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD11	16	0.15
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD12	16	0.15
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD13	16	0.15
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD11	16	0.15
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD12	16	0.15
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD13	16	0.15
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD11	16	0.15
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD12	16	0.15
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD13	16	0.15
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD21	13	0.15
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD22	13	0.15
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD23	13	0.15
(1,731)	1:148:A:LEU:HD21	1:151:A:LYS:HE2	17	0.15
(1,731)	1:148:A:LEU:HD22	1:151:A:LYS:HE2	17	0.15
(1,731)	1:148:A:LEU:HD23	1:151:A:LYS:HE2	17	0.15
(1,719)	1:144:A:LEU:HB2	1:141:A:TYR:HA	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,716)	1:148:A:LEU:HD21	1:147:A:GLU:HG2	18	0.15
(1,716)	1:148:A:LEU:HD22	1:147:A:GLU:HG2	18	0.15
(1,716)	1:148:A:LEU:HD23	1:147:A:GLU:HG2	18	0.15
(1,711)	1:139:A:THR:HG21	1:143:A:ASN:HB2	4	0.15
(1,711)	1:139:A:THR:HG22	1:143:A:ASN:HB2	4	0.15
(1,711)	1:139:A:THR:HG23	1:143:A:ASN:HB2	4	0.15
(1,605)	1:107:A:ASP:HB3	1:110:A:SER:HB3	18	0.15
(1,602)	1:55:A:LEU:HD11	1:100:A:LEU:HG	4	0.15
(1,602)	1:55:A:LEU:HD12	1:100:A:LEU:HG	4	0.15
(1,602)	1:55:A:LEU:HD13	1:100:A:LEU:HG	4	0.15
(1,583)	1:151:A:LYS:HG2	1:151:A:LYS:H	5	0.15
(1,536)	1:70:A:LEU:HD21	1:68:A:LYS:HE2	10	0.15
(1,536)	1:70:A:LEU:HD22	1:68:A:LYS:HE2	10	0.15
(1,536)	1:70:A:LEU:HD23	1:68:A:LYS:HE2	10	0.15
(1,536)	1:70:A:LEU:HD21	1:68:A:LYS:HE3	10	0.15
(1,536)	1:70:A:LEU:HD22	1:68:A:LYS:HE3	10	0.15
(1,536)	1:70:A:LEU:HD23	1:68:A:LYS:HE3	10	0.15
(1,531)	1:92:A:LYS:HD3	1:92:A:LYS:HB2	18	0.15
(1,514)	1:115:A:LYS:H	1:115:A:LYS:HG2	6	0.15
(1,436)	1:6:A:ARG:HG3	1:7:A:PRO:HD2	20	0.15
(1,363)	1:75:A:ARG:HD3	1:75:A:ARG:HB2	3	0.15
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD2	5	0.15
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD3	5	0.15
(1,323)	1:114:A:ARG:HB3	1:115:A:LYS:H	8	0.15
(1,322)	1:115:A:LYS:H	1:114:A:ARG:HB2	13	0.15
(1,312)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	13	0.15
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	14	0.15
(1,300)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	19	0.15
(1,297)	1:99:A:GLU:HG3	1:99:A:GLU:HB2	2	0.15
(1,254)	1:82:A:PRO:HD2	1:81:A:MET:HG2	4	0.15
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD11	16	0.15
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD12	16	0.15
(1,235)	1:23:A:LYS:HB3	1:26:A:ILE:HD13	16	0.15
(1,220)	1:131:A:GLU:HG3	1:131:A:GLU:HB3	12	0.15
(1,213)	1:159:A:THR:H	1:158:A:LYS:HB2	3	0.15
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	12	0.15
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	12	0.15
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	12	0.15
(1,153)	1:103:A:GLU:HG3	1:104:A:LYS:H	7	0.15
(1,122)	1:94:A:ASP:HB3	1:97:A:ILE:HB	16	0.15
(1,112)	1:53:A:ASN:H	1:52:A:GLU:HG3	13	0.15
(1,105)	1:31:A:ASN:HB3	1:32:A:PHE:H	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,105)	1:31:A:ASN:HB3	1:32:A:PHE:H	12	0.15
(1,98)	1:121:A:LEU:HD11	1:141:A:TYR:HB2	5	0.15
(1,98)	1:121:A:LEU:HD12	1:141:A:TYR:HB2	5	0.15
(1,98)	1:121:A:LEU:HD13	1:141:A:TYR:HB2	5	0.15
(1,95)	1:35:A:ASP:HB3	1:34:A:LEU:HB3	15	0.15
(1,91)	1:57:A:TYR:HE1	1:64:A:ASP:HB2	9	0.15
(1,91)	1:57:A:TYR:HE2	1:64:A:ASP:HB2	9	0.15
(1,46)	1:46:A:LEU:HB2	1:47:A:ASP:HA	9	0.15
(1,46)	1:46:A:LEU:HB2	1:47:A:ASP:HA	13	0.15
(1,46)	1:46:A:LEU:HB2	1:47:A:ASP:HA	16	0.15
(1,30)	1:6:A:ARG:HA	1:6:A:ARG:HD2	2	0.15
(1,30)	1:6:A:ARG:HA	1:6:A:ARG:HD3	2	0.15
(1,19)	1:28:A:ARG:HD3	1:28:A:ARG:HA	18	0.15
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB1	8	0.15
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB2	8	0.15
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB3	8	0.15
(1,3)	1:15:A:LYS:HD3	1:8:A:GLY:HA2	18	0.15
(1,1988)	1:156:A:HIS:H	1:156:A:HIS:HD2	19	0.14
(1,1972)	1:20:A:ARG:HB3	1:44:A:PHE:HZ	7	0.14
(1,1969)	1:24:A:SER:HB3	1:44:A:PHE:HZ	17	0.14
(1,1931)	1:58:A:TYR:HD1	1:59:A:LEU:H	5	0.14
(1,1931)	1:58:A:TYR:HD2	1:59:A:LEU:H	5	0.14
(1,1906)	1:57:A:TYR:HD1	1:64:A:ASP:HB2	5	0.14
(1,1906)	1:57:A:TYR:HD2	1:64:A:ASP:HB2	5	0.14
(1,1901)	1:103:A:GLU:H	1:102:A:TYR:HD1	18	0.14
(1,1901)	1:103:A:GLU:H	1:102:A:TYR:HD2	18	0.14
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	2	0.14
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	4	0.14
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	5	0.14
(1,1888)	1:129:A:GLY:H	1:130:A:GLU:H	8	0.14
(1,1887)	1:126:A:HIS:H	1:129:A:GLY:H	2	0.14
(1,1887)	1:126:A:HIS:H	1:129:A:GLY:H	9	0.14
(1,1887)	1:126:A:HIS:H	1:129:A:GLY:H	10	0.14
(1,1872)	1:8:A:GLY:H	1:8:A:GLY:HA2	14	0.14
(1,1838)	1:114:A:ARG:HB3	1:114:A:ARG:H	15	0.14
(1,1806)	1:24:A:SER:H	1:23:A:LYS:HB2	4	0.14
(1,1802)	1:24:A:SER:H	1:25:A:LEU:HG	15	0.14
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	3	0.14
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	6	0.14
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	15	0.14
(1,1718)	1:142:A:VAL:HG21	1:143:A:ASN:H	15	0.14
(1,1718)	1:142:A:VAL:HG22	1:143:A:ASN:H	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1718)	1:142:A:VAL:HG23	1:143:A:ASN:H	15	0.14
(1,1669)	1:93:A:LEU:HB3	1:94:A:ASP:H	6	0.14
(1,1656)	1:122:A:LYS:H	1:122:A:LYS:HG2	3	0.14
(1,1656)	1:122:A:LYS:H	1:122:A:LYS:HG2	7	0.14
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	17	0.14
(1,1633)	1:87:A:CYS:H	1:87:A:CYS:HB3	2	0.14
(1,1633)	1:87:A:CYS:H	1:87:A:CYS:HB3	15	0.14
(1,1614)	1:25:A:LEU:HD11	1:40:A:GLU:H	9	0.14
(1,1614)	1:25:A:LEU:HD12	1:40:A:GLU:H	9	0.14
(1,1614)	1:25:A:LEU:HD13	1:40:A:GLU:H	9	0.14
(1,1613)	1:40:A:GLU:H	1:39:A:LYS:HB3	12	0.14
(1,1604)	1:54:A:ARG:HB3	1:54:A:ARG:H	10	0.14
(1,1604)	1:54:A:ARG:HB3	1:54:A:ARG:H	15	0.14
(1,1585)	1:142:A:VAL:H	1:143:A:ASN:HB2	12	0.14
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	3	0.14
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	3	0.14
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	3	0.14
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	11	0.14
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	11	0.14
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	11	0.14
(1,1548)	1:130:A:GLU:H	1:128:A:TRP:HB3	4	0.14
(1,1524)	1:117:A:ARG:H	1:116:A:MET:H	9	0.14
(1,1522)	1:131:A:GLU:H	1:130:A:GLU:HB3	13	0.14
(1,1511)	1:25:A:LEU:H	1:25:A:LEU:HG	1	0.14
(1,1511)	1:25:A:LEU:H	1:25:A:LEU:HG	4	0.14
(1,1511)	1:25:A:LEU:H	1:25:A:LEU:HG	12	0.14
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	16	0.14
(1,1473)	1:101:A:LYS:HB2	1:102:A:TYR:H	14	0.14
(1,1453)	1:37:A:ILE:H	1:33:A:SER:HA	4	0.14
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	16	0.14
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	19	0.14
(1,1387)	1:103:A:GLU:H	1:103:A:GLU:HB2	15	0.14
(1,1365)	1:26:A:ILE:HB	1:27:A:ASP:H	4	0.14
(1,1352)	1:25:A:LEU:HA	1:27:A:ASP:H	1	0.14
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	14	0.14
(1,1329)	1:121:A:LEU:H	1:118:A:VAL:H	1	0.14
(1,1329)	1:121:A:LEU:H	1:118:A:VAL:H	18	0.14
(1,1311)	1:107:A:ASP:H	1:107:A:ASP:HB2	14	0.14
(1,1310)	1:107:A:ASP:HB3	1:107:A:ASP:H	12	0.14
(1,1308)	1:67:A:THR:HG21	1:66:A:ALA:H	17	0.14
(1,1308)	1:67:A:THR:HG22	1:66:A:ALA:H	17	0.14
(1,1308)	1:67:A:THR:HG23	1:66:A:ALA:H	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1237)	1:81:A:MET:HB3	1:82:A:PRO:HD3	12	0.14
(1,1202)	1:59:A:LEU:HA	1:69:A:ILE:HD11	15	0.14
(1,1202)	1:59:A:LEU:HA	1:69:A:ILE:HD12	15	0.14
(1,1202)	1:59:A:LEU:HA	1:69:A:ILE:HD13	15	0.14
(1,1177)	1:86:A:ILE:HD11	1:81:A:MET:H	3	0.14
(1,1177)	1:86:A:ILE:HD12	1:81:A:MET:H	3	0.14
(1,1177)	1:86:A:ILE:HD13	1:81:A:MET:H	3	0.14
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	5	0.14
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	7	0.14
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	7	0.14
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	18	0.14
(1,1110)	1:116:A:MET:HA	1:117:A:ARG:HD2	15	0.14
(1,1105)	1:103:A:GLU:HA	1:104:A:LYS:HG2	5	0.14
(1,1101)	1:158:A:LYS:HA	1:158:A:LYS:HG3	7	0.14
(1,1062)	1:29:A:GLY:H	1:25:A:LEU:HA	4	0.14
(1,1038)	1:121:A:LEU:HD11	1:121:A:LEU:HA	10	0.14
(1,1038)	1:121:A:LEU:HD12	1:121:A:LEU:HA	10	0.14
(1,1038)	1:121:A:LEU:HD13	1:121:A:LEU:HA	10	0.14
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE1	6	0.14
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE2	6	0.14
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE3	6	0.14
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE1	17	0.14
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE2	17	0.14
(1,1020)	1:15:A:LYS:HD3	1:84:A:MET:HE3	17	0.14
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	8	0.14
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	8	0.14
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	8	0.14
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	10	0.14
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	10	0.14
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	10	0.14
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD2	4	0.14
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD3	4	0.14
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD2	7	0.14
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD3	7	0.14
(1,979)	1:119:A:ALA:HB1	1:122:A:LYS:HD2	5	0.14
(1,979)	1:119:A:ALA:HB2	1:122:A:LYS:HD2	5	0.14
(1,979)	1:119:A:ALA:HB3	1:122:A:LYS:HD2	5	0.14
(1,964)	1:69:A:ILE:HA	1:70:A:LEU:HA	4	0.14
(1,964)	1:69:A:ILE:HA	1:70:A:LEU:HA	17	0.14
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB1	13	0.14
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB2	13	0.14
(1,961)	1:107:A:ASP:HB3	1:109:A:ALA:HB3	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,951)	1:126:A:HIS:HA	1:126:A:HIS:HB2	7	0.14
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	5	0.14
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	15	0.14
(1,910)	1:108:A:LEU:H	1:153:A:ALA:HB1	18	0.14
(1,910)	1:108:A:LEU:H	1:153:A:ALA:HB2	18	0.14
(1,910)	1:108:A:LEU:H	1:153:A:ALA:HB3	18	0.14
(1,906)	1:82:A:PRO:HB3	1:83:A:ALA:HB1	10	0.14
(1,906)	1:82:A:PRO:HB3	1:83:A:ALA:HB2	10	0.14
(1,906)	1:82:A:PRO:HB3	1:83:A:ALA:HB3	10	0.14
(1,904)	1:83:A:ALA:HB1	1:19:A:ASN:HD22	6	0.14
(1,904)	1:83:A:ALA:HB2	1:19:A:ASN:HD22	6	0.14
(1,904)	1:83:A:ALA:HB3	1:19:A:ASN:HD22	6	0.14
(1,897)	1:52:A:GLU:HA	1:52:A:GLU:HG2	2	0.14
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG21	5	0.14
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG22	5	0.14
(1,866)	1:52:A:GLU:HA	1:13:A:VAL:HG23	5	0.14
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG11	19	0.14
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG12	19	0.14
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG13	19	0.14
(1,810)	1:112:A:ASP:HB3	1:111:A:VAL:HA	8	0.14
(1,797)	1:138:A:LYS:HA	1:138:A:LYS:HG2	17	0.14
(1,786)	1:75:A:ARG:HA	1:75:A:ARG:HD2	15	0.14
(1,765)	1:155:A:THR:H	1:155:A:THR:HG21	19	0.14
(1,765)	1:155:A:THR:H	1:155:A:THR:HG22	19	0.14
(1,765)	1:155:A:THR:H	1:155:A:THR:HG23	19	0.14
(1,719)	1:144:A:LEU:HB2	1:141:A:TYR:HA	14	0.14
(1,711)	1:139:A:THR:HG21	1:143:A:ASN:HB2	13	0.14
(1,711)	1:139:A:THR:HG22	1:143:A:ASN:HB2	13	0.14
(1,711)	1:139:A:THR:HG23	1:143:A:ASN:HB2	13	0.14
(1,677)	1:59:A:LEU:HB3	1:56:A:CYS:HA	1	0.14
(1,582)	1:151:A:LYS:H	1:151:A:LYS:HG3	14	0.14
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD11	2	0.14
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD12	2	0.14
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD13	2	0.14
(1,566)	1:46:A:LEU:HD11	1:43:A:SER:HB3	4	0.14
(1,566)	1:46:A:LEU:HD12	1:43:A:SER:HB3	4	0.14
(1,566)	1:46:A:LEU:HD13	1:43:A:SER:HB3	4	0.14
(1,552)	1:31:A:ASN:HD21	1:33:A:SER:HB2	15	0.14
(1,534)	1:23:A:LYS:HA	1:23:A:LYS:HG3	4	0.14
(1,513)	1:121:A:LEU:HD21	1:138:A:LYS:HG2	2	0.14
(1,513)	1:121:A:LEU:HD22	1:138:A:LYS:HG2	2	0.14
(1,513)	1:121:A:LEU:HD23	1:138:A:LYS:HG2	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,513)	1:121:A:LEU:HD21	1:138:A:LYS:HG3	2	0.14
(1,513)	1:121:A:LEU:HD22	1:138:A:LYS:HG3	2	0.14
(1,513)	1:121:A:LEU:HD23	1:138:A:LYS:HG3	2	0.14
(1,439)	1:147:A:GLU:HG2	1:144:A:LEU:HG	20	0.14
(1,417)	1:93:A:LEU:HG	1:90:A:LEU:HA	4	0.14
(1,415)	1:113:A:LEU:H	1:113:A:LEU:HG	8	0.14
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD2	13	0.14
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD3	13	0.14
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	18	0.14
(1,289)	1:67:A:THR:HB	1:67:A:THR:H	1	0.14
(1,254)	1:82:A:PRO:HD2	1:81:A:MET:HG2	15	0.14
(1,252)	1:151:A:LYS:HB3	1:152:A:TYR:HD1	1	0.14
(1,252)	1:151:A:LYS:HB3	1:152:A:TYR:HD2	1	0.14
(1,234)	1:26:A:ILE:HD11	1:23:A:LYS:HB2	9	0.14
(1,234)	1:26:A:ILE:HD12	1:23:A:LYS:HB2	9	0.14
(1,234)	1:26:A:ILE:HD13	1:23:A:LYS:HB2	9	0.14
(1,220)	1:131:A:GLU:HG3	1:131:A:GLU:HB3	2	0.14
(1,188)	1:96:A:GLN:HA	1:96:A:GLN:HG2	10	0.14
(1,168)	1:17:A:PHE:H	1:16:A:GLU:HG2	4	0.14
(1,163)	1:2:A:GLU:HA	1:2:A:GLU:HG2	5	0.14
(1,146)	1:88:A:GLU:HA	1:88:A:GLU:HG2	18	0.14
(1,142)	1:88:A:GLU:HG3	1:89:A:LYS:H	11	0.14
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG21	3	0.14
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG22	3	0.14
(1,113)	1:52:A:GLU:HG3	1:13:A:VAL:HG23	3	0.14
(1,105)	1:31:A:ASN:HB3	1:32:A:PHE:H	18	0.14
(1,76)	1:140:A:ASP:HB2	1:135:A:CYS:HA	2	0.14
(1,48)	1:86:A:ILE:HG21	1:89:A:LYS:HE3	6	0.14
(1,48)	1:86:A:ILE:HG22	1:89:A:LYS:HE3	6	0.14
(1,48)	1:86:A:ILE:HG23	1:89:A:LYS:HE3	6	0.14
(1,46)	1:46:A:LEU:HB2	1:47:A:ASP:HA	5	0.14
(1,16)	1:20:A:ARG:HD2	1:20:A:ARG:HB2	3	0.14
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB1	7	0.14
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB2	7	0.14
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB3	7	0.14
(1,12)	1:28:A:ARG:H	1:28:A:ARG:HD2	16	0.14
(1,12)	1:28:A:ARG:H	1:28:A:ARG:HD3	16	0.14
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	11	0.14
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	11	0.14
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	11	0.14
(1,2013)	1:151:A:LYS:HE3	1:152:A:TYR:HE1	2	0.13
(1,2013)	1:151:A:LYS:HE3	1:152:A:TYR:HE2	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2002)	1:22:A:TYR:HA	1:22:A:TYR:HE1	4	0.13
(1,2002)	1:22:A:TYR:HA	1:22:A:TYR:HE2	4	0.13
(1,1988)	1:156:A:HIS:H	1:156:A:HIS:HD2	3	0.13
(1,1979)	1:148:A:LEU:HB3	1:128:A:TRP:HH2	15	0.13
(1,1965)	1:26:A:ILE:HG13	1:32:A:PHE:HZ	4	0.13
(1,1964)	1:21:A:PHE:HD1	1:44:A:PHE:HZ	9	0.13
(1,1964)	1:21:A:PHE:HD2	1:44:A:PHE:HZ	9	0.13
(1,1964)	1:21:A:PHE:HD1	1:44:A:PHE:HZ	13	0.13
(1,1964)	1:21:A:PHE:HD2	1:44:A:PHE:HZ	13	0.13
(1,1954)	1:44:A:PHE:HE1	1:20:A:ARG:HB2	19	0.13
(1,1954)	1:44:A:PHE:HE2	1:20:A:ARG:HB2	19	0.13
(1,1913)	1:141:A:TYR:H	1:141:A:TYR:HD1	14	0.13
(1,1913)	1:141:A:TYR:H	1:141:A:TYR:HD2	14	0.13
(1,1908)	1:58:A:TYR:H	1:57:A:TYR:HD1	5	0.13
(1,1908)	1:58:A:TYR:H	1:57:A:TYR:HD2	5	0.13
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	7	0.13
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	17	0.13
(1,1887)	1:126:A:HIS:H	1:129:A:GLY:H	14	0.13
(1,1879)	1:4:A:GLY:HA3	1:5:A:GLY:H	13	0.13
(1,1876)	1:49:A:LYS:HB3	1:50:A:GLY:H	12	0.13
(1,1872)	1:8:A:GLY:H	1:8:A:GLY:HA2	1	0.13
(1,1872)	1:8:A:GLY:H	1:8:A:GLY:HA2	10	0.13
(1,1839)	1:114:A:ARG:H	1:114:A:ARG:HG3	19	0.13
(1,1835)	1:114:A:ARG:H	1:114:A:ARG:HD2	11	0.13
(1,1822)	1:97:A:ILE:HD11	1:96:A:GLN:HE21	9	0.13
(1,1822)	1:97:A:ILE:HD12	1:96:A:GLN:HE21	9	0.13
(1,1822)	1:97:A:ILE:HD13	1:96:A:GLN:HE21	9	0.13
(1,1818)	1:36:A:THR:HG21	1:31:A:ASN:HD22	3	0.13
(1,1818)	1:36:A:THR:HG22	1:31:A:ASN:HD22	3	0.13
(1,1818)	1:36:A:THR:HG23	1:31:A:ASN:HD22	3	0.13
(1,1818)	1:36:A:THR:HG21	1:31:A:ASN:HD22	11	0.13
(1,1818)	1:36:A:THR:HG22	1:31:A:ASN:HD22	11	0.13
(1,1818)	1:36:A:THR:HG23	1:31:A:ASN:HD22	11	0.13
(1,1818)	1:36:A:THR:HG21	1:31:A:ASN:HD22	20	0.13
(1,1818)	1:36:A:THR:HG22	1:31:A:ASN:HD22	20	0.13
(1,1818)	1:36:A:THR:HG23	1:31:A:ASN:HD22	20	0.13
(1,1806)	1:24:A:SER:H	1:23:A:LYS:HB2	15	0.13
(1,1802)	1:24:A:SER:H	1:25:A:LEU:HG	3	0.13
(1,1802)	1:24:A:SER:H	1:25:A:LEU:HG	6	0.13
(1,1802)	1:24:A:SER:H	1:25:A:LEU:HG	10	0.13
(1,1771)	1:35:A:ASP:H	1:34:A:LEU:HB3	6	0.13
(1,1760)	1:120:A:GLU:H	1:120:A:GLU:HB3	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1718)	1:142:A:VAL:HG21	1:143:A:ASN:H	7	0.13
(1,1718)	1:142:A:VAL:HG22	1:143:A:ASN:H	7	0.13
(1,1718)	1:142:A:VAL:HG23	1:143:A:ASN:H	7	0.13
(1,1667)	1:30:A:VAL:HG11	1:28:A:ARG:HE	5	0.13
(1,1667)	1:30:A:VAL:HG12	1:28:A:ARG:HE	5	0.13
(1,1667)	1:30:A:VAL:HG13	1:28:A:ARG:HE	5	0.13
(1,1666)	1:30:A:VAL:HB	1:28:A:ARG:HE	18	0.13
(1,1633)	1:87:A:CYS:H	1:87:A:CYS:HB3	6	0.13
(1,1633)	1:87:A:CYS:H	1:87:A:CYS:HB3	12	0.13
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	7	0.13
(1,1614)	1:25:A:LEU:HD11	1:40:A:GLU:H	11	0.13
(1,1614)	1:25:A:LEU:HD12	1:40:A:GLU:H	11	0.13
(1,1614)	1:25:A:LEU:HD13	1:40:A:GLU:H	11	0.13
(1,1614)	1:25:A:LEU:HD11	1:40:A:GLU:H	17	0.13
(1,1614)	1:25:A:LEU:HD12	1:40:A:GLU:H	17	0.13
(1,1614)	1:25:A:LEU:HD13	1:40:A:GLU:H	17	0.13
(1,1614)	1:25:A:LEU:HD11	1:40:A:GLU:H	20	0.13
(1,1614)	1:25:A:LEU:HD12	1:40:A:GLU:H	20	0.13
(1,1614)	1:25:A:LEU:HD13	1:40:A:GLU:H	20	0.13
(1,1609)	1:49:A:LYS:H	1:49:A:LYS:HB2	3	0.13
(1,1604)	1:54:A:ARG:HB3	1:54:A:ARG:H	1	0.13
(1,1604)	1:54:A:ARG:HB3	1:54:A:ARG:H	2	0.13
(1,1590)	1:55:A:LEU:H	1:100:A:LEU:HG	1	0.13
(1,1586)	1:143:A:ASN:HB3	1:142:A:VAL:H	17	0.13
(1,1576)	1:28:A:ARG:H	1:30:A:VAL:H	4	0.13
(1,1553)	1:93:A:LEU:H	1:92:A:LYS:HB2	1	0.13
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	5	0.13
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	15	0.13
(1,1527)	1:116:A:MET:H	1:115:A:LYS:HB2	4	0.13
(1,1527)	1:116:A:MET:H	1:115:A:LYS:HB2	9	0.13
(1,1527)	1:116:A:MET:H	1:115:A:LYS:HB2	11	0.13
(1,1524)	1:117:A:ARG:H	1:116:A:MET:H	11	0.13
(1,1524)	1:117:A:ARG:H	1:116:A:MET:H	12	0.13
(1,1517)	1:89:A:LYS:H	1:90:A:LEU:HD21	4	0.13
(1,1517)	1:89:A:LYS:H	1:90:A:LEU:HD22	4	0.13
(1,1517)	1:89:A:LYS:H	1:90:A:LEU:HD23	4	0.13
(1,1511)	1:25:A:LEU:H	1:25:A:LEU:HG	9	0.13
(1,1511)	1:25:A:LEU:H	1:25:A:LEU:HG	16	0.13
(1,1511)	1:25:A:LEU:H	1:25:A:LEU:HG	18	0.13
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB2	6	0.13
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB3	6	0.13
(1,1483)	1:22:A:TYR:H	1:22:A:TYR:HB3	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1471)	1:102:A:TYR:H	1:101:A:LYS:HA	11	0.13
(1,1471)	1:102:A:TYR:H	1:101:A:LYS:HA	12	0.13
(1,1471)	1:102:A:TYR:H	1:101:A:LYS:HA	16	0.13
(1,1471)	1:102:A:TYR:H	1:101:A:LYS:HA	17	0.13
(1,1471)	1:102:A:TYR:H	1:101:A:LYS:HA	19	0.13
(1,1446)	1:96:A:GLN:HG3	1:96:A:GLN:H	1	0.13
(1,1446)	1:96:A:GLN:HG3	1:96:A:GLN:H	12	0.13
(1,1429)	1:155:A:THR:HB	1:156:A:HIS:H	13	0.13
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	1	0.13
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	2	0.13
(1,1368)	1:113:A:LEU:H	1:112:A:ASP:H	1	0.13
(1,1359)	1:63:A:LYS:HB3	1:65:A:ALA:H	3	0.13
(1,1359)	1:63:A:LYS:HB3	1:65:A:ALA:H	8	0.13
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	10	0.13
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	13	0.13
(1,1329)	1:121:A:LEU:H	1:118:A:VAL:H	6	0.13
(1,1329)	1:121:A:LEU:H	1:118:A:VAL:H	8	0.13
(1,1329)	1:121:A:LEU:H	1:118:A:VAL:H	12	0.13
(1,1329)	1:121:A:LEU:H	1:118:A:VAL:H	14	0.13
(1,1311)	1:107:A:ASP:H	1:107:A:ASP:HB2	18	0.13
(1,1310)	1:107:A:ASP:HB3	1:107:A:ASP:H	10	0.13
(1,1278)	1:127:A:SER:HB3	1:128:A:TRP:HE1	13	0.13
(1,1219)	1:155:A:THR:H	1:154:A:ALA:HA	8	0.13
(1,1197)	1:156:A:HIS:HA	1:157:A:PRO:HD2	2	0.13
(1,1161)	1:119:A:ALA:HA	1:122:A:LYS:HG2	18	0.13
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD11	4	0.13
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD12	4	0.13
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD13	4	0.13
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	8	0.13
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	10	0.13
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	10	0.13
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	10	0.13
(1,1101)	1:158:A:LYS:HA	1:158:A:LYS:HG3	2	0.13
(1,1101)	1:158:A:LYS:HA	1:158:A:LYS:HG3	12	0.13
(1,1091)	1:14:A:CYS:HA	1:97:A:ILE:HG21	14	0.13
(1,1091)	1:14:A:CYS:HA	1:97:A:ILE:HG22	14	0.13
(1,1091)	1:14:A:CYS:HA	1:97:A:ILE:HG23	14	0.13
(1,1064)	1:77:A:MET:HE1	1:22:A:TYR:HA	15	0.13
(1,1064)	1:77:A:MET:HE2	1:22:A:TYR:HA	15	0.13
(1,1064)	1:77:A:MET:HE3	1:22:A:TYR:HA	15	0.13
(1,1049)	1:140:A:ASP:HB3	1:140:A:ASP:HA	10	0.13
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE1	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE2	9	0.13
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE3	9	0.13
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE1	11	0.13
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE2	11	0.13
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE3	11	0.13
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE1	12	0.13
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE2	12	0.13
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE3	12	0.13
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE1	2	0.13
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE2	2	0.13
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE3	2	0.13
(1,1019)	1:84:A:MET:HE1	1:15:A:LYS:HD2	13	0.13
(1,1019)	1:84:A:MET:HE2	1:15:A:LYS:HD2	13	0.13
(1,1019)	1:84:A:MET:HE3	1:15:A:LYS:HD2	13	0.13
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD2	2	0.13
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD3	2	0.13
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD2	20	0.13
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD3	20	0.13
(1,999)	1:114:A:ARG:HA	1:114:A:ARG:HB2	2	0.13
(1,979)	1:119:A:ALA:HB1	1:122:A:LYS:HD2	8	0.13
(1,979)	1:119:A:ALA:HB2	1:122:A:LYS:HD2	8	0.13
(1,979)	1:119:A:ALA:HB3	1:122:A:LYS:HD2	8	0.13
(1,951)	1:126:A:HIS:HA	1:126:A:HIS:HB2	2	0.13
(1,931)	1:153:A:ALA:HB1	1:154:A:ALA:H	18	0.13
(1,931)	1:153:A:ALA:HB2	1:154:A:ALA:H	18	0.13
(1,931)	1:153:A:ALA:HB3	1:154:A:ALA:H	18	0.13
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	13	0.13
(1,910)	1:108:A:LEU:H	1:153:A:ALA:HB1	20	0.13
(1,910)	1:108:A:LEU:H	1:153:A:ALA:HB2	20	0.13
(1,910)	1:108:A:LEU:H	1:153:A:ALA:HB3	20	0.13
(1,906)	1:82:A:PRO:HB3	1:83:A:ALA:HB1	19	0.13
(1,906)	1:82:A:PRO:HB3	1:83:A:ALA:HB2	19	0.13
(1,906)	1:82:A:PRO:HB3	1:83:A:ALA:HB3	19	0.13
(1,904)	1:83:A:ALA:HB1	1:19:A:ASN:HD22	7	0.13
(1,904)	1:83:A:ALA:HB2	1:19:A:ASN:HD22	7	0.13
(1,904)	1:83:A:ALA:HB3	1:19:A:ASN:HD22	7	0.13
(1,884)	1:61:A:ALA:HB1	1:56:A:CYS:HB2	6	0.13
(1,884)	1:61:A:ALA:HB2	1:56:A:CYS:HB2	6	0.13
(1,884)	1:61:A:ALA:HB3	1:56:A:CYS:HB2	6	0.13
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG11	16	0.13
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG12	16	0.13
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG13	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,790)	1:95:A:SER:HA	1:91:A:LYS:HA	5	0.13
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD11	13	0.13
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD12	13	0.13
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD13	13	0.13
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD11	13	0.13
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD12	13	0.13
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD13	13	0.13
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD11	13	0.13
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD12	13	0.13
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD13	13	0.13
(1,765)	1:155:A:THR:H	1:155:A:THR:HG21	13	0.13
(1,765)	1:155:A:THR:H	1:155:A:THR:HG22	13	0.13
(1,765)	1:155:A:THR:H	1:155:A:THR:HG23	13	0.13
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB1	12	0.13
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB2	12	0.13
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB3	12	0.13
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB1	13	0.13
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB2	13	0.13
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB3	13	0.13
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB1	17	0.13
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB2	17	0.13
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB3	17	0.13
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB1	18	0.13
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB2	18	0.13
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB3	18	0.13
(1,642)	1:54:A:ARG:HD3	1:100:A:LEU:HD21	17	0.13
(1,642)	1:54:A:ARG:HD3	1:100:A:LEU:HD22	17	0.13
(1,642)	1:54:A:ARG:HD3	1:100:A:LEU:HD23	17	0.13
(1,622)	1:51:A:LYS:HA	1:100:A:LEU:HD21	5	0.13
(1,622)	1:51:A:LYS:HA	1:100:A:LEU:HD22	5	0.13
(1,622)	1:51:A:LYS:HA	1:100:A:LEU:HD23	5	0.13
(1,590)	1:63:A:LYS:H	1:63:A:LYS:HG2	4	0.13
(1,590)	1:63:A:LYS:H	1:63:A:LYS:HG3	4	0.13
(1,583)	1:151:A:LYS:HG2	1:151:A:LYS:H	3	0.13
(1,573)	1:106:A:LEU:HD21	1:108:A:LEU:HA	17	0.13
(1,573)	1:106:A:LEU:HD22	1:108:A:LEU:HA	17	0.13
(1,573)	1:106:A:LEU:HD23	1:108:A:LEU:HA	17	0.13
(1,566)	1:46:A:LEU:HD11	1:43:A:SER:HB3	12	0.13
(1,566)	1:46:A:LEU:HD12	1:43:A:SER:HB3	12	0.13
(1,566)	1:46:A:LEU:HD13	1:43:A:SER:HB3	12	0.13
(1,557)	1:158:A:LYS:HE3	1:158:A:LYS:HG3	4	0.13
(1,557)	1:158:A:LYS:HE2	1:158:A:LYS:HG3	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	1:13:A:VAL:HA	1:55:A:LEU:HD11	17	0.13
(1,522)	1:13:A:VAL:HA	1:55:A:LEU:HD12	17	0.13
(1,522)	1:13:A:VAL:HA	1:55:A:LEU:HD13	17	0.13
(1,514)	1:115:A:LYS:H	1:115:A:LYS:HG2	19	0.13
(1,513)	1:121:A:LEU:HD21	1:138:A:LYS:HG2	8	0.13
(1,513)	1:121:A:LEU:HD22	1:138:A:LYS:HG2	8	0.13
(1,513)	1:121:A:LEU:HD23	1:138:A:LYS:HG2	8	0.13
(1,513)	1:121:A:LEU:HD21	1:138:A:LYS:HG3	8	0.13
(1,513)	1:121:A:LEU:HD22	1:138:A:LYS:HG3	8	0.13
(1,513)	1:121:A:LEU:HD23	1:138:A:LYS:HG3	8	0.13
(1,466)	1:90:A:LEU:HD11	1:90:A:LEU:H	16	0.13
(1,466)	1:90:A:LEU:HD12	1:90:A:LEU:H	16	0.13
(1,466)	1:90:A:LEU:HD13	1:90:A:LEU:H	16	0.13
(1,438)	1:6:A:ARG:HG3	1:6:A:ARG:HB3	18	0.13
(1,422)	1:106:A:LEU:HG	1:107:A:ASP:H	12	0.13
(1,415)	1:113:A:LEU:H	1:113:A:LEU:HG	1	0.13
(1,409)	1:161:A:LEU:H	1:161:A:LEU:HG	7	0.13
(1,409)	1:161:A:LEU:H	1:161:A:LEU:HG	18	0.13
(1,390)	1:117:A:ARG:HG3	1:117:A:ARG:HA	5	0.13
(1,386)	1:77:A:MET:H	1:76:A:PRO:HG3	10	0.13
(1,340)	1:36:A:THR:HA	1:39:A:LYS:HD2	2	0.13
(1,340)	1:36:A:THR:HA	1:39:A:LYS:HD3	2	0.13
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD2	7	0.13
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD2	7	0.13
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD2	7	0.13
(1,338)	1:13:A:VAL:HG11	1:101:A:LYS:HD3	7	0.13
(1,338)	1:13:A:VAL:HG12	1:101:A:LYS:HD3	7	0.13
(1,338)	1:13:A:VAL:HG13	1:101:A:LYS:HD3	7	0.13
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	14	0.13
(1,323)	1:114:A:ARG:HB3	1:115:A:LYS:H	1	0.13
(1,313)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	11	0.13
(1,312)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	3	0.13
(1,244)	1:85:A:LYS:HB3	1:81:A:MET:HG2	19	0.13
(1,237)	1:148:A:LEU:HA	1:151:A:LYS:HB3	2	0.13
(1,219)	1:131:A:GLU:HB3	1:131:A:GLU:HG2	13	0.13
(1,198)	1:112:A:ASP:H	1:111:A:VAL:HB	13	0.13
(1,178)	1:136:A:ALA:HB1	1:137:A:GLU:HG2	14	0.13
(1,178)	1:136:A:ALA:HB2	1:137:A:GLU:HG2	14	0.13
(1,178)	1:136:A:ALA:HB3	1:137:A:GLU:HG2	14	0.13
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	20	0.13
(1,169)	1:16:A:GLU:HA	1:16:A:GLU:HG2	4	0.13
(1,61)	1:122:A:LYS:HE3	1:141:A:TYR:HE1	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,61)	1:122:A:LYS:HE3	1:141:A:TYR:HE2	13	0.13
(1,46)	1:46:A:LEU:HB2	1:47:A:ASP:HA	14	0.13
(1,46)	1:46:A:LEU:HB2	1:47:A:ASP:HA	18	0.13
(1,43)	1:51:A:LYS:HE2	1:51:A:LYS:HG2	20	0.13
(1,30)	1:6:A:ARG:HA	1:6:A:ARG:HD2	9	0.13
(1,30)	1:6:A:ARG:HA	1:6:A:ARG:HD3	9	0.13
(1,26)	1:117:A:ARG:HB3	1:117:A:ARG:HD2	13	0.13
(1,17)	1:20:A:ARG:HB3	1:20:A:ARG:HD2	15	0.13
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB1	6	0.13
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB2	6	0.13
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB3	6	0.13
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB1	19	0.13
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB2	19	0.13
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB3	19	0.13
(1,12)	1:28:A:ARG:H	1:28:A:ARG:HD2	5	0.13
(1,12)	1:28:A:ARG:H	1:28:A:ARG:HD3	5	0.13
(1,12)	1:28:A:ARG:H	1:28:A:ARG:HD2	10	0.13
(1,12)	1:28:A:ARG:H	1:28:A:ARG:HD3	10	0.13
(1,9)	1:8:A:GLY:HA2	1:15:A:LYS:HE2	20	0.13
(1,9)	1:8:A:GLY:HA3	1:15:A:LYS:HE2	20	0.13
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG11	10	0.12
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG12	10	0.12
(1,1997)	1:141:A:TYR:HE1	1:118:A:VAL:HG13	10	0.12
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG11	10	0.12
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG12	10	0.12
(1,1997)	1:141:A:TYR:HE2	1:118:A:VAL:HG13	10	0.12
(1,1986)	1:156:A:HIS:HA	1:156:A:HIS:HD2	8	0.12
(1,1964)	1:21:A:PHE:HD1	1:44:A:PHE:HZ	17	0.12
(1,1964)	1:21:A:PHE:HD2	1:44:A:PHE:HZ	17	0.12
(1,1964)	1:21:A:PHE:HD1	1:44:A:PHE:HZ	19	0.12
(1,1964)	1:21:A:PHE:HD2	1:44:A:PHE:HZ	19	0.12
(1,1939)	1:55:A:LEU:HD21	1:17:A:PHE:HE1	19	0.12
(1,1939)	1:55:A:LEU:HD21	1:17:A:PHE:HE2	19	0.12
(1,1939)	1:55:A:LEU:HD22	1:17:A:PHE:HE1	19	0.12
(1,1939)	1:55:A:LEU:HD22	1:17:A:PHE:HE2	19	0.12
(1,1939)	1:55:A:LEU:HD23	1:17:A:PHE:HE1	19	0.12
(1,1939)	1:55:A:LEU:HD23	1:17:A:PHE:HE2	19	0.12
(1,1907)	1:64:A:ASP:HB3	1:57:A:TYR:HD1	17	0.12
(1,1907)	1:64:A:ASP:HB3	1:57:A:TYR:HD2	17	0.12
(1,1887)	1:126:A:HIS:H	1:129:A:GLY:H	4	0.12
(1,1887)	1:126:A:HIS:H	1:129:A:GLY:H	6	0.12
(1,1887)	1:126:A:HIS:H	1:129:A:GLY:H	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1883)	1:49:A:LYS:H	1:48:A:THR:H	9	0.12
(1,1872)	1:8:A:GLY:H	1:8:A:GLY:HA2	2	0.12
(1,1872)	1:8:A:GLY:H	1:8:A:GLY:HA2	15	0.12
(1,1872)	1:8:A:GLY:H	1:8:A:GLY:HA2	19	0.12
(1,1851)	1:155:A:THR:H	1:153:A:ALA:HB1	17	0.12
(1,1851)	1:155:A:THR:H	1:153:A:ALA:HB2	17	0.12
(1,1851)	1:155:A:THR:H	1:153:A:ALA:HB3	17	0.12
(1,1818)	1:36:A:THR:HG21	1:31:A:ASN:HD22	15	0.12
(1,1818)	1:36:A:THR:HG22	1:31:A:ASN:HD22	15	0.12
(1,1818)	1:36:A:THR:HG23	1:31:A:ASN:HD22	15	0.12
(1,1818)	1:36:A:THR:HG21	1:31:A:ASN:HD22	19	0.12
(1,1818)	1:36:A:THR:HG22	1:31:A:ASN:HD22	19	0.12
(1,1818)	1:36:A:THR:HG23	1:31:A:ASN:HD22	19	0.12
(1,1806)	1:24:A:SER:H	1:23:A:LYS:HB2	20	0.12
(1,1802)	1:24:A:SER:H	1:25:A:LEU:HG	9	0.12
(1,1750)	1:18:A:LEU:HB3	1:18:A:LEU:H	15	0.12
(1,1750)	1:18:A:LEU:HB3	1:18:A:LEU:H	20	0.12
(1,1718)	1:142:A:VAL:HG21	1:143:A:ASN:H	4	0.12
(1,1718)	1:142:A:VAL:HG22	1:143:A:ASN:H	4	0.12
(1,1718)	1:142:A:VAL:HG23	1:143:A:ASN:H	4	0.12
(1,1718)	1:142:A:VAL:HG21	1:143:A:ASN:H	13	0.12
(1,1718)	1:142:A:VAL:HG22	1:143:A:ASN:H	13	0.12
(1,1718)	1:142:A:VAL:HG23	1:143:A:ASN:H	13	0.12
(1,1718)	1:142:A:VAL:HG21	1:143:A:ASN:H	14	0.12
(1,1718)	1:142:A:VAL:HG22	1:143:A:ASN:H	14	0.12
(1,1718)	1:142:A:VAL:HG23	1:143:A:ASN:H	14	0.12
(1,1718)	1:142:A:VAL:HG21	1:143:A:ASN:H	17	0.12
(1,1718)	1:142:A:VAL:HG22	1:143:A:ASN:H	17	0.12
(1,1718)	1:142:A:VAL:HG23	1:143:A:ASN:H	17	0.12
(1,1686)	1:13:A:VAL:HG21	1:52:A:GLU:H	12	0.12
(1,1686)	1:13:A:VAL:HG22	1:52:A:GLU:H	12	0.12
(1,1686)	1:13:A:VAL:HG23	1:52:A:GLU:H	12	0.12
(1,1660)	1:39:A:LYS:H	1:38:A:GLU:HB2	3	0.12
(1,1656)	1:122:A:LYS:H	1:122:A:LYS:HG2	12	0.12
(1,1656)	1:122:A:LYS:H	1:122:A:LYS:HG2	15	0.12
(1,1648)	1:94:A:ASP:HB3	1:97:A:ILE:H	4	0.12
(1,1647)	1:97:A:ILE:H	1:94:A:ASP:HB2	2	0.12
(1,1614)	1:25:A:LEU:HD11	1:40:A:GLU:H	19	0.12
(1,1614)	1:25:A:LEU:HD12	1:40:A:GLU:H	19	0.12
(1,1614)	1:25:A:LEU:HD13	1:40:A:GLU:H	19	0.12
(1,1613)	1:40:A:GLU:H	1:39:A:LYS:HB3	3	0.12
(1,1613)	1:40:A:GLU:H	1:39:A:LYS:HB3	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1604)	1:54:A:ARG:HB3	1:54:A:ARG:H	4	0.12
(1,1590)	1:55:A:LEU:H	1:100:A:LEU:HG	17	0.12
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD21	2	0.12
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD22	2	0.12
(1,1577)	1:117:A:ARG:H	1:121:A:LEU:HD23	2	0.12
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	8	0.12
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	10	0.12
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	13	0.12
(1,1529)	1:131:A:GLU:H	1:131:A:GLU:HB2	4	0.12
(1,1527)	1:116:A:MET:H	1:115:A:LYS:HB2	6	0.12
(1,1527)	1:116:A:MET:H	1:115:A:LYS:HB2	12	0.12
(1,1524)	1:117:A:ARG:H	1:116:A:MET:H	15	0.12
(1,1511)	1:25:A:LEU:H	1:25:A:LEU:HG	5	0.12
(1,1511)	1:25:A:LEU:H	1:25:A:LEU:HG	6	0.12
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB2	14	0.12
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB3	14	0.12
(1,1471)	1:102:A:TYR:H	1:101:A:LYS:HA	3	0.12
(1,1471)	1:102:A:TYR:H	1:101:A:LYS:HA	7	0.12
(1,1429)	1:155:A:THR:HB	1:156:A:HIS:H	18	0.12
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	12	0.12
(1,1413)	1:123:A:GLN:HB3	1:124:A:ILE:H	17	0.12
(1,1379)	1:158:A:LYS:H	1:157:A:PRO:HB3	5	0.12
(1,1379)	1:158:A:LYS:H	1:157:A:PRO:HB3	18	0.12
(1,1359)	1:63:A:LYS:HB3	1:65:A:ALA:H	14	0.12
(1,1353)	1:25:A:LEU:HB3	1:27:A:ASP:H	10	0.12
(1,1352)	1:25:A:LEU:HA	1:27:A:ASP:H	16	0.12
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	1	0.12
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	19	0.12
(1,1329)	1:121:A:LEU:H	1:118:A:VAL:H	3	0.12
(1,1329)	1:121:A:LEU:H	1:118:A:VAL:H	4	0.12
(1,1329)	1:121:A:LEU:H	1:118:A:VAL:H	7	0.12
(1,1328)	1:2:A:GLU:HB2	1:2:A:GLU:H	8	0.12
(1,1328)	1:2:A:GLU:HB2	1:2:A:GLU:H	17	0.12
(1,1295)	1:108:A:LEU:H	1:107:A:ASP:H	13	0.12
(1,1295)	1:108:A:LEU:H	1:107:A:ASP:H	19	0.12
(1,1218)	1:67:A:THR:H	1:66:A:ALA:HA	4	0.12
(1,1174)	1:49:A:LYS:HA	1:49:A:LYS:HG2	11	0.12
(1,1174)	1:49:A:LYS:HA	1:49:A:LYS:HG3	11	0.12
(1,1174)	1:49:A:LYS:HA	1:49:A:LYS:HG2	13	0.12
(1,1174)	1:49:A:LYS:HA	1:49:A:LYS:HG3	13	0.12
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	2	0.12
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	15	0.12
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD11	6	0.12
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD12	6	0.12
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD13	6	0.12
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD11	9	0.12
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD12	9	0.12
(1,1141)	1:121:A:LEU:HB2	1:145:A:ILE:HD13	9	0.12
(1,1125)	1:104:A:LYS:HA	1:104:A:LYS:HG2	14	0.12
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE1	3	0.12
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE2	3	0.12
(1,1116)	1:79:A:VAL:HG21	1:81:A:MET:HE3	3	0.12
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE1	3	0.12
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE2	3	0.12
(1,1116)	1:79:A:VAL:HG22	1:81:A:MET:HE3	3	0.12
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE1	3	0.12
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE2	3	0.12
(1,1116)	1:79:A:VAL:HG23	1:81:A:MET:HE3	3	0.12
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	9	0.12
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	9	0.12
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	9	0.12
(1,1111)	1:117:A:ARG:HD3	1:116:A:MET:HA	6	0.12
(1,1103)	1:103:A:GLU:HA	1:103:A:GLU:HG2	15	0.12
(1,1101)	1:158:A:LYS:HA	1:158:A:LYS:HG3	17	0.12
(1,1027)	1:124:A:ILE:HG21	1:116:A:MET:HE1	2	0.12
(1,1027)	1:124:A:ILE:HG21	1:116:A:MET:HE2	2	0.12
(1,1027)	1:124:A:ILE:HG21	1:116:A:MET:HE3	2	0.12
(1,1027)	1:124:A:ILE:HG22	1:116:A:MET:HE1	2	0.12
(1,1027)	1:124:A:ILE:HG22	1:116:A:MET:HE2	2	0.12
(1,1027)	1:124:A:ILE:HG22	1:116:A:MET:HE3	2	0.12
(1,1027)	1:124:A:ILE:HG23	1:116:A:MET:HE1	2	0.12
(1,1027)	1:124:A:ILE:HG23	1:116:A:MET:HE2	2	0.12
(1,1027)	1:124:A:ILE:HG23	1:116:A:MET:HE3	2	0.12
(1,1027)	1:124:A:ILE:HG21	1:116:A:MET:HE1	6	0.12
(1,1027)	1:124:A:ILE:HG21	1:116:A:MET:HE2	6	0.12
(1,1027)	1:124:A:ILE:HG21	1:116:A:MET:HE3	6	0.12
(1,1027)	1:124:A:ILE:HG22	1:116:A:MET:HE1	6	0.12
(1,1027)	1:124:A:ILE:HG22	1:116:A:MET:HE2	6	0.12
(1,1027)	1:124:A:ILE:HG22	1:116:A:MET:HE3	6	0.12
(1,1027)	1:124:A:ILE:HG23	1:116:A:MET:HE1	6	0.12
(1,1027)	1:124:A:ILE:HG23	1:116:A:MET:HE2	6	0.12
(1,1027)	1:124:A:ILE:HG23	1:116:A:MET:HE3	6	0.12
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE1	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE2	19	0.12
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE3	19	0.12
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE1	17	0.12
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE2	17	0.12
(1,1024)	1:113:A:LEU:HA	1:116:A:MET:HE3	17	0.12
(1,1019)	1:84:A:MET:HE1	1:15:A:LYS:HD2	18	0.12
(1,1019)	1:84:A:MET:HE2	1:15:A:LYS:HD2	18	0.12
(1,1019)	1:84:A:MET:HE3	1:15:A:LYS:HD2	18	0.12
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	4	0.12
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	4	0.12
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	4	0.12
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	5	0.12
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	5	0.12
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	5	0.12
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD2	15	0.12
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD3	15	0.12
(1,999)	1:114:A:ARG:HA	1:114:A:ARG:HB2	11	0.12
(1,979)	1:119:A:ALA:HB1	1:122:A:LYS:HD2	1	0.12
(1,979)	1:119:A:ALA:HB2	1:122:A:LYS:HD2	1	0.12
(1,979)	1:119:A:ALA:HB3	1:122:A:LYS:HD2	1	0.12
(1,942)	1:79:A:VAL:HG21	1:80:A:HIS:H	3	0.12
(1,942)	1:79:A:VAL:HG22	1:80:A:HIS:H	3	0.12
(1,942)	1:79:A:VAL:HG23	1:80:A:HIS:H	3	0.12
(1,941)	1:9:A:ALA:HB1	1:8:A:GLY:H	19	0.12
(1,941)	1:9:A:ALA:HB2	1:8:A:GLY:H	19	0.12
(1,941)	1:9:A:ALA:HB3	1:8:A:GLY:H	19	0.12
(1,904)	1:83:A:ALA:HB1	1:19:A:ASN:HD22	2	0.12
(1,904)	1:83:A:ALA:HB2	1:19:A:ASN:HD22	2	0.12
(1,904)	1:83:A:ALA:HB3	1:19:A:ASN:HD22	2	0.12
(1,904)	1:83:A:ALA:HB1	1:19:A:ASN:HD22	8	0.12
(1,904)	1:83:A:ALA:HB2	1:19:A:ASN:HD22	8	0.12
(1,904)	1:83:A:ALA:HB3	1:19:A:ASN:HD22	8	0.12
(1,887)	1:65:A:ALA:HB1	1:57:A:TYR:HE1	7	0.12
(1,887)	1:65:A:ALA:HB1	1:57:A:TYR:HE2	7	0.12
(1,887)	1:65:A:ALA:HB2	1:57:A:TYR:HE1	7	0.12
(1,887)	1:65:A:ALA:HB2	1:57:A:TYR:HE2	7	0.12
(1,887)	1:65:A:ALA:HB3	1:57:A:TYR:HE1	7	0.12
(1,887)	1:65:A:ALA:HB3	1:57:A:TYR:HE2	7	0.12
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG11	12	0.12
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG12	12	0.12
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG13	12	0.12
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG11	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG12	15	0.12
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG13	15	0.12
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG21	16	0.12
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG22	16	0.12
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG23	16	0.12
(1,765)	1:155:A:THR:H	1:155:A:THR:HG21	12	0.12
(1,765)	1:155:A:THR:H	1:155:A:THR:HG22	12	0.12
(1,765)	1:155:A:THR:H	1:155:A:THR:HG23	12	0.12
(1,762)	1:105:A:THR:H	1:105:A:THR:HG21	18	0.12
(1,762)	1:105:A:THR:H	1:105:A:THR:HG22	18	0.12
(1,762)	1:105:A:THR:H	1:105:A:THR:HG23	18	0.12
(1,747)	1:105:A:THR:HA	1:106:A:LEU:HB3	17	0.12
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD21	19	0.12
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD22	19	0.12
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD23	19	0.12
(1,731)	1:148:A:LEU:HD21	1:151:A:LYS:HE2	8	0.12
(1,731)	1:148:A:LEU:HD22	1:151:A:LYS:HE2	8	0.12
(1,731)	1:148:A:LEU:HD23	1:151:A:LYS:HE2	8	0.12
(1,719)	1:144:A:LEU:HB2	1:141:A:TYR:HA	20	0.12
(1,603)	1:111:A:VAL:H	1:110:A:SER:HB3	12	0.12
(1,585)	1:101:A:LYS:HG3	1:102:A:TYR:H	6	0.12
(1,577)	1:106:A:LEU:HD11	1:124:A:ILE:HG12	1	0.12
(1,577)	1:106:A:LEU:HD12	1:124:A:ILE:HG12	1	0.12
(1,577)	1:106:A:LEU:HD13	1:124:A:ILE:HG12	1	0.12
(1,577)	1:106:A:LEU:HD21	1:124:A:ILE:HG12	1	0.12
(1,577)	1:106:A:LEU:HD22	1:124:A:ILE:HG12	1	0.12
(1,577)	1:106:A:LEU:HD23	1:124:A:ILE:HG12	1	0.12
(1,559)	1:158:A:LYS:HE3	1:158:A:LYS:HG2	11	0.12
(1,532)	1:92:A:LYS:HB3	1:92:A:LYS:HD3	5	0.12
(1,531)	1:92:A:LYS:HD3	1:92:A:LYS:HB2	10	0.12
(1,497)	1:93:A:LEU:HD11	1:90:A:LEU:HA	2	0.12
(1,497)	1:93:A:LEU:HD12	1:90:A:LEU:HA	2	0.12
(1,497)	1:93:A:LEU:HD13	1:90:A:LEU:HA	2	0.12
(1,445)	1:90:A:LEU:HD11	1:73:A:VAL:H	18	0.12
(1,445)	1:90:A:LEU:HD12	1:73:A:VAL:H	18	0.12
(1,445)	1:90:A:LEU:HD13	1:73:A:VAL:H	18	0.12
(1,438)	1:6:A:ARG:HG3	1:6:A:ARG:HB3	16	0.12
(1,435)	1:7:A:PRO:HD2	1:6:A:ARG:HG2	8	0.12
(1,422)	1:106:A:LEU:HG	1:107:A:ASP:H	13	0.12
(1,409)	1:161:A:LEU:H	1:161:A:LEU:HG	10	0.12
(1,409)	1:161:A:LEU:H	1:161:A:LEU:HG	11	0.12
(1,409)	1:161:A:LEU:H	1:161:A:LEU:HG	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,405)	1:145:A:ILE:HG12	1:142:A:VAL:HA	2	0.12
(1,390)	1:117:A:ARG:HG3	1:117:A:ARG:HA	13	0.12
(1,390)	1:117:A:ARG:HG3	1:117:A:ARG:HA	17	0.12
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD2	14	0.12
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD3	14	0.12
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD2	16	0.12
(1,343)	1:137:A:GLU:HA	1:138:A:LYS:HD3	16	0.12
(1,331)	1:20:A:ARG:H	1:20:A:ARG:HG3	17	0.12
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG21	17	0.12
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG22	17	0.12
(1,325)	1:114:A:ARG:HB3	1:142:A:VAL:HG23	17	0.12
(1,323)	1:114:A:ARG:HB3	1:115:A:LYS:H	12	0.12
(1,323)	1:114:A:ARG:HB3	1:115:A:LYS:H	17	0.12
(1,310)	1:95:A:SER:HA	1:91:A:LYS:HD2	3	0.12
(1,307)	1:89:A:LYS:H	1:88:A:GLU:HB3	4	0.12
(1,299)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	6	0.12
(1,292)	1:105:A:THR:HB	1:105:A:THR:HA	10	0.12
(1,262)	1:84:A:MET:H	1:85:A:LYS:HB2	13	0.12
(1,262)	1:84:A:MET:H	1:85:A:LYS:HB3	13	0.12
(1,260)	1:86:A:ILE:HA	1:89:A:LYS:HB2	6	0.12
(1,260)	1:86:A:ILE:HA	1:89:A:LYS:HB3	6	0.12
(1,260)	1:86:A:ILE:HA	1:89:A:LYS:HB2	13	0.12
(1,260)	1:86:A:ILE:HA	1:89:A:LYS:HB3	13	0.12
(1,257)	1:81:A:MET:HG3	1:86:A:ILE:H	14	0.12
(1,256)	1:86:A:ILE:H	1:81:A:MET:HG2	4	0.12
(1,198)	1:112:A:ASP:H	1:111:A:VAL:HB	16	0.12
(1,198)	1:112:A:ASP:H	1:111:A:VAL:HB	18	0.12
(1,198)	1:112:A:ASP:H	1:111:A:VAL:HB	20	0.12
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB1	19	0.12
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB2	19	0.12
(1,179)	1:137:A:GLU:HG3	1:136:A:ALA:HB3	19	0.12
(1,161)	1:3:A:ALA:HB1	1:2:A:GLU:HG2	3	0.12
(1,161)	1:3:A:ALA:HB2	1:2:A:GLU:HG2	3	0.12
(1,161)	1:3:A:ALA:HB3	1:2:A:GLU:HG2	3	0.12
(1,161)	1:3:A:ALA:HB1	1:2:A:GLU:HG3	3	0.12
(1,161)	1:3:A:ALA:HB2	1:2:A:GLU:HG3	3	0.12
(1,161)	1:3:A:ALA:HB3	1:2:A:GLU:HG3	3	0.12
(1,122)	1:94:A:ASP:HB3	1:97:A:ILE:HB	14	0.12
(1,50)	1:158:A:LYS:HE3	1:159:A:THR:H	19	0.12
(1,30)	1:6:A:ARG:HA	1:6:A:ARG:HD2	3	0.12
(1,30)	1:6:A:ARG:HA	1:6:A:ARG:HD3	3	0.12
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB1	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB2	10	0.12
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB3	10	0.12
(1,12)	1:28:A:ARG:H	1:28:A:ARG:HD2	1	0.12
(1,12)	1:28:A:ARG:H	1:28:A:ARG:HD3	1	0.12
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB1	15	0.12
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB2	15	0.12
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB3	15	0.12
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB1	16	0.12
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB2	16	0.12
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB3	16	0.12
(1,2015)	1:148:A:LEU:HD11	1:152:A:TYR:HE1	9	0.11
(1,2015)	1:148:A:LEU:HD11	1:152:A:TYR:HE2	9	0.11
(1,2015)	1:148:A:LEU:HD12	1:152:A:TYR:HE1	9	0.11
(1,2015)	1:148:A:LEU:HD12	1:152:A:TYR:HE2	9	0.11
(1,2015)	1:148:A:LEU:HD13	1:152:A:TYR:HE1	9	0.11
(1,2015)	1:148:A:LEU:HD13	1:152:A:TYR:HE2	9	0.11
(1,1988)	1:156:A:HIS:H	1:156:A:HIS:HD2	1	0.11
(1,1988)	1:156:A:HIS:H	1:156:A:HIS:HD2	7	0.11
(1,1988)	1:156:A:HIS:H	1:156:A:HIS:HD2	18	0.11
(1,1971)	1:44:A:PHE:HZ	1:20:A:ARG:HB2	16	0.11
(1,1964)	1:21:A:PHE:HD1	1:44:A:PHE:HZ	1	0.11
(1,1964)	1:21:A:PHE:HD2	1:44:A:PHE:HZ	1	0.11
(1,1964)	1:21:A:PHE:HD1	1:44:A:PHE:HZ	5	0.11
(1,1964)	1:21:A:PHE:HD2	1:44:A:PHE:HZ	5	0.11
(1,1964)	1:21:A:PHE:HD1	1:44:A:PHE:HZ	14	0.11
(1,1964)	1:21:A:PHE:HD2	1:44:A:PHE:HZ	14	0.11
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE1	1	0.11
(1,1945)	1:18:A:LEU:HA	1:17:A:PHE:HE2	1	0.11
(1,1937)	1:58:A:TYR:HD1	1:97:A:ILE:HG13	15	0.11
(1,1937)	1:58:A:TYR:HD2	1:97:A:ILE:HG13	15	0.11
(1,1930)	1:25:A:LEU:HD21	1:22:A:TYR:HD1	19	0.11
(1,1930)	1:25:A:LEU:HD21	1:22:A:TYR:HD2	19	0.11
(1,1930)	1:25:A:LEU:HD22	1:22:A:TYR:HD1	19	0.11
(1,1930)	1:25:A:LEU:HD22	1:22:A:TYR:HD2	19	0.11
(1,1930)	1:25:A:LEU:HD23	1:22:A:TYR:HD1	19	0.11
(1,1930)	1:25:A:LEU:HD23	1:22:A:TYR:HD2	19	0.11
(1,1887)	1:126:A:HIS:H	1:129:A:GLY:H	12	0.11
(1,1883)	1:49:A:LYS:H	1:48:A:THR:H	1	0.11
(1,1883)	1:49:A:LYS:H	1:48:A:THR:H	5	0.11
(1,1883)	1:49:A:LYS:H	1:48:A:THR:H	16	0.11
(1,1883)	1:49:A:LYS:H	1:48:A:THR:H	19	0.11
(1,1876)	1:49:A:LYS:HB3	1:50:A:GLY:H	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1872)	1:8:A:GLY:H	1:8:A:GLY:HA2	13	0.11
(1,1872)	1:8:A:GLY:H	1:8:A:GLY:HA2	20	0.11
(1,1838)	1:114:A:ARG:HB3	1:114:A:ARG:H	3	0.11
(1,1828)	1:16:A:GLU:HA	1:19:A:ASN:HD22	1	0.11
(1,1824)	1:31:A:ASN:HD21	1:32:A:PHE:HA	17	0.11
(1,1815)	1:33:A:SER:HB2	1:31:A:ASN:HD22	20	0.11
(1,1806)	1:24:A:SER:H	1:23:A:LYS:HB2	14	0.11
(1,1802)	1:24:A:SER:H	1:25:A:LEU:HG	1	0.11
(1,1802)	1:24:A:SER:H	1:25:A:LEU:HG	5	0.11
(1,1796)	1:59:A:LEU:HB3	1:59:A:LEU:H	13	0.11
(1,1775)	1:28:A:ARG:H	1:28:A:ARG:HB3	2	0.11
(1,1771)	1:35:A:ASP:H	1:34:A:LEU:HB3	3	0.11
(1,1718)	1:142:A:VAL:HG21	1:143:A:ASN:H	10	0.11
(1,1718)	1:142:A:VAL:HG22	1:143:A:ASN:H	10	0.11
(1,1718)	1:142:A:VAL:HG23	1:143:A:ASN:H	10	0.11
(1,1666)	1:30:A:VAL:HB	1:28:A:ARG:HE	7	0.11
(1,1666)	1:30:A:VAL:HB	1:28:A:ARG:HE	11	0.11
(1,1666)	1:30:A:VAL:HB	1:28:A:ARG:HE	13	0.11
(1,1666)	1:30:A:VAL:HB	1:28:A:ARG:HE	17	0.11
(1,1633)	1:87:A:CYS:H	1:87:A:CYS:HB3	16	0.11
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	9	0.11
(1,1614)	1:25:A:LEU:HD11	1:40:A:GLU:H	1	0.11
(1,1614)	1:25:A:LEU:HD12	1:40:A:GLU:H	1	0.11
(1,1614)	1:25:A:LEU:HD13	1:40:A:GLU:H	1	0.11
(1,1614)	1:25:A:LEU:HD11	1:40:A:GLU:H	7	0.11
(1,1614)	1:25:A:LEU:HD12	1:40:A:GLU:H	7	0.11
(1,1614)	1:25:A:LEU:HD13	1:40:A:GLU:H	7	0.11
(1,1614)	1:25:A:LEU:HD11	1:40:A:GLU:H	12	0.11
(1,1614)	1:25:A:LEU:HD12	1:40:A:GLU:H	12	0.11
(1,1614)	1:25:A:LEU:HD13	1:40:A:GLU:H	12	0.11
(1,1614)	1:25:A:LEU:HD11	1:40:A:GLU:H	14	0.11
(1,1614)	1:25:A:LEU:HD12	1:40:A:GLU:H	14	0.11
(1,1614)	1:25:A:LEU:HD13	1:40:A:GLU:H	14	0.11
(1,1590)	1:55:A:LEU:H	1:100:A:LEU:HG	2	0.11
(1,1590)	1:55:A:LEU:H	1:100:A:LEU:HG	9	0.11
(1,1590)	1:55:A:LEU:H	1:100:A:LEU:HG	20	0.11
(1,1558)	1:90:A:LEU:HD21	1:93:A:LEU:H	4	0.11
(1,1558)	1:90:A:LEU:HD22	1:93:A:LEU:H	4	0.11
(1,1558)	1:90:A:LEU:HD23	1:93:A:LEU:H	4	0.11
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	1	0.11
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	3	0.11
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	16	0.11
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	17	0.11
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	18	0.11
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	20	0.11
(1,1526)	1:116:A:MET:HG3	1:116:A:MET:H	2	0.11
(1,1524)	1:117:A:ARG:H	1:116:A:MET:H	7	0.11
(1,1511)	1:25:A:LEU:H	1:25:A:LEU:HG	10	0.11
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB2	18	0.11
(1,1500)	1:90:A:LEU:H	1:89:A:LYS:HB3	18	0.11
(1,1497)	1:90:A:LEU:H	1:91:A:LYS:H	2	0.11
(1,1473)	1:101:A:LYS:HB2	1:102:A:TYR:H	1	0.11
(1,1472)	1:102:A:TYR:HB2	1:102:A:TYR:H	13	0.11
(1,1471)	1:102:A:TYR:H	1:101:A:LYS:HA	4	0.11
(1,1461)	1:107:A:ASP:HA	1:109:A:ALA:H	14	0.11
(1,1429)	1:155:A:THR:HB	1:156:A:HIS:H	16	0.11
(1,1429)	1:155:A:THR:HB	1:156:A:HIS:H	19	0.11
(1,1423)	1:121:A:LEU:H	1:121:A:LEU:HG	4	0.11
(1,1408)	1:128:A:TRP:H	1:128:A:TRP:HB3	3	0.11
(1,1387)	1:103:A:GLU:H	1:103:A:GLU:HB2	17	0.11
(1,1379)	1:158:A:LYS:H	1:157:A:PRO:HB3	8	0.11
(1,1366)	1:26:A:ILE:HG12	1:27:A:ASP:H	9	0.11
(1,1333)	1:118:A:VAL:H	1:118:A:VAL:HB	4	0.11
(1,1329)	1:121:A:LEU:H	1:118:A:VAL:H	16	0.11
(1,1329)	1:121:A:LEU:H	1:118:A:VAL:H	20	0.11
(1,1322)	1:46:A:LEU:H	1:43:A:SER:HB2	1	0.11
(1,1322)	1:46:A:LEU:H	1:43:A:SER:HB3	1	0.11
(1,1322)	1:46:A:LEU:H	1:43:A:SER:HB2	3	0.11
(1,1322)	1:46:A:LEU:H	1:43:A:SER:HB3	3	0.11
(1,1322)	1:46:A:LEU:H	1:43:A:SER:HB2	5	0.11
(1,1322)	1:46:A:LEU:H	1:43:A:SER:HB3	5	0.11
(1,1322)	1:46:A:LEU:H	1:43:A:SER:HB2	9	0.11
(1,1322)	1:46:A:LEU:H	1:43:A:SER:HB3	9	0.11
(1,1322)	1:46:A:LEU:H	1:43:A:SER:HB2	17	0.11
(1,1322)	1:46:A:LEU:H	1:43:A:SER:HB3	17	0.11
(1,1319)	1:8:A:GLY:HA3	1:9:A:ALA:H	4	0.11
(1,1311)	1:107:A:ASP:H	1:107:A:ASP:HB2	4	0.11
(1,1311)	1:107:A:ASP:H	1:107:A:ASP:HB2	20	0.11
(1,1295)	1:108:A:LEU:H	1:107:A:ASP:H	2	0.11
(1,1295)	1:108:A:LEU:H	1:107:A:ASP:H	10	0.11
(1,1295)	1:108:A:LEU:H	1:107:A:ASP:H	11	0.11
(1,1224)	1:26:A:ILE:HD11	1:26:A:ILE:H	4	0.11
(1,1224)	1:26:A:ILE:HD12	1:26:A:ILE:H	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	1:26:A:ILE:HD13	1:26:A:ILE:H	4	0.11
(1,1218)	1:67:A:THR:H	1:66:A:ALA:HA	6	0.11
(1,1217)	1:37:A:ILE:HD11	1:25:A:LEU:HD21	4	0.11
(1,1217)	1:37:A:ILE:HD11	1:25:A:LEU:HD22	4	0.11
(1,1217)	1:37:A:ILE:HD11	1:25:A:LEU:HD23	4	0.11
(1,1217)	1:37:A:ILE:HD12	1:25:A:LEU:HD21	4	0.11
(1,1217)	1:37:A:ILE:HD12	1:25:A:LEU:HD22	4	0.11
(1,1217)	1:37:A:ILE:HD12	1:25:A:LEU:HD23	4	0.11
(1,1217)	1:37:A:ILE:HD13	1:25:A:LEU:HD21	4	0.11
(1,1217)	1:37:A:ILE:HD13	1:25:A:LEU:HD22	4	0.11
(1,1217)	1:37:A:ILE:HD13	1:25:A:LEU:HD23	4	0.11
(1,1202)	1:59:A:LEU:HA	1:69:A:ILE:HD11	19	0.11
(1,1202)	1:59:A:LEU:HA	1:69:A:ILE:HD12	19	0.11
(1,1202)	1:59:A:LEU:HA	1:69:A:ILE:HD13	19	0.11
(1,1176)	1:95:A:SER:H	1:94:A:ASP:HA	2	0.11
(1,1174)	1:49:A:LYS:HA	1:49:A:LYS:HG2	18	0.11
(1,1174)	1:49:A:LYS:HA	1:49:A:LYS:HG3	18	0.11
(1,1167)	1:106:A:LEU:HA	1:106:A:LEU:HB3	14	0.11
(1,1137)	1:142:A:VAL:HA	1:145:A:ILE:HD11	14	0.11
(1,1137)	1:142:A:VAL:HA	1:145:A:ILE:HD12	14	0.11
(1,1137)	1:142:A:VAL:HA	1:145:A:ILE:HD13	14	0.11
(1,1113)	1:111:A:VAL:HB	1:108:A:LEU:HA	16	0.11
(1,1104)	1:103:A:GLU:HG3	1:103:A:GLU:HA	16	0.11
(1,1101)	1:158:A:LYS:HA	1:158:A:LYS:HG3	13	0.11
(1,1091)	1:14:A:CYS:HA	1:97:A:ILE:HG21	6	0.11
(1,1091)	1:14:A:CYS:HA	1:97:A:ILE:HG22	6	0.11
(1,1091)	1:14:A:CYS:HA	1:97:A:ILE:HG23	6	0.11
(1,1090)	1:81:A:MET:HB2	1:81:A:MET:HE1	3	0.11
(1,1090)	1:81:A:MET:HB2	1:81:A:MET:HE2	3	0.11
(1,1090)	1:81:A:MET:HB2	1:81:A:MET:HE3	3	0.11
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE1	10	0.11
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE2	10	0.11
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE3	10	0.11
(1,1064)	1:77:A:MET:HE1	1:22:A:TYR:HA	17	0.11
(1,1064)	1:77:A:MET:HE2	1:22:A:TYR:HA	17	0.11
(1,1064)	1:77:A:MET:HE3	1:22:A:TYR:HA	17	0.11
(1,1049)	1:140:A:ASP:HB3	1:140:A:ASP:HA	2	0.11
(1,1049)	1:140:A:ASP:HB3	1:140:A:ASP:HA	9	0.11
(1,1049)	1:140:A:ASP:HB3	1:140:A:ASP:HA	15	0.11
(1,1049)	1:140:A:ASP:HB3	1:140:A:ASP:HA	16	0.11
(1,1049)	1:140:A:ASP:HB3	1:140:A:ASP:HA	20	0.11
(1,1047)	1:77:A:MET:HE1	1:22:A:TYR:HB3	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1047)	1:77:A:MET:HE2	1:22:A:TYR:HB3	16	0.11
(1,1047)	1:77:A:MET:HE3	1:22:A:TYR:HB3	16	0.11
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE1	1	0.11
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE2	1	0.11
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE3	1	0.11
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE1	13	0.11
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE2	13	0.11
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE3	13	0.11
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE1	15	0.11
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE2	15	0.11
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE3	15	0.11
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE1	20	0.11
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE2	20	0.11
(1,1025)	1:116:A:MET:HG3	1:116:A:MET:HE3	20	0.11
(1,1019)	1:84:A:MET:HE1	1:15:A:LYS:HD2	2	0.11
(1,1019)	1:84:A:MET:HE2	1:15:A:LYS:HD2	2	0.11
(1,1019)	1:84:A:MET:HE3	1:15:A:LYS:HD2	2	0.11
(1,1015)	1:125:A:LEU:HD11	1:125:A:LEU:HA	16	0.11
(1,1015)	1:125:A:LEU:HD12	1:125:A:LEU:HA	16	0.11
(1,1015)	1:125:A:LEU:HD13	1:125:A:LEU:HA	16	0.11
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD2	9	0.11
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD3	9	0.11
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD2	14	0.11
(1,1011)	1:151:A:LYS:HA	1:151:A:LYS:HD3	14	0.11
(1,1007)	1:85:A:LYS:HA	1:88:A:GLU:H	18	0.11
(1,1003)	1:124:A:ILE:HB	1:125:A:LEU:HA	6	0.11
(1,979)	1:119:A:ALA:HB1	1:122:A:LYS:HD2	16	0.11
(1,979)	1:119:A:ALA:HB2	1:122:A:LYS:HD2	16	0.11
(1,979)	1:119:A:ALA:HB3	1:122:A:LYS:HD2	16	0.11
(1,931)	1:153:A:ALA:HB1	1:154:A:ALA:H	16	0.11
(1,931)	1:153:A:ALA:HB2	1:154:A:ALA:H	16	0.11
(1,931)	1:153:A:ALA:HB3	1:154:A:ALA:H	16	0.11
(1,928)	1:23:A:LYS:HA	1:23:A:LYS:HB2	20	0.11
(1,910)	1:108:A:LEU:H	1:153:A:ALA:HB1	14	0.11
(1,910)	1:108:A:LEU:H	1:153:A:ALA:HB2	14	0.11
(1,910)	1:108:A:LEU:H	1:153:A:ALA:HB3	14	0.11
(1,904)	1:83:A:ALA:HB1	1:19:A:ASN:HD22	12	0.11
(1,904)	1:83:A:ALA:HB2	1:19:A:ASN:HD22	12	0.11
(1,904)	1:83:A:ALA:HB3	1:19:A:ASN:HD22	12	0.11
(1,902)	1:18:A:LEU:H	1:83:A:ALA:HB1	3	0.11
(1,902)	1:18:A:LEU:H	1:83:A:ALA:HB2	3	0.11
(1,902)	1:18:A:LEU:H	1:83:A:ALA:HB3	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	1	0.11
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	1	0.11
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	1	0.11
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB1	17	0.11
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB2	17	0.11
(1,891)	1:64:A:ASP:HB3	1:65:A:ALA:HB3	17	0.11
(1,884)	1:61:A:ALA:HB1	1:56:A:CYS:HB2	1	0.11
(1,884)	1:61:A:ALA:HB2	1:56:A:CYS:HB2	1	0.11
(1,884)	1:61:A:ALA:HB3	1:56:A:CYS:HB2	1	0.11
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG11	1	0.11
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG12	1	0.11
(1,848)	1:122:A:LYS:HE3	1:118:A:VAL:HG13	1	0.11
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG11	7	0.11
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG12	7	0.11
(1,825)	1:112:A:ASP:H	1:111:A:VAL:HG13	7	0.11
(1,786)	1:75:A:ARG:HA	1:75:A:ARG:HD2	2	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG21	4	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG22	4	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG23	4	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG21	5	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG22	5	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG23	5	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG21	6	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG22	6	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG23	6	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG21	8	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG22	8	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG23	8	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG21	10	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG22	10	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG23	10	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG21	11	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG22	11	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG23	11	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG21	17	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG22	17	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG23	17	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG21	20	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG22	20	0.11
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG23	20	0.11
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB1	9	0.11
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB2	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB3	9	0.11
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB1	16	0.11
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB2	16	0.11
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB3	16	0.11
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD21	10	0.11
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD22	10	0.11
(1,732)	1:151:A:LYS:HE3	1:148:A:LEU:HD23	10	0.11
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB2	20	0.11
(1,697)	1:75:A:ARG:HD3	1:71:A:SER:HB3	20	0.11
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	3	0.11
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	3	0.11
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	3	0.11
(1,647)	1:118:A:VAL:HG21	1:137:A:GLU:HA	13	0.11
(1,647)	1:118:A:VAL:HG22	1:137:A:GLU:HA	13	0.11
(1,647)	1:118:A:VAL:HG23	1:137:A:GLU:HA	13	0.11
(1,637)	1:26:A:ILE:HD11	1:26:A:ILE:HA	9	0.11
(1,637)	1:26:A:ILE:HD12	1:26:A:ILE:HA	9	0.11
(1,637)	1:26:A:ILE:HD13	1:26:A:ILE:HA	9	0.11
(1,603)	1:111:A:VAL:H	1:110:A:SER:HB3	1	0.11
(1,603)	1:111:A:VAL:H	1:110:A:SER:HB3	9	0.11
(1,577)	1:106:A:LEU:HD11	1:124:A:ILE:HG12	9	0.11
(1,577)	1:106:A:LEU:HD12	1:124:A:ILE:HG12	9	0.11
(1,577)	1:106:A:LEU:HD13	1:124:A:ILE:HG12	9	0.11
(1,577)	1:106:A:LEU:HD21	1:124:A:ILE:HG12	9	0.11
(1,577)	1:106:A:LEU:HD22	1:124:A:ILE:HG12	9	0.11
(1,577)	1:106:A:LEU:HD23	1:124:A:ILE:HG12	9	0.11
(1,573)	1:106:A:LEU:HD21	1:108:A:LEU:HA	15	0.11
(1,573)	1:106:A:LEU:HD22	1:108:A:LEU:HA	15	0.11
(1,573)	1:106:A:LEU:HD23	1:108:A:LEU:HA	15	0.11
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD11	13	0.11
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD12	13	0.11
(1,572)	1:108:A:LEU:HA	1:106:A:LEU:HD13	13	0.11
(1,568)	1:34:A:LEU:HD11	1:75:A:ARG:HD2	7	0.11
(1,568)	1:34:A:LEU:HD12	1:75:A:ARG:HD2	7	0.11
(1,568)	1:34:A:LEU:HD13	1:75:A:ARG:HD2	7	0.11
(1,531)	1:92:A:LYS:HD3	1:92:A:LYS:HB2	1	0.11
(1,529)	1:92:A:LYS:H	1:92:A:LYS:HD2	5	0.11
(1,529)	1:92:A:LYS:H	1:92:A:LYS:HD3	5	0.11
(1,529)	1:92:A:LYS:H	1:92:A:LYS:HD2	15	0.11
(1,529)	1:92:A:LYS:H	1:92:A:LYS:HD3	15	0.11
(1,522)	1:13:A:VAL:HA	1:55:A:LEU:HD11	9	0.11
(1,522)	1:13:A:VAL:HA	1:55:A:LEU:HD12	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	1:13:A:VAL:HA	1:55:A:LEU:HD13	9	0.11
(1,512)	1:115:A:LYS:HG2	1:115:A:LYS:HE2	8	0.11
(1,512)	1:115:A:LYS:HG2	1:115:A:LYS:HE3	8	0.11
(1,500)	1:152:A:TYR:H	1:150:A:PRO:HA	11	0.11
(1,477)	1:76:A:PRO:HA	1:79:A:VAL:H	3	0.11
(1,422)	1:106:A:LEU:HG	1:107:A:ASP:H	6	0.11
(1,418)	1:6:A:ARG:H	1:6:A:ARG:HG2	9	0.11
(1,415)	1:113:A:LEU:H	1:113:A:LEU:HG	16	0.11
(1,412)	1:125:A:LEU:HG	1:126:A:HIS:HB2	19	0.11
(1,412)	1:125:A:LEU:HG	1:126:A:HIS:HB3	19	0.11
(1,390)	1:117:A:ARG:HG3	1:117:A:ARG:HA	10	0.11
(1,390)	1:117:A:ARG:HG3	1:117:A:ARG:HA	16	0.11
(1,387)	1:86:A:ILE:HG21	1:76:A:PRO:HG3	16	0.11
(1,387)	1:86:A:ILE:HG22	1:76:A:PRO:HG3	16	0.11
(1,387)	1:86:A:ILE:HG23	1:76:A:PRO:HG3	16	0.11
(1,386)	1:77:A:MET:H	1:76:A:PRO:HG3	5	0.11
(1,385)	1:121:A:LEU:HB3	1:118:A:VAL:HA	20	0.11
(1,380)	1:81:A:MET:HG3	1:86:A:ILE:HG12	18	0.11
(1,322)	1:115:A:LYS:H	1:114:A:ARG:HB2	16	0.11
(1,302)	1:155:A:THR:HB	1:155:A:THR:HA	2	0.11
(1,300)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	6	0.11
(1,290)	1:67:A:THR:HB	1:67:A:THR:HA	5	0.11
(1,262)	1:84:A:MET:H	1:85:A:LYS:HB2	6	0.11
(1,262)	1:84:A:MET:H	1:85:A:LYS:HB3	6	0.11
(1,262)	1:84:A:MET:H	1:85:A:LYS:HB2	19	0.11
(1,262)	1:84:A:MET:H	1:85:A:LYS:HB3	19	0.11
(1,251)	1:63:A:LYS:HB3	1:63:A:LYS:HE3	16	0.11
(1,250)	1:63:A:LYS:HE3	1:63:A:LYS:HB2	1	0.11
(1,243)	1:81:A:MET:HG3	1:85:A:LYS:HB2	8	0.11
(1,243)	1:81:A:MET:HG2	1:85:A:LYS:HB2	8	0.11
(1,213)	1:159:A:THR:H	1:158:A:LYS:HB2	4	0.11
(1,203)	1:158:A:LYS:HB3	1:158:A:LYS:HE2	11	0.11
(1,198)	1:112:A:ASP:H	1:111:A:VAL:HB	14	0.11
(1,172)	1:139:A:THR:H	1:137:A:GLU:HG2	7	0.11
(1,169)	1:16:A:GLU:HA	1:16:A:GLU:HG2	5	0.11
(1,138)	1:42:A:ILE:HD11	1:38:A:GLU:HG2	9	0.11
(1,138)	1:42:A:ILE:HD12	1:38:A:GLU:HG2	9	0.11
(1,138)	1:42:A:ILE:HD13	1:38:A:GLU:HG2	9	0.11
(1,122)	1:94:A:ASP:HB3	1:97:A:ILE:HB	3	0.11
(1,41)	1:51:A:LYS:HE3	1:51:A:LYS:HG2	10	0.11
(1,21)	1:114:A:ARG:HD3	1:114:A:ARG:HB2	6	0.11
(1,21)	1:114:A:ARG:HD3	1:114:A:ARG:HB2	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:28:A:ARG:HA	1:28:A:ARG:HD2	5	0.11
(1,16)	1:20:A:ARG:HD2	1:20:A:ARG:HB2	17	0.11
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB1	3	0.11
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB2	3	0.11
(1,14)	1:148:A:LEU:HB3	1:149:A:ALA:HB3	3	0.11
(1,10)	1:15:A:LYS:HE3	1:8:A:GLY:HA2	12	0.11
(1,9)	1:8:A:GLY:HA2	1:15:A:LYS:HE2	15	0.11
(1,9)	1:8:A:GLY:HA3	1:15:A:LYS:HE2	15	0.11
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG21	15	0.11
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG22	15	0.11
(1,7)	1:60:A:GLY:HA2	1:69:A:ILE:HG23	15	0.11
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB1	6	0.11
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB2	6	0.11
(1,6)	1:8:A:GLY:HA3	1:9:A:ALA:HB3	6	0.11
(1,4)	1:8:A:GLY:HA3	1:15:A:LYS:HD3	14	0.11
(1,2007)	1:57:A:TYR:HE1	1:64:A:ASP:HB2	4	0.1
(1,2007)	1:57:A:TYR:HE2	1:64:A:ASP:HB2	4	0.1
(1,1930)	1:25:A:LEU:HD21	1:22:A:TYR:HD1	17	0.1
(1,1930)	1:25:A:LEU:HD21	1:22:A:TYR:HD2	17	0.1
(1,1930)	1:25:A:LEU:HD22	1:22:A:TYR:HD1	17	0.1
(1,1930)	1:25:A:LEU:HD22	1:22:A:TYR:HD2	17	0.1
(1,1930)	1:25:A:LEU:HD23	1:22:A:TYR:HD1	17	0.1
(1,1930)	1:25:A:LEU:HD23	1:22:A:TYR:HD2	17	0.1
(1,1901)	1:103:A:GLU:H	1:102:A:TYR:HD1	15	0.1
(1,1901)	1:103:A:GLU:H	1:102:A:TYR:HD2	15	0.1
(1,1890)	1:129:A:GLY:H	1:128:A:TRP:HB3	3	0.1
(1,1880)	1:4:A:GLY:H	1:3:A:ALA:HA	12	0.1
(1,1872)	1:8:A:GLY:H	1:8:A:GLY:HA2	4	0.1
(1,1872)	1:8:A:GLY:H	1:8:A:GLY:HA2	11	0.1
(1,1872)	1:8:A:GLY:H	1:8:A:GLY:HA2	17	0.1
(1,1824)	1:31:A:ASN:HD21	1:32:A:PHE:HA	2	0.1
(1,1818)	1:36:A:THR:HG21	1:31:A:ASN:HD22	5	0.1
(1,1818)	1:36:A:THR:HG22	1:31:A:ASN:HD22	5	0.1
(1,1818)	1:36:A:THR:HG23	1:31:A:ASN:HD22	5	0.1
(1,1818)	1:36:A:THR:HG21	1:31:A:ASN:HD22	14	0.1
(1,1818)	1:36:A:THR:HG22	1:31:A:ASN:HD22	14	0.1
(1,1818)	1:36:A:THR:HG23	1:31:A:ASN:HD22	14	0.1
(1,1806)	1:24:A:SER:H	1:23:A:LYS:HB2	11	0.1
(1,1802)	1:24:A:SER:H	1:25:A:LEU:HG	16	0.1
(1,1802)	1:24:A:SER:H	1:25:A:LEU:HG	20	0.1
(1,1781)	1:73:A:VAL:H	1:73:A:VAL:HB	13	0.1
(1,1749)	1:18:A:LEU:H	1:17:A:PHE:HB2	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1721)	1:32:A:PHE:H	1:33:A:SER:H	2	0.1
(1,1718)	1:142:A:VAL:HG21	1:143:A:ASN:H	3	0.1
(1,1718)	1:142:A:VAL:HG22	1:143:A:ASN:H	3	0.1
(1,1718)	1:142:A:VAL:HG23	1:143:A:ASN:H	3	0.1
(1,1718)	1:142:A:VAL:HG21	1:143:A:ASN:H	20	0.1
(1,1718)	1:142:A:VAL:HG22	1:143:A:ASN:H	20	0.1
(1,1718)	1:142:A:VAL:HG23	1:143:A:ASN:H	20	0.1
(1,1666)	1:30:A:VAL:HB	1:28:A:ARG:HE	5	0.1
(1,1649)	1:125:A:LEU:H	1:125:A:LEU:HB2	3	0.1
(1,1619)	1:126:A:HIS:H	1:125:A:LEU:HB2	20	0.1
(1,1614)	1:25:A:LEU:HD11	1:40:A:GLU:H	3	0.1
(1,1614)	1:25:A:LEU:HD12	1:40:A:GLU:H	3	0.1
(1,1614)	1:25:A:LEU:HD13	1:40:A:GLU:H	3	0.1
(1,1614)	1:25:A:LEU:HD11	1:40:A:GLU:H	18	0.1
(1,1614)	1:25:A:LEU:HD12	1:40:A:GLU:H	18	0.1
(1,1614)	1:25:A:LEU:HD13	1:40:A:GLU:H	18	0.1
(1,1604)	1:54:A:ARG:HB3	1:54:A:ARG:H	11	0.1
(1,1604)	1:54:A:ARG:HB3	1:54:A:ARG:H	20	0.1
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	7	0.1
(1,1546)	1:122:A:LYS:HG3	1:119:A:ALA:H	12	0.1
(1,1524)	1:117:A:ARG:H	1:116:A:MET:H	14	0.1
(1,1522)	1:131:A:GLU:H	1:130:A:GLU:HB3	18	0.1
(1,1461)	1:107:A:ASP:HA	1:109:A:ALA:H	4	0.1
(1,1311)	1:107:A:ASP:H	1:107:A:ASP:HB2	7	0.1
(1,1295)	1:108:A:LEU:H	1:107:A:ASP:H	15	0.1
(1,1197)	1:156:A:HIS:HA	1:157:A:PRO:HD2	11	0.1
(1,1197)	1:156:A:HIS:HA	1:157:A:PRO:HD2	14	0.1
(1,1197)	1:156:A:HIS:HA	1:157:A:PRO:HD2	17	0.1
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	3	0.1
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	13	0.1
(1,1127)	1:161:A:LEU:H	1:160:A:GLU:HA	19	0.1
(1,1114)	1:81:A:MET:HE1	1:82:A:PRO:HD3	5	0.1
(1,1114)	1:81:A:MET:HE2	1:82:A:PRO:HD3	5	0.1
(1,1114)	1:81:A:MET:HE3	1:82:A:PRO:HD3	5	0.1
(1,1113)	1:111:A:VAL:HB	1:108:A:LEU:HA	7	0.1
(1,1103)	1:103:A:GLU:HA	1:103:A:GLU:HG2	7	0.1
(1,1091)	1:14:A:CYS:HA	1:97:A:ILE:HG21	4	0.1
(1,1091)	1:14:A:CYS:HA	1:97:A:ILE:HG22	4	0.1
(1,1091)	1:14:A:CYS:HA	1:97:A:ILE:HG23	4	0.1
(1,1078)	1:61:A:ALA:HA	1:42:A:ILE:HG21	6	0.1
(1,1078)	1:61:A:ALA:HA	1:42:A:ILE:HG22	6	0.1
(1,1078)	1:61:A:ALA:HA	1:42:A:ILE:HG23	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE1	4	0.1
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE2	4	0.1
(1,1065)	1:18:A:LEU:HB2	1:77:A:MET:HE3	4	0.1
(1,1064)	1:77:A:MET:HE1	1:22:A:TYR:HA	20	0.1
(1,1064)	1:77:A:MET:HE2	1:22:A:TYR:HA	20	0.1
(1,1064)	1:77:A:MET:HE3	1:22:A:TYR:HA	20	0.1
(1,1049)	1:140:A:ASP:HB3	1:140:A:ASP:HA	3	0.1
(1,1049)	1:140:A:ASP:HB3	1:140:A:ASP:HA	13	0.1
(1,1027)	1:124:A:ILE:HG21	1:116:A:MET:HE1	5	0.1
(1,1027)	1:124:A:ILE:HG21	1:116:A:MET:HE2	5	0.1
(1,1027)	1:124:A:ILE:HG21	1:116:A:MET:HE3	5	0.1
(1,1027)	1:124:A:ILE:HG22	1:116:A:MET:HE1	5	0.1
(1,1027)	1:124:A:ILE:HG22	1:116:A:MET:HE2	5	0.1
(1,1027)	1:124:A:ILE:HG22	1:116:A:MET:HE3	5	0.1
(1,1027)	1:124:A:ILE:HG23	1:116:A:MET:HE1	5	0.1
(1,1027)	1:124:A:ILE:HG23	1:116:A:MET:HE2	5	0.1
(1,1027)	1:124:A:ILE:HG23	1:116:A:MET:HE3	5	0.1
(1,1003)	1:124:A:ILE:HB	1:125:A:LEU:HA	14	0.1
(1,931)	1:153:A:ALA:HB1	1:154:A:ALA:H	20	0.1
(1,931)	1:153:A:ALA:HB2	1:154:A:ALA:H	20	0.1
(1,931)	1:153:A:ALA:HB3	1:154:A:ALA:H	20	0.1
(1,911)	1:9:A:ALA:HB1	1:15:A:LYS:HD2	19	0.1
(1,911)	1:9:A:ALA:HB2	1:15:A:LYS:HD2	19	0.1
(1,911)	1:9:A:ALA:HB3	1:15:A:LYS:HD2	19	0.1
(1,807)	1:13:A:VAL:HG11	1:12:A:GLU:HB3	10	0.1
(1,807)	1:13:A:VAL:HG12	1:12:A:GLU:HB3	10	0.1
(1,807)	1:13:A:VAL:HG13	1:12:A:GLU:HB3	10	0.1
(1,786)	1:75:A:ARG:HA	1:75:A:ARG:HD2	7	0.1
(1,786)	1:75:A:ARG:HA	1:75:A:ARG:HD2	8	0.1
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG21	9	0.1
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG22	9	0.1
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG23	9	0.1
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG21	18	0.1
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG22	18	0.1
(1,783)	1:155:A:THR:HA	1:155:A:THR:HG23	18	0.1
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD11	4	0.1
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD12	4	0.1
(1,774)	1:30:A:VAL:HG21	1:25:A:LEU:HD13	4	0.1
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD11	4	0.1
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD12	4	0.1
(1,774)	1:30:A:VAL:HG22	1:25:A:LEU:HD13	4	0.1
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD11	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD12	4	0.1
(1,774)	1:30:A:VAL:HG23	1:25:A:LEU:HD13	4	0.1
(1,762)	1:105:A:THR:H	1:105:A:THR:HG21	11	0.1
(1,762)	1:105:A:THR:H	1:105:A:THR:HG22	11	0.1
(1,762)	1:105:A:THR:H	1:105:A:THR:HG23	11	0.1
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB1	19	0.1
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB2	19	0.1
(1,760)	1:135:A:CYS:HA	1:136:A:ALA:HB3	19	0.1
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG21	9	0.1
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG22	9	0.1
(1,712)	1:143:A:ASN:HB3	1:139:A:THR:HG23	9	0.1
(1,591)	1:49:A:LYS:HE2	1:49:A:LYS:HG2	5	0.1
(1,591)	1:49:A:LYS:HE3	1:49:A:LYS:HG2	5	0.1
(1,591)	1:49:A:LYS:HE2	1:49:A:LYS:HG2	7	0.1
(1,591)	1:49:A:LYS:HE3	1:49:A:LYS:HG2	7	0.1
(1,591)	1:49:A:LYS:HE2	1:49:A:LYS:HG2	14	0.1
(1,591)	1:49:A:LYS:HE3	1:49:A:LYS:HG2	14	0.1
(1,577)	1:106:A:LEU:HD11	1:124:A:ILE:HG12	6	0.1
(1,577)	1:106:A:LEU:HD12	1:124:A:ILE:HG12	6	0.1
(1,577)	1:106:A:LEU:HD13	1:124:A:ILE:HG12	6	0.1
(1,577)	1:106:A:LEU:HD21	1:124:A:ILE:HG12	6	0.1
(1,577)	1:106:A:LEU:HD22	1:124:A:ILE:HG12	6	0.1
(1,577)	1:106:A:LEU:HD23	1:124:A:ILE:HG12	6	0.1
(1,577)	1:106:A:LEU:HD11	1:124:A:ILE:HG12	13	0.1
(1,577)	1:106:A:LEU:HD12	1:124:A:ILE:HG12	13	0.1
(1,577)	1:106:A:LEU:HD13	1:124:A:ILE:HG12	13	0.1
(1,577)	1:106:A:LEU:HD21	1:124:A:ILE:HG12	13	0.1
(1,577)	1:106:A:LEU:HD22	1:124:A:ILE:HG12	13	0.1
(1,577)	1:106:A:LEU:HD23	1:124:A:ILE:HG12	13	0.1
(1,577)	1:106:A:LEU:HD11	1:124:A:ILE:HG12	20	0.1
(1,577)	1:106:A:LEU:HD12	1:124:A:ILE:HG12	20	0.1
(1,577)	1:106:A:LEU:HD13	1:124:A:ILE:HG12	20	0.1
(1,577)	1:106:A:LEU:HD21	1:124:A:ILE:HG12	20	0.1
(1,577)	1:106:A:LEU:HD22	1:124:A:ILE:HG12	20	0.1
(1,577)	1:106:A:LEU:HD23	1:124:A:ILE:HG12	20	0.1
(1,566)	1:46:A:LEU:HD11	1:43:A:SER:HB3	13	0.1
(1,566)	1:46:A:LEU:HD12	1:43:A:SER:HB3	13	0.1
(1,566)	1:46:A:LEU:HD13	1:43:A:SER:HB3	13	0.1
(1,537)	1:70:A:LEU:HD21	1:68:A:LYS:HG2	6	0.1
(1,537)	1:70:A:LEU:HD22	1:68:A:LYS:HG2	6	0.1
(1,537)	1:70:A:LEU:HD23	1:68:A:LYS:HG2	6	0.1
(1,537)	1:70:A:LEU:HD21	1:68:A:LYS:HG3	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,537)	1:70:A:LEU:HD22	1:68:A:LYS:HG3	6	0.1
(1,537)	1:70:A:LEU:HD23	1:68:A:LYS:HG3	6	0.1
(1,512)	1:115:A:LYS:HG2	1:115:A:LYS:HE2	4	0.1
(1,512)	1:115:A:LYS:HG2	1:115:A:LYS:HE3	4	0.1
(1,496)	1:108:A:LEU:HD11	1:124:A:ILE:HG21	3	0.1
(1,496)	1:108:A:LEU:HD11	1:124:A:ILE:HG22	3	0.1
(1,496)	1:108:A:LEU:HD11	1:124:A:ILE:HG23	3	0.1
(1,496)	1:108:A:LEU:HD12	1:124:A:ILE:HG21	3	0.1
(1,496)	1:108:A:LEU:HD12	1:124:A:ILE:HG22	3	0.1
(1,496)	1:108:A:LEU:HD12	1:124:A:ILE:HG23	3	0.1
(1,496)	1:108:A:LEU:HD13	1:124:A:ILE:HG21	3	0.1
(1,496)	1:108:A:LEU:HD13	1:124:A:ILE:HG22	3	0.1
(1,496)	1:108:A:LEU:HD13	1:124:A:ILE:HG23	3	0.1
(1,469)	1:36:A:THR:HA	1:39:A:LYS:HE2	10	0.1
(1,469)	1:36:A:THR:HA	1:39:A:LYS:HE3	10	0.1
(1,453)	1:148:A:LEU:HB3	1:145:A:ILE:HA	14	0.1
(1,422)	1:106:A:LEU:HG	1:107:A:ASP:H	10	0.1
(1,419)	1:6:A:ARG:HG3	1:6:A:ARG:H	7	0.1
(1,409)	1:161:A:LEU:H	1:161:A:LEU:HG	8	0.1
(1,409)	1:161:A:LEU:H	1:161:A:LEU:HG	9	0.1
(1,390)	1:117:A:ARG:HG3	1:117:A:ARG:HA	4	0.1
(1,353)	1:139:A:THR:HB	1:137:A:GLU:HG2	12	0.1
(1,340)	1:36:A:THR:HA	1:39:A:LYS:HD2	20	0.1
(1,340)	1:36:A:THR:HA	1:39:A:LYS:HD3	20	0.1
(1,324)	1:142:A:VAL:HG21	1:114:A:ARG:HB2	2	0.1
(1,324)	1:142:A:VAL:HG22	1:114:A:ARG:HB2	2	0.1
(1,324)	1:142:A:VAL:HG23	1:114:A:ARG:HB2	2	0.1
(1,321)	1:89:A:LYS:H	1:88:A:GLU:HB2	1	0.1
(1,302)	1:155:A:THR:HB	1:155:A:THR:HA	15	0.1
(1,292)	1:105:A:THR:HB	1:105:A:THR:HA	17	0.1
(1,254)	1:82:A:PRO:HD2	1:81:A:MET:HG2	8	0.1
(1,237)	1:148:A:LEU:HA	1:151:A:LYS:HB3	20	0.1
(1,198)	1:112:A:ASP:H	1:111:A:VAL:HB	2	0.1
(1,198)	1:112:A:ASP:H	1:111:A:VAL:HB	10	0.1
(1,135)	1:74:A:THR:HG21	1:38:A:GLU:HG2	14	0.1
(1,135)	1:74:A:THR:HG22	1:38:A:GLU:HG2	14	0.1
(1,135)	1:74:A:THR:HG23	1:38:A:GLU:HG2	14	0.1
(1,46)	1:46:A:LEU:HB2	1:47:A:ASP:HA	7	0.1
(1,30)	1:6:A:ARG:HA	1:6:A:ARG:HD2	17	0.1
(1,30)	1:6:A:ARG:HA	1:6:A:ARG:HD3	17	0.1
(1,21)	1:114:A:ARG:HD3	1:114:A:ARG:HB2	7	0.1
(1,19)	1:28:A:ARG:HD3	1:28:A:ARG:HA	3	0.1

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

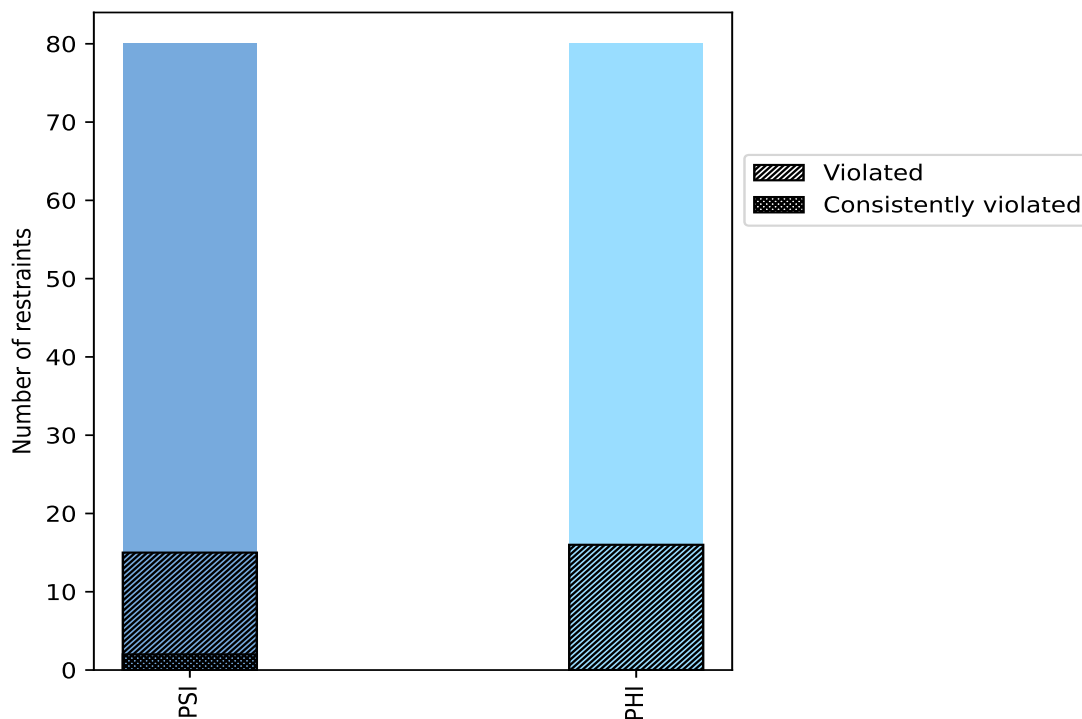
### 10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% <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>
PSI	80	50.0	15	18.8	9.4	2	2.5	1.2
PHI	80	50.0	16	20.0	10.0	0	0.0	0.0
Total	160	100.0	31	19.4	19.4	2	1.2	1.2

<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](#)



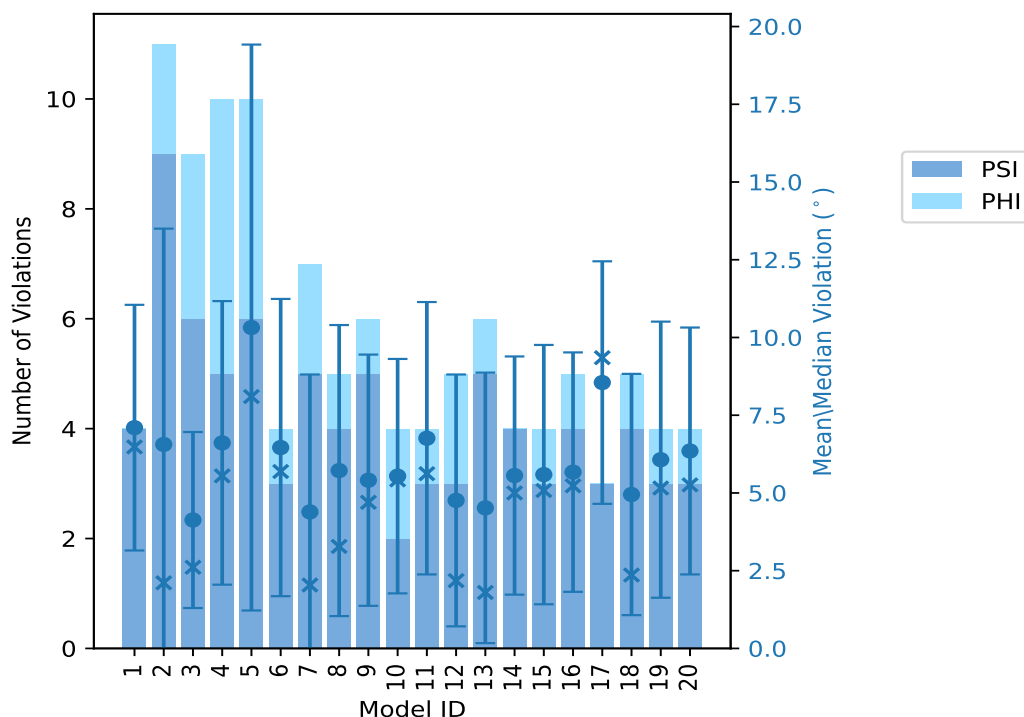
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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 (°)
	PSI	PHI	Total				
1	4	0	4	7.1	12.79	3.95	6.48
2	9	2	11	6.56	20.04	6.94	2.11
3	6	3	9	4.13	9.2	2.83	2.61
4	5	5	10	6.61	13.89	4.56	5.55
5	6	4	10	10.32	30.82	9.1	8.1
6	3	1	4	6.46	13.35	4.78	5.69
7	5	2	7	4.39	13.47	4.42	2.04
8	4	1	5	5.72	12.44	4.68	3.28
9	5	1	6	5.41	11.95	4.04	4.7
10	2	2	4	5.54	9.96	3.77	5.42
11	3	1	4	6.76	13.12	4.38	5.62
12	3	2	5	4.76	11.27	4.05	2.18
13	5	1	6	4.52	12.24	4.35	1.8
14	4	0	4	5.56	10.91	3.83	5.0
15	3	1	4	5.59	10.95	4.17	5.08
16	4	1	5	5.67	10.81	3.85	5.23
17	3	0	3	8.55	12.87	3.9	9.35
18	4	1	5	4.95	11.41	3.88	2.36
19	3	1	4	6.07	12.8	4.44	5.16
20	3	1	4	6.35	12.41	3.97	5.26

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
5	11	16	1	5.0
3	2	5	2	10.0
1	0	1	3	15.0
1	1	2	4	20.0
2	1	3	5	25.0
0	1	1	6	30.0
0	0	0	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

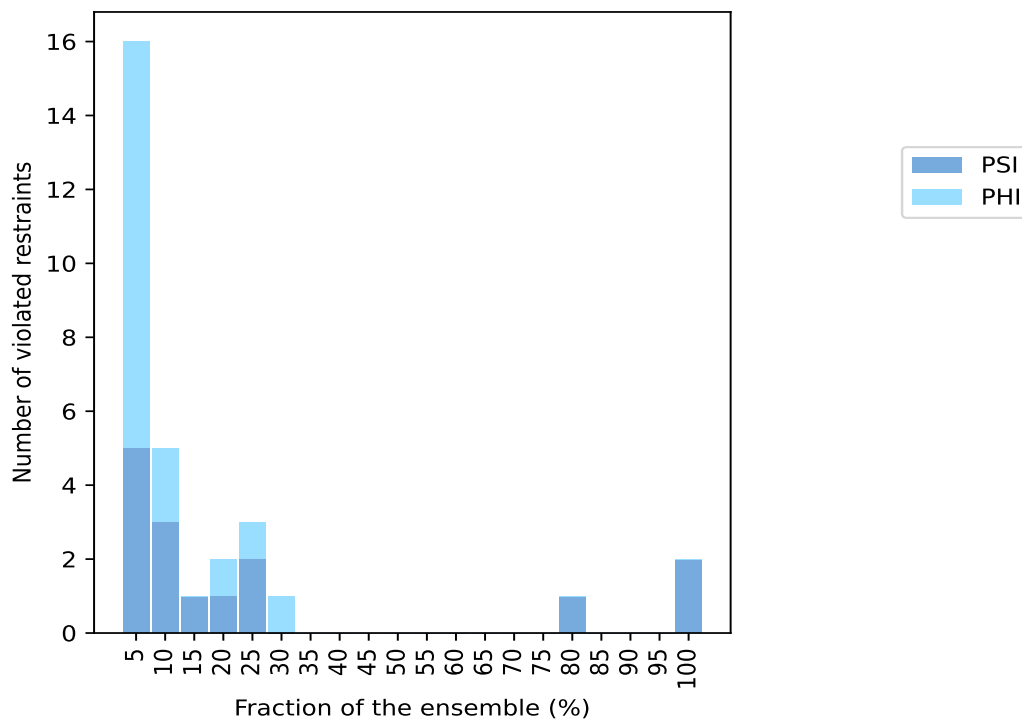
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
1	0	1	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
2	0	2	20	100.0

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

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

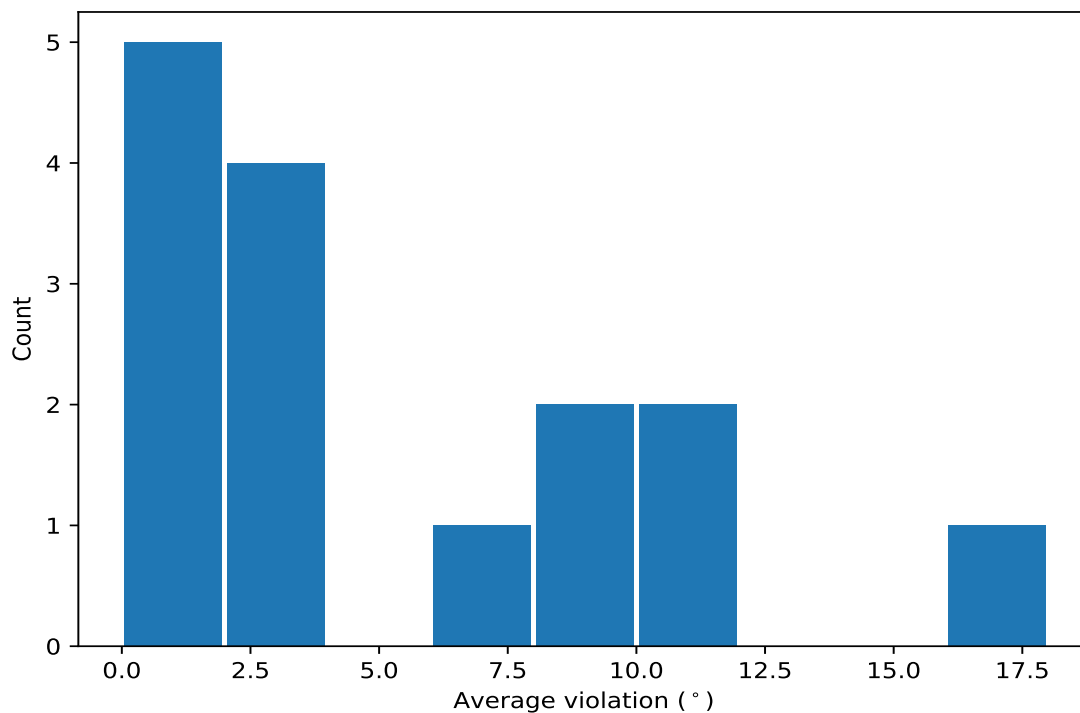


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 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.

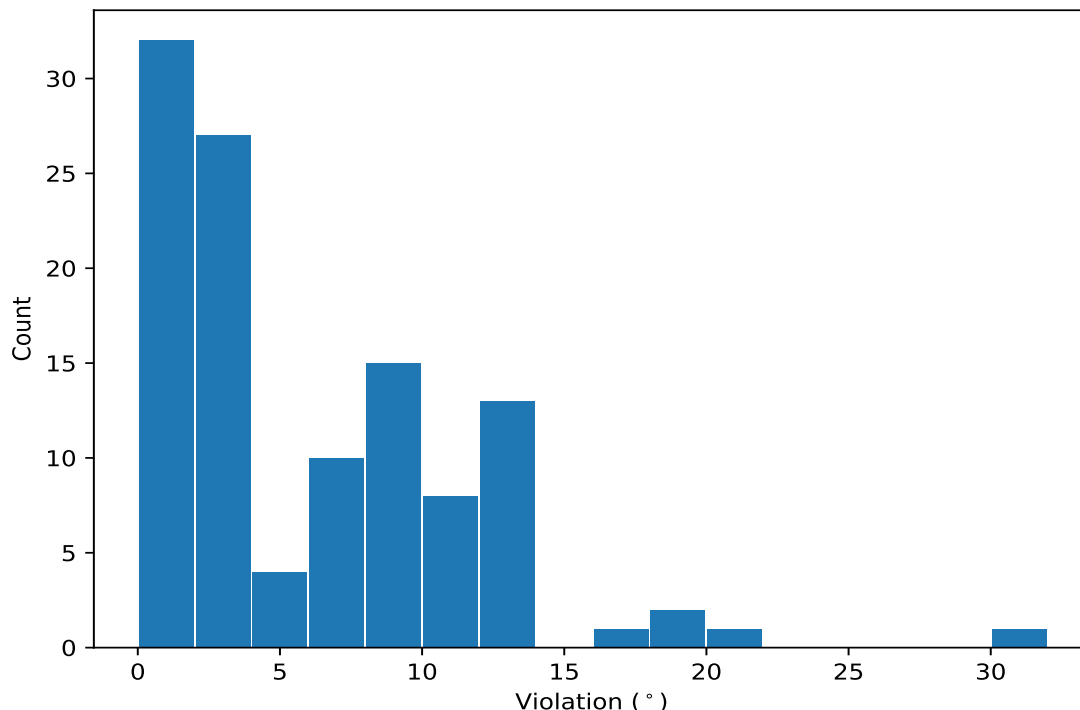
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	20	11.91	1.17	12.12
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	20	8.3	0.74	8.35
(1,14)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:HIS:N	16	2.82	1.06	2.6
(1,21)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	6	1.6	0.42	1.68
(1,102)	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	1:72:A:GLU:N	5	2.27	0.95	1.9
(1,22)	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	1:103:A:GLU:N	5	2.02	1.15	1.62
(1,101)	1:70:A:LEU:C	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	5	1.84	0.63	1.68
(1,82)	1:84:A:MET:N	1:84:A:MET:CA	1:84:A:MET:C	1:85:A:LYS:N	4	2.05	0.21	2.09
(1,105)	1:69:A:ILE:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	4	1.43	0.26	1.37
(1,32)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:LYS:N	3	11.6	7.02	13.84
(1,45)	1:90:A:LEU:C	1:91:A:LYS:N	1:91:A:LYS:CA	1:91:A:LYS:C	2	16.96	3.07	16.96
(1,26)	1:96:A:GLN:N	1:96:A:GLN:CA	1:96:A:GLN:C	1:97:A:ILE:N	2	8.78	7.72	8.78
(1,104)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:VAL:N	2	6.25	1.02	6.25
(1,37)	1:80:A:HIS:C	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	2	1.86	0.48	1.86
(1,86)	1:83:A:ALA:N	1:83:A:ALA:CA	1:83:A:ALA:C	1:84:A:MET:N	2	1.16	0.03	1.16

<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 [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,25)	1:95:A:SER:C	1:96:A:GLN:N	1:96:A:GLN:CA	1:96:A:GLN:C	5	30.82
(1,45)	1:90:A:LEU:C	1:91:A:LYS:N	1:91:A:LYS:CA	1:91:A:LYS:C	2	20.04
(1,32)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:LYS:N	2	18.86
(1,12)	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	1:96:A:GLN:N	5	18.55
(1,26)	1:96:A:GLN:N	1:96:A:GLN:CA	1:96:A:GLN:C	1:97:A:ILE:N	5	16.51
(1,45)	1:90:A:LEU:C	1:91:A:LYS:N	1:91:A:LYS:CA	1:91:A:LYS:C	4	13.89
(1,32)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:LYS:N	4	13.84
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	7	13.47
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	5	13.42
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	6	13.35
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	11	13.12
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	17	12.87
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	19	12.8
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	1	12.79

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	8	12.44
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	20	12.41
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	13	12.24
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	2	12.01
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	9	11.95
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	18	11.41
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	12	11.27
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	15	10.95
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	14	10.91
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	4	10.87
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	16	10.81
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	8	10.2
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	10	9.96
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	17	9.35
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	16	9.26
(1,38)	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	1:82:A:PRO:N	3	9.2
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	13	8.75
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	1	8.69
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	7	8.6
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	10	8.58
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	11	8.54
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	2	8.39
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	9	8.35
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	15	8.35
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	6	8.31
(1,7)	1:96:A:GLN:C	1:97:A:ILE:N	1:97:A:ILE:CA	1:97:A:ILE:C	5	8.28
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	3	8.01
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	5	7.93
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	12	7.75
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	4	7.62
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	18	7.42
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	14	7.41
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	20	7.35
(1,104)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:VAL:N	9	7.27
(1,120)	1:128:A:TRP:N	1:128:A:TRP:CA	1:128:A:TRP:C	1:129:A:GLY:N	19	7.13
(1,57)	1:25:A:LEU:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	4	6.68
(1,14)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:HIS:N	3	6.41
(1,104)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:VAL:N	16	5.23
(1,79)	1:26:A:ILE:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	4	4.42
(1,22)	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	1:103:A:GLU:N	1	4.27
(1,46)	1:91:A:LYS:N	1:91:A:LYS:CA	1:91:A:LYS:C	1:92:A:LYS:N	2	4.0
(1,102)	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	1:72:A:GLU:N	3	3.97
(1,14)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:HIS:N	17	3.43
(1,14)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:HIS:N	8	3.28
(1,91)	1:87:A:CYS:C	1:88:A:GLU:N	1:88:A:GLU:CA	1:88:A:GLU:C	4	3.25
(1,14)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:HIS:N	19	3.18
(1,14)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:HIS:N	20	3.18
(1,14)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:HIS:N	6	3.07
(1,101)	1:70:A:LEU:C	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	11	2.7
(1,14)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:HIS:N	1	2.67
(1,14)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:HIS:N	11	2.66

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,85)	1:82:A:PRO:C	1:83:A:ALA:N	1:83:A:ALA:CA	1:83:A:ALA:C	3	2.61
(1,102)	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	1:72:A:GLU:N	14	2.6
(1,14)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:HIS:N	7	2.54
(1,101)	1:70:A:LEU:C	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	20	2.44
(1,14)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:HIS:N	5	2.44
(1,14)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:HIS:N	18	2.36
(1,37)	1:80:A:HIS:C	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	3	2.34
(1,82)	1:84:A:MET:N	1:84:A:MET:CA	1:84:A:MET:C	1:85:A:LYS:N	18	2.3
(1,21)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	10	2.26
(1,14)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:HIS:N	12	2.18
(1,14)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:HIS:N	9	2.14
(1,82)	1:84:A:MET:N	1:84:A:MET:CA	1:84:A:MET:C	1:85:A:LYS:N	2	2.11
(1,32)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:LYS:N	3	2.1
(1,82)	1:84:A:MET:N	1:84:A:MET:CA	1:84:A:MET:C	1:85:A:LYS:N	13	2.07
(1,14)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:HIS:N	2	2.05
(1,61)	1:50:A:GLY:C	1:51:A:LYS:N	1:51:A:LYS:CA	1:51:A:LYS:C	7	2.04
(1,14)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:HIS:N	4	2.02
(1,102)	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	1:72:A:GLU:N	16	1.9
(1,105)	1:69:A:ILE:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	15	1.8
(1,22)	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	1:103:A:GLU:N	4	1.8
(1,21)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	5	1.8
(1,21)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	4	1.75
(1,82)	1:84:A:MET:N	1:84:A:MET:CA	1:84:A:MET:C	1:85:A:LYS:N	5	1.73
(1,101)	1:70:A:LEU:C	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	5	1.68
(1,22)	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	1:103:A:GLU:N	8	1.62
(1,21)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	7	1.61
(1,14)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:HIS:N	13	1.54
(1,105)	1:69:A:ILE:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	12	1.53
(1,102)	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	1:72:A:GLU:N	9	1.48
(1,102)	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	1:72:A:GLU:N	2	1.41
(1,37)	1:80:A:HIS:C	1:81:A:MET:N	1:81:A:MET:CA	1:81:A:MET:C	10	1.38
(1,106)	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	1:71:A:SER:N	14	1.33
(1,22)	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	1:103:A:GLU:N	7	1.32
(1,3)	1:77:A:MET:C	1:78:A:SER:N	1:78:A:SER:CA	1:78:A:SER:C	3	1.3
(1,50)	1:23:A:LYS:N	1:23:A:LYS:CA	1:23:A:LYS:C	1:24:A:SER:N	13	1.29
(1,101)	1:70:A:LEU:C	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	9	1.27
(1,4)	1:78:A:SER:N	1:78:A:SER:CA	1:78:A:SER:C	1:79:A:VAL:N	15	1.26
(1,159)	1:132:A:CYS:C	1:133:A:ARG:N	1:133:A:ARG:CA	1:133:A:ARG:C	18	1.24
(1,105)	1:69:A:ILE:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	13	1.21
(1,86)	1:83:A:ALA:N	1:83:A:ALA:CA	1:83:A:ALA:C	1:84:A:MET:N	3	1.19
(1,105)	1:69:A:ILE:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	19	1.17
(1,153)	1:130:A:GLU:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	16	1.16
(1,86)	1:83:A:ALA:N	1:83:A:ALA:CA	1:83:A:ALA:C	1:84:A:MET:N	7	1.13
(1,101)	1:70:A:LEU:C	1:71:A:SER:N	1:71:A:SER:CA	1:71:A:SER:C	6	1.09
(1,43)	1:85:A:LYS:C	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	2	1.09
(1,22)	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	1:103:A:GLU:N	2	1.09
(1,21)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	12	1.09
(1,26)	1:96:A:GLN:N	1:96:A:GLN:CA	1:96:A:GLN:C	1:97:A:ILE:N	2	1.06
(1,21)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	8	1.06