Full wwPDB NMR Structure Validation Report (i)

Mar 1, 2026 – 05:22 PM UTC

PDB ID	:	2LGO / pdb_00002lgo
BMRB ID	:	17818
Title	:	Solution NMR structure of a FKBP-type peptidyl-prolyl cis-trans isomerase from Giardia lamblia, Seattle Structural Genomics Center for Infectious Disease target GilaA.00840.a
Authors	:	Buchko, G.W.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2011-07-29

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

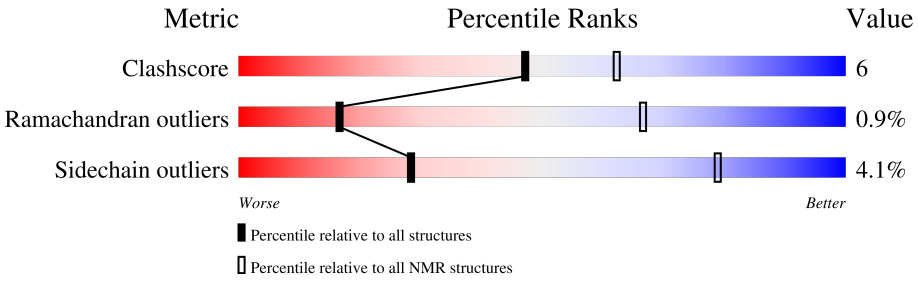
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 77%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	130	73% 7% • 18%

2 Ensemble composition and analysis

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:25-A:130 (106)	0.92	14

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

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

The models can be grouped into 5 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1996 atoms, of which 998 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called FKBP.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	130	1996	637	998	175	182	4	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q8I6M8
A	2	ALA	-	expression tag	UNP Q8I6M8
A	3	HIS	-	expression tag	UNP Q8I6M8
A	4	HIS	-	expression tag	UNP Q8I6M8
A	5	HIS	-	expression tag	UNP Q8I6M8
A	6	HIS	-	expression tag	UNP Q8I6M8
A	7	HIS	-	expression tag	UNP Q8I6M8
A	8	HIS	-	expression tag	UNP Q8I6M8
A	9	MET	-	expression tag	UNP Q8I6M8
A	10	GLY	-	expression tag	UNP Q8I6M8
A	11	THR	-	expression tag	UNP Q8I6M8
A	12	LEU	-	expression tag	UNP Q8I6M8
A	13	GLU	-	expression tag	UNP Q8I6M8
A	14	ALA	-	expression tag	UNP Q8I6M8
A	15	GLN	-	expression tag	UNP Q8I6M8
A	16	THR	-	expression tag	UNP Q8I6M8
A	17	GLN	-	expression tag	UNP Q8I6M8
A	18	GLY	-	expression tag	UNP Q8I6M8
A	19	PRO	-	expression tag	UNP Q8I6M8
A	20	GLY	-	expression tag	UNP Q8I6M8
A	21	SER	-	expression tag	UNP Q8I6M8

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: FKBP

Chain A:

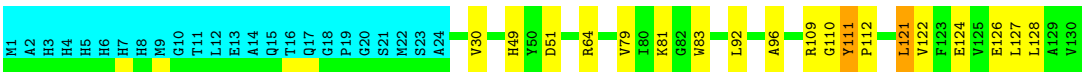
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: FKBP

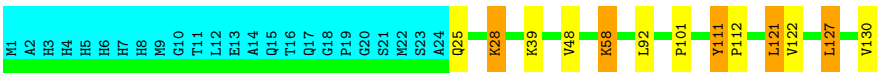
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: FKBP

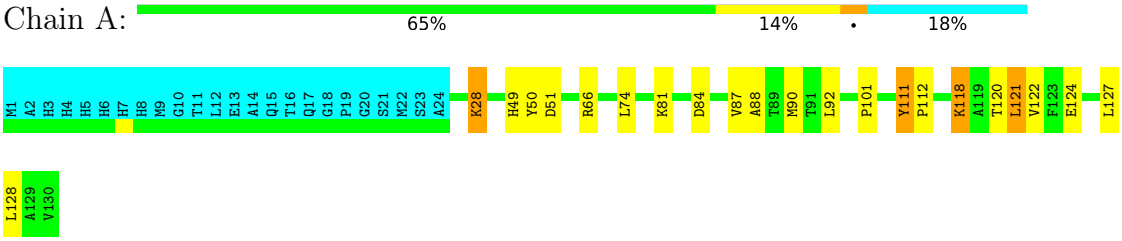
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: FKBP

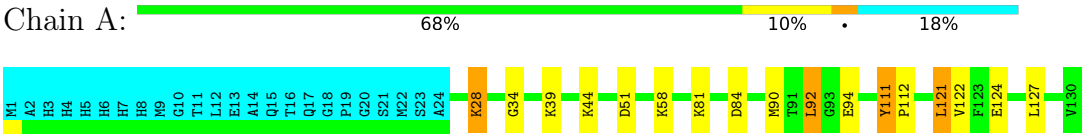
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: FKBP

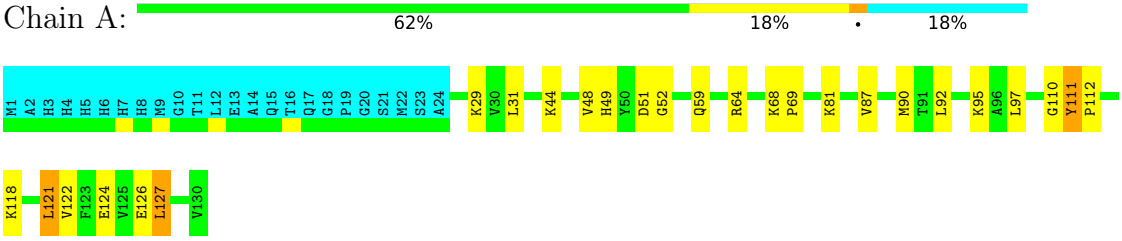
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: FKBP

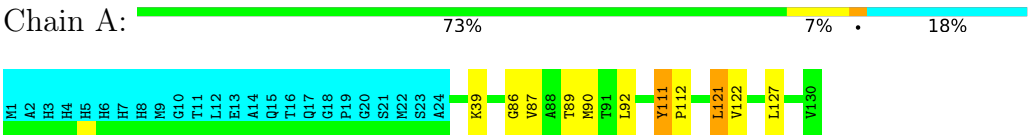
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: FKBP

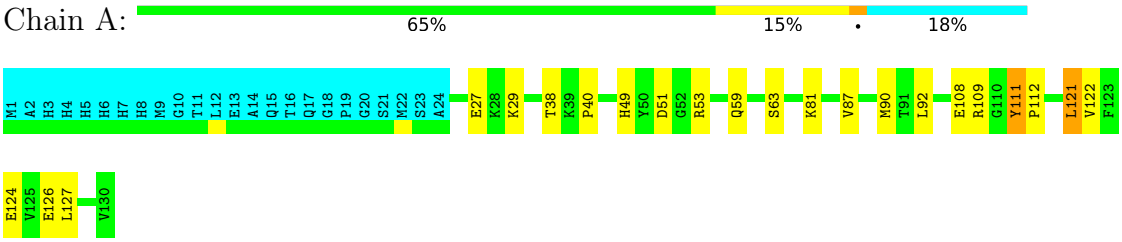
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: FKBP

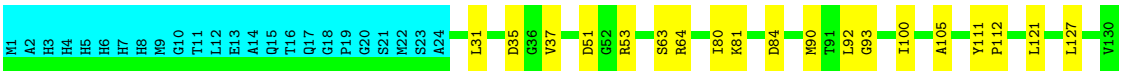
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: FKBP

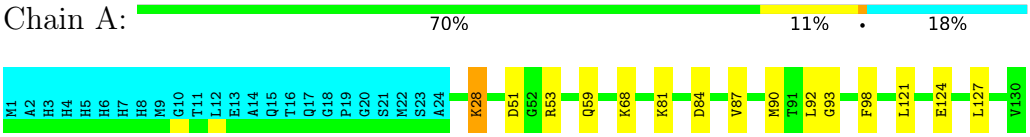
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: FKBP

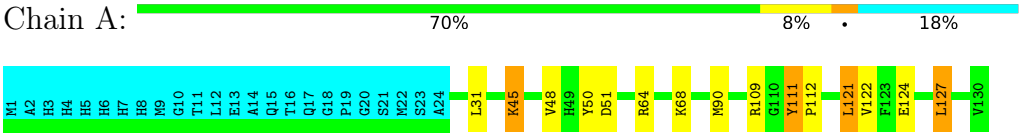
Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: FKBP

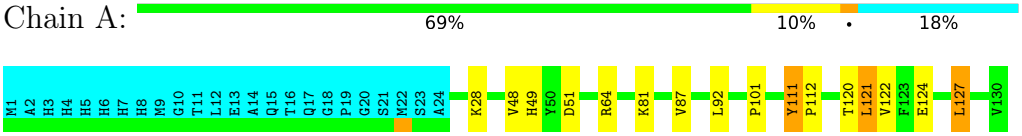
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: FKBP

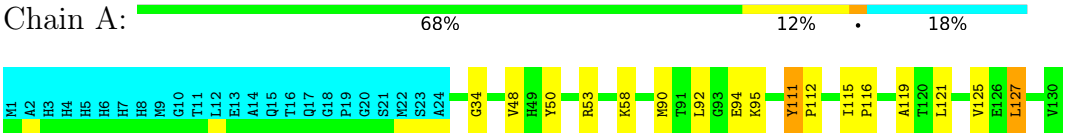
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: FKBP

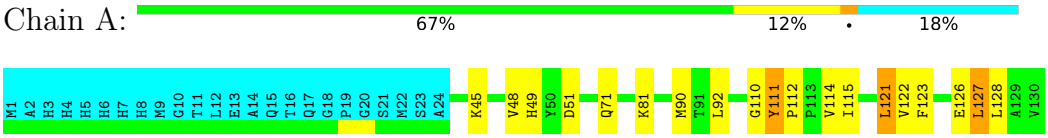
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: FKBP

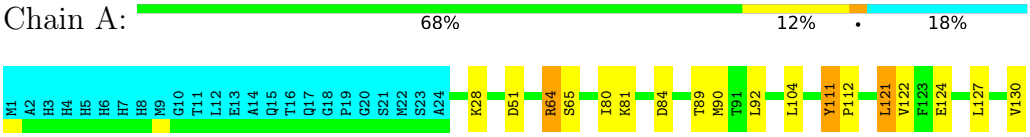
Chain A:



4.2.14 Score per residue for model 14 (medoid)

• Molecule 1: FKBP

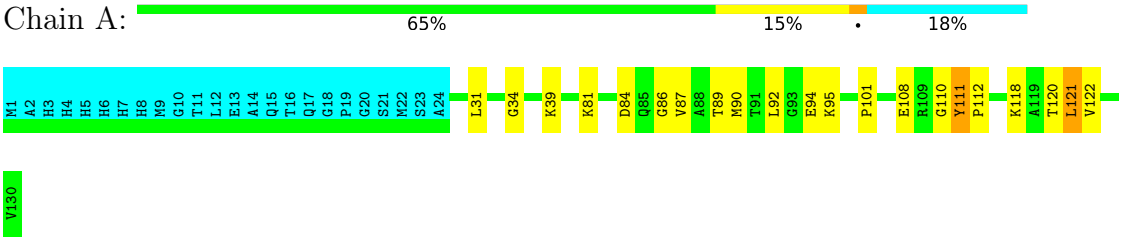
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: FKBP

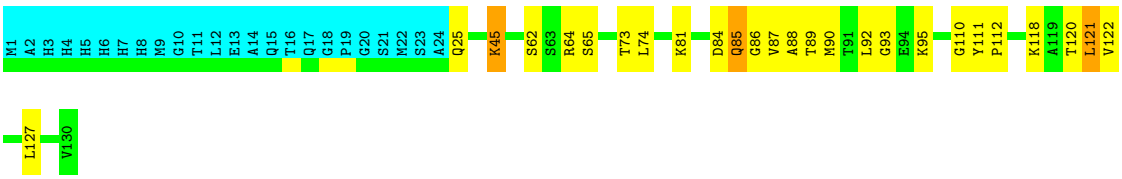
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: FKBP

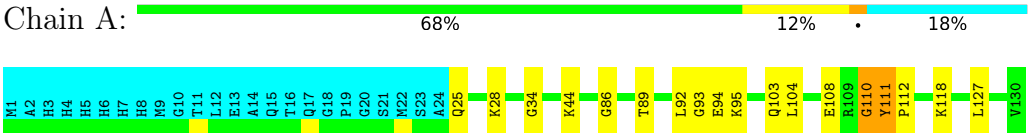
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: FKBP

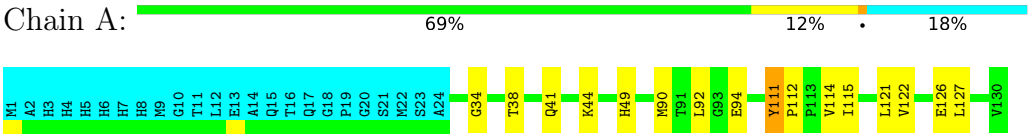
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: FKBP

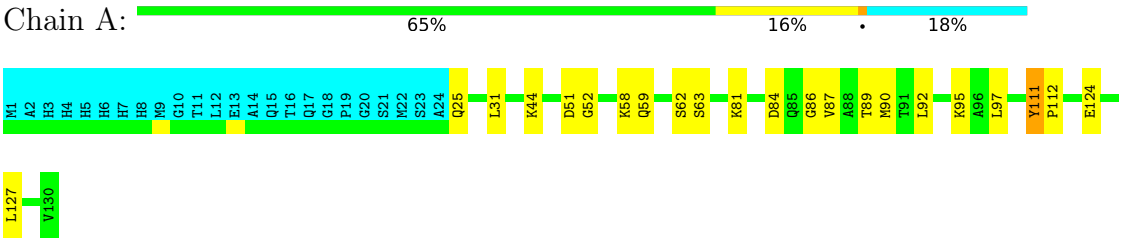
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: FKBP

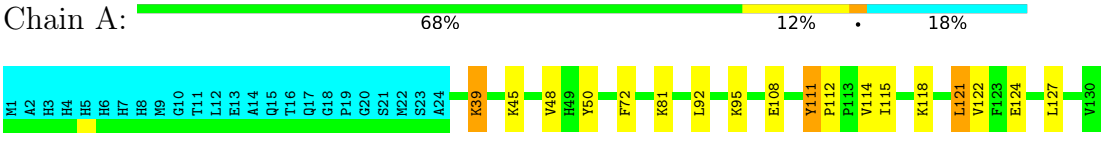
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: FKBP

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

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

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

Software name	Classification	Version
CYANA	structure solution	3.0
CNS	refinement	1.1
CYANA	refinement	

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	1218
Number of shifts mapped to atoms	1218
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	819	833	832	10±2
All	All	16380	16660	16640	197

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:MET:SD	1:A:127:LEU:HB2	0.77	2.19	4	10
1:A:92:LEU:HA	1:A:127:LEU:HD12	0.71	1.62	8	17
1:A:51:ASP:HB2	1:A:124:GLU:HB2	0.66	1.65	11	6
1:A:81:LYS:HA	1:A:84:ASP:HB3	0.64	1.69	8	7
1:A:48:VAL:HG12	1:A:127:LEU:HD22	0.63	1.71	11	5
1:A:51:ASP:HB3	1:A:124:GLU:HB3	0.63	1.70	9	2
1:A:111:TYR:HB2	1:A:112:PRO:HD3	0.63	1.71	12	16
1:A:108:GLU:HA	1:A:118:LYS:HA	0.61	1.72	15	3
1:A:118:LYS:NZ	1:A:118:LYS:HB2	0.60	2.11	3	2
1:A:28:LYS:N	1:A:28:LYS:HD3	0.59	2.11	3	1
1:A:85:GLN:HE21	1:A:85:GLN:HA	0.58	1.57	16	1
1:A:49:HIS:CE1	1:A:64:ARG:HA	0.58	2.33	1	2
1:A:74:LEU:HD11	1:A:88:ALA:HB2	0.58	1.73	3	2
1:A:49:HIS:HB2	1:A:126:GLU:HB3	0.56	1.77	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:HIS:HB3	1:A:126:GLU:HB3	0.53	1.81	1	3
1:A:87:VAL:O	1:A:90:MET:HG2	0.53	2.04	6	8
1:A:112:PRO:HG2	1:A:115:ILE:HB	0.53	1.81	13	1
1:A:121:LEU:HD13	1:A:122:VAL:N	0.52	2.19	15	15
1:A:86:GLY:O	1:A:89:THR:HG22	0.51	2.06	19	5
1:A:27:GLU:HB3	1:A:29:LYS:HE3	0.51	1.83	7	1
1:A:51:ASP:HA	1:A:63:SER:HB2	0.51	1.81	8	3
1:A:25:GLN:HB2	1:A:120:THR:HG21	0.51	1.81	16	1
1:A:114:VAL:HG23	1:A:115:ILE:HG12	0.50	1.84	13	3
1:A:45:LYS:HB2	1:A:45:LYS:HZ3	0.50	1.67	10	1
1:A:80:ILE:HD12	1:A:105:ALA:HA	0.49	1.85	8	1
1:A:45:LYS:HD2	1:A:71:GLN:HB3	0.49	1.83	13	1
1:A:52:GLY:O	1:A:59:GLN:HB2	0.49	2.08	19	2
1:A:110:GLY:O	1:A:111:TYR:HB2	0.49	2.07	5	4
1:A:31:LEU:HD23	1:A:95:LYS:HD3	0.48	1.84	5	1
1:A:50:TYR:HA	1:A:124:GLU:O	0.48	2.09	20	3
1:A:31:LEU:HD11	1:A:97:LEU:HB2	0.47	1.87	19	1
1:A:66:ARG:HA	1:A:66:ARG:HE	0.47	1.69	3	1
1:A:45:LYS:NZ	1:A:73:THR:OG1	0.47	2.48	16	1
1:A:53:ARG:HG3	1:A:59:GLN:HB3	0.46	1.86	9	2
1:A:101:PRO:HA	1:A:120:THR:HG23	0.46	1.87	11	3
1:A:118:LYS:HB2	1:A:118:LYS:HZ2	0.46	1.69	3	1
1:A:111:TYR:H	1:A:112:PRO:HD2	0.46	1.71	18	1
1:A:28:LYS:HD3	1:A:28:LYS:H	0.46	1.71	4	1
1:A:116:PRO:HG2	1:A:119:ALA:HB2	0.46	1.86	12	1
1:A:34:GLY:HA3	1:A:94:GLU:HB2	0.46	1.87	12	5
1:A:49:HIS:ND1	1:A:128:LEU:HD21	0.45	2.25	13	1
1:A:110:GLY:O	1:A:112:PRO:HD2	0.45	2.11	5	2
1:A:39:LYS:HB3	1:A:39:LYS:NZ	0.45	2.26	6	2
1:A:62:SER:OG	1:A:64:ARG:HG3	0.45	2.10	16	1
1:A:92:LEU:HD23	1:A:93:GLY:N	0.44	2.25	16	4
1:A:64:ARG:HD2	1:A:65:SER:N	0.44	2.28	16	1
1:A:118:LYS:HB3	1:A:118:LYS:NZ	0.44	2.28	16	1
1:A:28:LYS:HB3	1:A:98:PHE:CD2	0.44	2.48	9	1
1:A:25:GLN:H	1:A:101:PRO:HB3	0.43	1.72	2	1
1:A:38:THR:O	1:A:40:PRO:HD3	0.43	2.13	7	1
1:A:127:LEU:HD11	1:A:130:VAL:HB	0.43	1.90	14	1
1:A:53:ARG:NH2	1:A:64:ARG:NH2	0.43	2.66	8	1
1:A:112:PRO:HD2	1:A:115:ILE:HB	0.43	1.91	12	1
1:A:49:HIS:HB2	1:A:128:LEU:HD21	0.43	1.91	1	1
1:A:87:VAL:HG23	1:A:127:LEU:HD23	0.43	1.89	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:VAL:HB	1:A:83:TRP:HE3	0.43	1.73	1	1
1:A:35:ASP:HB3	1:A:37:VAL:HG22	0.43	1.91	8	1
1:A:59:GLN:NE2	1:A:62:SER:HA	0.43	2.29	19	1
1:A:49:HIS:HB3	1:A:128:LEU:HD21	0.43	1.90	3	1
1:A:38:THR:HG21	1:A:92:LEU:HB2	0.42	1.90	18	1
1:A:103:GLN:HG3	1:A:104:LEU:HG	0.42	1.90	17	1
1:A:100:ILE:HG22	1:A:105:ALA:HB2	0.42	1.92	8	1
1:A:30:VAL:HA	1:A:96:ALA:HA	0.42	1.91	1	1
1:A:81:LYS:HD3	1:A:81:LYS:O	0.42	2.15	1	2
1:A:28:LYS:NZ	1:A:89:THR:OG1	0.42	2.51	14	1
1:A:64:ARG:HG2	1:A:65:SER:N	0.42	2.30	14	1
1:A:68:LYS:HD2	1:A:69:PRO:HD2	0.42	1.92	5	1
1:A:51:ASP:O	1:A:123:PHE:HA	0.42	2.14	13	1
1:A:58:LYS:NZ	1:A:58:LYS:HB2	0.41	2.30	2	1
1:A:80:ILE:HD12	1:A:104:LEU:O	0.41	2.14	14	1
1:A:39:LYS:NZ	1:A:39:LYS:HB2	0.41	2.30	2	2
1:A:108:GLU:HG3	1:A:109:ARG:N	0.41	2.30	7	1
1:A:51:ASP:HB3	1:A:124:GLU:HB2	0.41	1.92	7	1
1:A:48:VAL:HG11	1:A:87:VAL:HG21	0.41	1.92	5	1
1:A:111:TYR:CB	1:A:112:PRO:HD3	0.41	2.44	15	1
1:A:45:LYS:HA	1:A:73:THR:HA	0.41	1.93	16	1
1:A:41:GLN:HG2	1:A:44:LYS:HE2	0.41	1.93	18	1
1:A:92:LEU:HD12	1:A:130:VAL:HG23	0.41	1.92	2	1
1:A:29:LYS:HB2	1:A:97:LEU:HB3	0.41	1.92	5	1
1:A:50:TYR:HD1	1:A:125:VAL:HG12	0.41	1.75	12	1
1:A:92:LEU:HD23	1:A:130:VAL:HG12	0.41	1.93	14	1
1:A:48:VAL:HG21	1:A:72:PHE:CE2	0.41	2.50	20	1
1:A:28:LYS:HD3	1:A:28:LYS:N	0.40	2.31	2	1
1:A:45:LYS:HB2	1:A:45:LYS:NZ	0.40	2.30	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	105/130 (81%)	101±2 (96±2%)	3±2 (3±2%)	1±0 (1±0%)	16 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2100/2600 (81%)	2024 (96%)	57 (3%)	19 (1%)	16 66

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

Mol	Chain	Res	Type	Models (Total)
1	A	111	TYR	17
1	A	110	GLY	2

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	86/104 (83%)	82±2 (96±2%)	4±2 (4±2%)	28 79
All	All	1720/2080 (83%)	1649 (96%)	71 (4%)	28 79

All 20 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	121	LEU	17
1	A	28	LYS	6
1	A	127	LEU	6
1	A	95	LYS	6
1	A	81	LYS	5
1	A	58	LYS	4
1	A	44	LYS	4
1	A	64	ARG	3
1	A	31	LEU	3
1	A	45	LYS	3
1	A	109	ARG	2
1	A	39	LYS	2
1	A	92	LEU	2
1	A	68	LYS	2
1	A	51	ASP	1
1	A	118	LYS	1
1	A	53	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	84	ASP	1
1	A	85	GLN	1
1	A	25	GLN	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 77% for the well-defined parts and 70% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1218
Number of shifts mapped to atoms	1218
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	121	-0.13 ± 0.12	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	104	-0.12 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	111	-0.20 ± 0.57	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 77%, i.e. 1105 atoms were assigned a chemical shift out of a possible 1433. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	396/525 (75%)	196/216 (91%)	104/212 (49%)	96/97 (99%)
Sidechain	639/792 (81%)	430/516 (83%)	205/248 (83%)	4/28 (14%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	70/116 (60%)	38/56 (68%)	31/57 (54%)	1/3 (33%)
Overall	1105/1433 (77%)	664/788 (84%)	340/517 (66%)	101/128 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 70%, i.e. 1217 atoms were assigned a chemical shift out of a possible 1729. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	457/646 (71%)	225/266 (85%)	121/260 (47%)	111/120 (92%)
Sidechain	690/919 (75%)	460/601 (77%)	226/288 (78%)	4/30 (13%)
Aromatic	70/164 (43%)	38/80 (48%)	31/69 (45%)	1/15 (7%)
Overall	1217/1729 (70%)	723/947 (76%)	378/617 (61%)	116/165 (70%)

7.1.4 Statistically unusual chemical shifts (i)

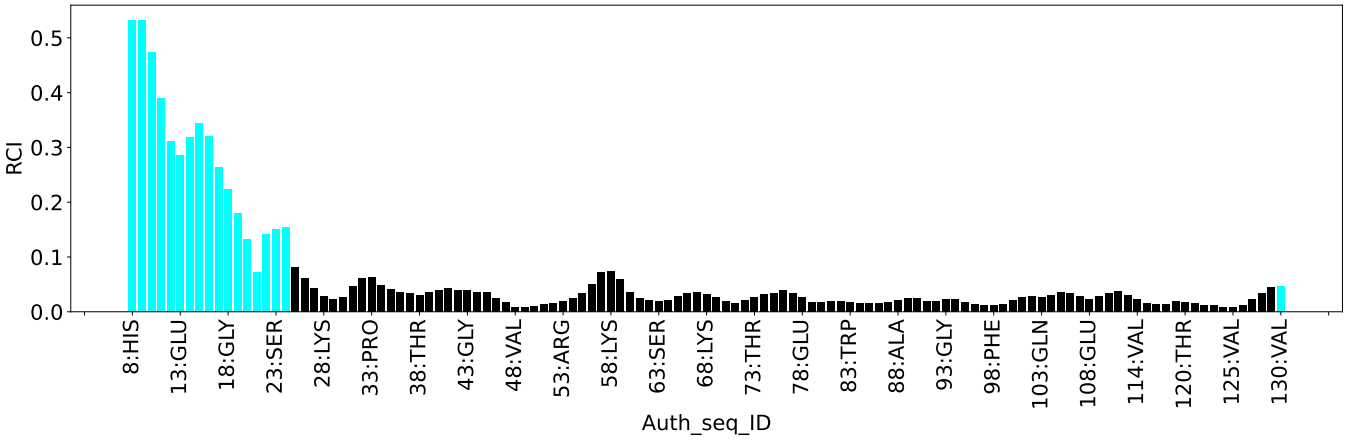
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	118	LYS	HG3	-0.09	0.04 – 2.67	-5.5

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:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
8:HIS
13:GLU
18:GLY
23:SER
28:LYS
33:PRO
38:THR
43:GLY
48:VAL
53:ARG
58:LYS
63:SER
68:LYS
73:THR
78:GLU
83:TRP
88:ALA
93:GLY
98:PHE
103:GLN
108:GLU
114:VAL
120:THR
125:VAL
130:VAL
Auth_seq_ID

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	1739
Intra-residue (|i-j|=0)	395
Sequential (|i-j|=1)	468
Medium range (|i-j|>1 and |i-j|<5)	251
Long range (|i-j|≥5)	549
Inter-chain	0
Hydrogen bond restraints	76
Disulfide bond restraints	0
Total dihedral-angle restraints	150
Number of unmapped restraints	0
Number of restraints per residue	14.5
Number of long range restraints per residue[1]	4.7

[1]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)	44.5	0.2
0.2-0.5 (Medium)	86.6	0.5
>0.5 (Large)	157.0	5.69

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)	0.1	1.85
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

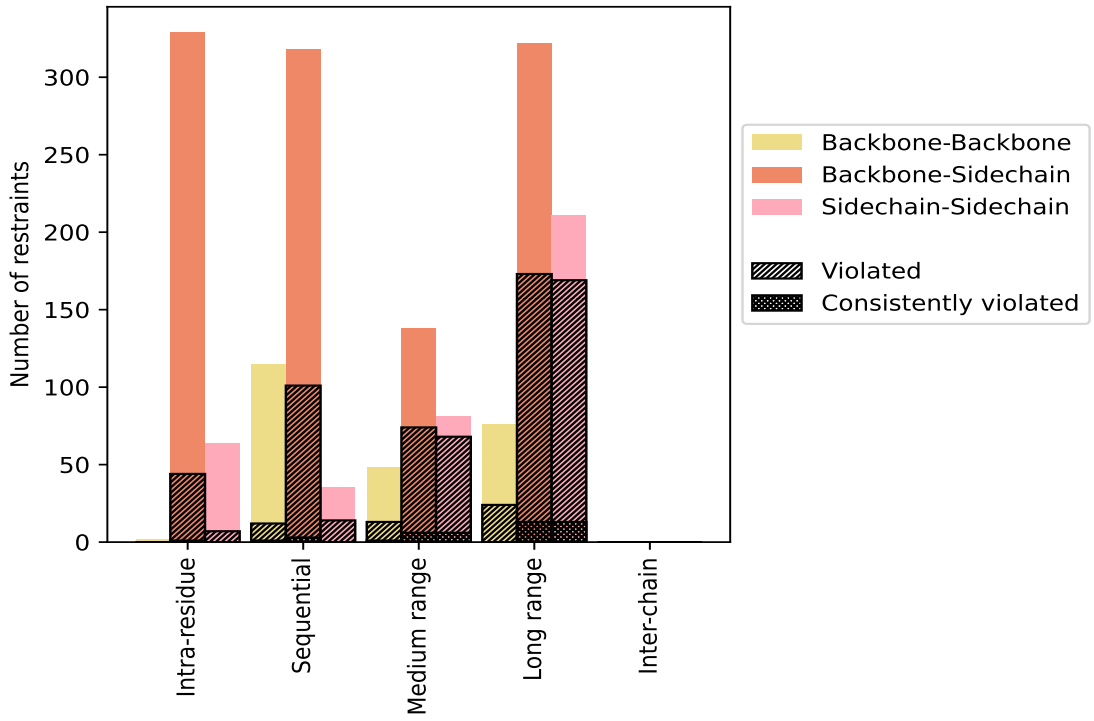
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	395	22.7	51	12.9	2.9	1	0.3	0.1
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	329	18.9	44	13.4	2.5	1	0.3	0.1
Sidechain-Sidechain	64	3.7	7	10.9	0.4	0	0.0	0.0
Sequential (|i-j|=1)	468	26.9	127	27.1	7.3	4	0.9	0.2
Backbone-Backbone	115	6.6	12	10.4	0.7	1	0.9	0.1
Backbone-Sidechain	318	18.3	101	31.8	5.8	3	0.9	0.2
Sidechain-Sidechain	35	2.0	14	40.0	0.8	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	251	14.4	155	61.8	8.9	13	5.2	0.7
Backbone-Backbone	48	2.8	13	27.1	0.7	1	2.1	0.1
Backbone-Sidechain	122	7.0	74	60.7	4.3	6	4.9	0.3
Sidechain-Sidechain	81	4.7	68	84.0	3.9	6	7.4	0.3
Long range (|i-j|≥5)	549	31.6	366	66.7	21.0	26	4.7	1.5
Backbone-Backbone	76	4.4	24	31.6	1.4	0	0.0	0.0
Backbone-Sidechain	262	15.1	173	66.0	9.9	13	5.0	0.7
Sidechain-Sidechain	211	12.1	169	80.1	9.7	13	6.2	0.7
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	76	4.4	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1739	100.0	699	40.2	40.2	44	2.5	2.5
Backbone-Backbone	241	13.9	49	20.3	2.8	2	0.8	0.1
Backbone-Sidechain	1107	63.7	392	35.4	22.5	23	2.1	1.3
Sidechain-Sidechain	391	22.5	258	66.0	14.8	19	4.9	1.1

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	12	49	54	181	0	296	0.88	3.51	0.74	0.64
2	15	38	73	160	0	286	0.85	4.95	0.84	0.56
3	13	51	72	177	0	313	0.98	4.66	0.91	0.68
4	16	50	70	196	0	332	0.96	4.98	0.89	0.64
5	16	40	52	143	0	251	0.89	5.15	0.91	0.57
6	10	52	64	166	0	292	0.75	4.56	0.77	0.5
7	17	47	56	176	0	296	0.98	5.38	0.91	0.66
8	14	42	73	152	0	281	0.87	5.4	0.91	0.58
9	12	50	74	169	0	305	0.95	5.47	0.93	0.55
10	11	41	61	157	0	270	0.87	4.2	0.86	0.5

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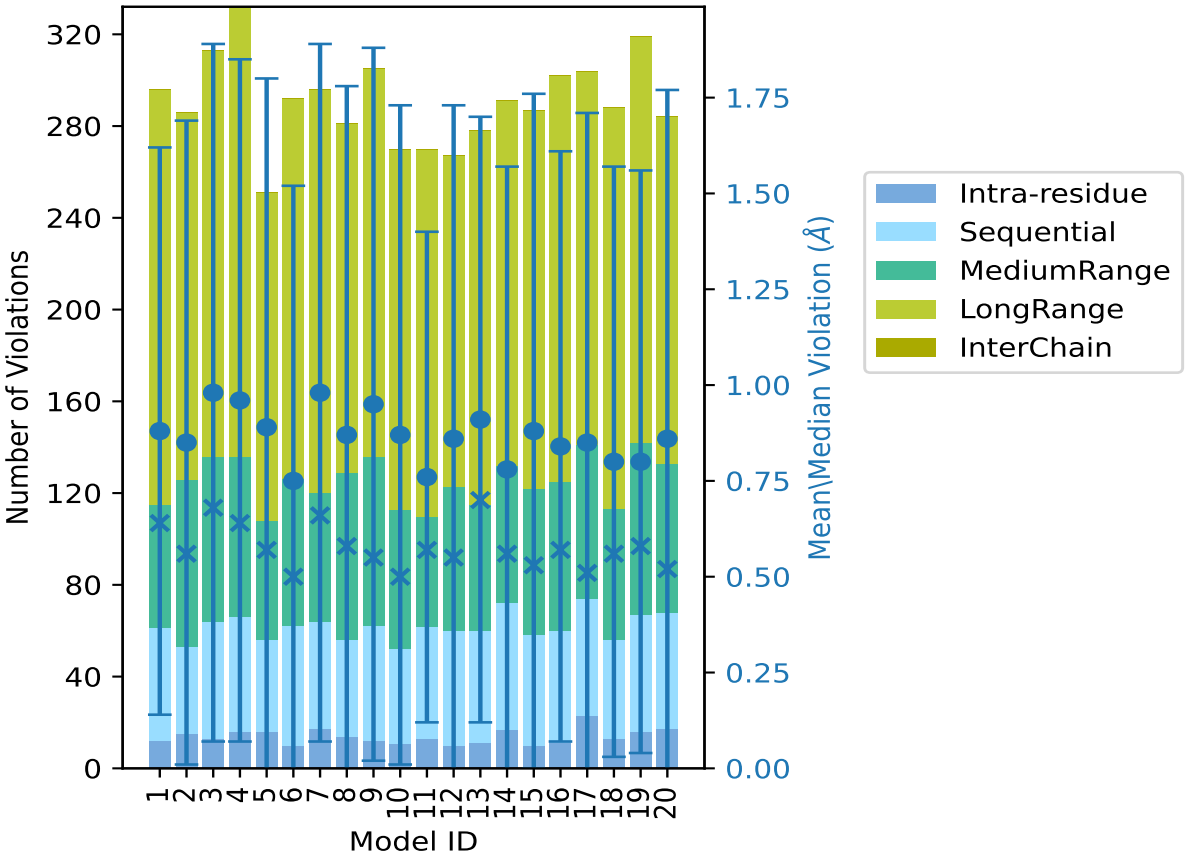
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	13	49	48	160	0	270	0.76	3.16	0.64	0.57
12	10	50	63	144	0	267	0.86	4.97	0.87	0.55
13	11	49	55	163	0	278	0.91	4.91	0.79	0.7
14	17	55	60	159	0	291	0.78	5.18	0.79	0.56
15	10	48	64	165	0	287	0.88	4.3	0.88	0.53
16	11	49	65	177	0	302	0.84	4.24	0.77	0.57
17	23	51	67	163	0	304	0.85	4.6	0.86	0.51
18	13	43	57	175	0	288	0.8	4.49	0.77	0.56
19	16	51	75	177	0	319	0.8	4.47	0.76	0.58
20	17	51	65	151	0	284	0.86	5.69	0.91	0.52

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model



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

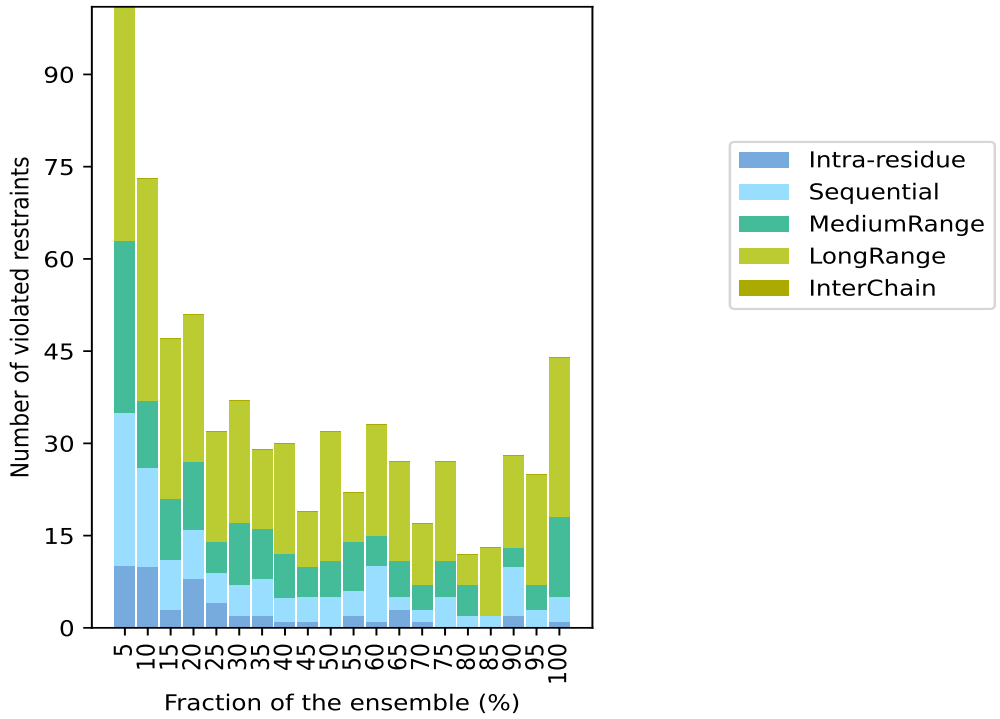
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 964(IR:344, SQ:341, MR:96, LR:183, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
10	25	28	38	0	101	1	5.0
10	16	11	36	0	73	2	10.0
3	8	10	26	0	47	3	15.0
8	8	11	24	0	51	4	20.0
4	5	5	18	0	32	5	25.0
2	5	10	20	0	37	6	30.0
2	6	8	13	0	29	7	35.0
1	4	7	18	0	30	8	40.0
1	4	5	9	0	19	9	45.0
0	5	6	21	0	32	10	50.0
2	4	8	8	0	22	11	55.0
1	9	5	18	0	33	12	60.0
3	2	6	16	0	27	13	65.0
1	2	4	10	0	17	14	70.0
0	5	6	16	0	27	15	75.0
0	2	5	5	0	12	16	80.0
0	2	0	11	0	13	17	85.0
2	8	3	15	0	28	18	90.0
0	3	4	18	0	25	19	95.0
1	4	13	26	0	44	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

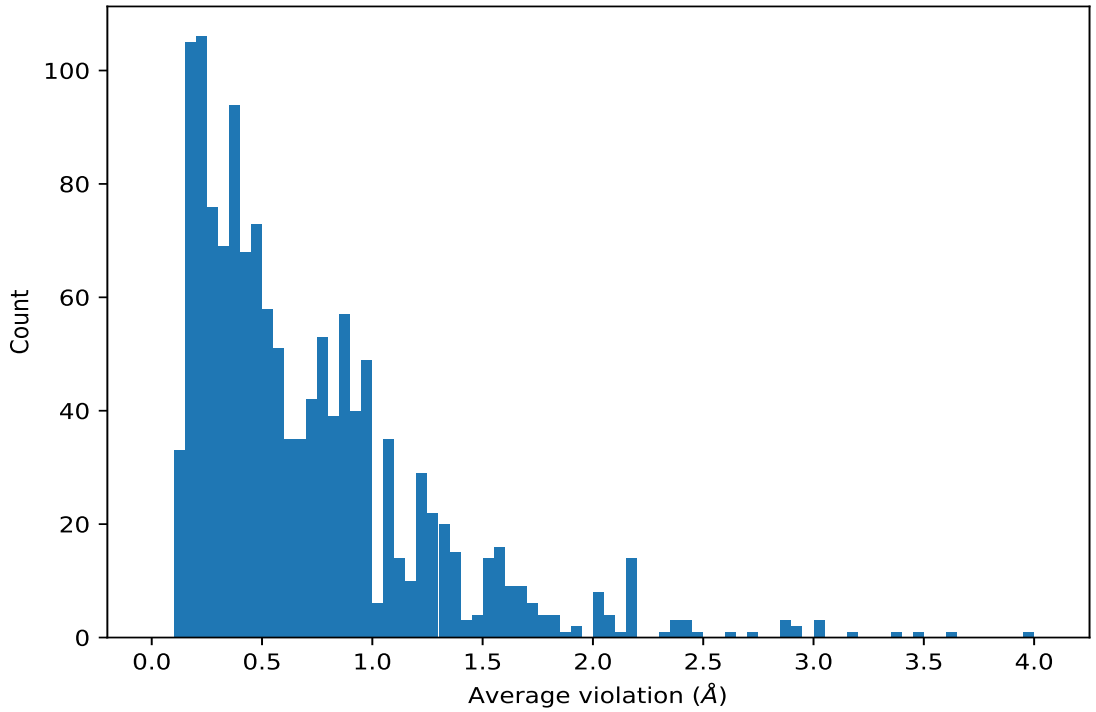
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	20	3.96	0.9	4.05
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	20	3.62	0.9	3.67
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	20	3.49	1.31	3.89
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	20	3.38	0.83	3.44
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	20	2.9	1.11	3.11
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	20	2.9	1.11	3.11
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	20	1.91	0.65	1.62
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	20	1.89	0.87	1.93
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	20	1.74	0.43	1.88
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	20	1.72	0.74	1.9
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	20	1.69	0.56	1.81
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	20	1.66	1.0	1.52
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	20	1.59	0.43	1.86
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	20	1.51	0.37	1.54
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	20	1.51	0.37	1.54
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	20	1.51	0.37	1.54

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	20	1.51	0.56	1.66
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	20	1.51	0.56	1.66
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	20	1.51	0.56	1.66
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	20	1.51	0.56	1.66
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	20	1.51	0.56	1.66
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	20	1.51	0.56	1.66
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	20	1.48	0.59	1.28
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	20	1.48	0.59	1.28
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	20	1.48	0.59	1.28
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	20	1.38	0.68	1.1
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	20	1.36	0.46	1.27
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	20	1.36	0.46	1.27
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	20	1.36	0.46	1.27
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	20	1.34	0.74	1.2
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	20	1.34	0.74	1.2
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	20	1.34	0.74	1.2
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	20	1.33	0.55	1.3
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	20	1.16	0.31	1.14
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	20	1.16	0.31	1.14
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	20	1.16	0.31	1.14
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	20	1.12	0.26	1.13
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	20	1.12	0.26	1.13
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	20	1.12	0.26	1.13
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	20	1.12	0.26	1.13
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	20	1.12	0.26	1.13
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	20	1.12	0.26	1.13
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	20	1.09	0.36	1.04
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	20	1.09	0.36	1.04
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	20	1.09	0.36	1.04
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	20	1.08	0.48	0.98
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	20	1.08	0.45	1.05
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	20	1.08	0.45	1.05
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	20	1.08	0.45	1.05
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	20	1.08	0.45	1.05
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	20	1.08	0.45	1.05
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	20	1.08	0.45	1.05
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	20	1.06	0.69	0.94
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	20	1.06	0.69	0.94
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	20	1.06	0.69	0.94
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	20	0.98	0.37	0.95
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	20	0.97	0.28	1.0
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	20	0.94	0.6	0.8

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	20	0.94	0.6	0.8
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	20	0.94	0.6	0.8
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	20	0.92	0.39	0.8
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	20	0.92	0.39	0.8
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	20	0.92	0.39	0.8
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	20	0.9	0.61	0.6
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	20	0.87	0.46	1.02
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	20	0.87	0.46	1.02
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	20	0.87	0.46	1.02
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	20	0.86	0.5	0.81
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	20	0.86	0.5	0.81
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	20	0.86	0.5	0.81
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	20	0.86	0.5	0.81
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	20	0.86	0.5	0.81
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	20	0.86	0.5	0.81
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	20	0.86	0.5	0.81
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	20	0.86	0.5	0.81
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	20	0.86	0.5	0.81
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	20	0.85	0.32	0.79
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	20	0.78	0.38	0.64
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	20	0.75	0.39	0.72
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	20	0.75	0.39	0.72
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	20	0.75	0.39	0.72
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	20	0.72	0.33	0.79
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	20	0.69	0.25	0.62
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	20	0.65	0.17	0.63
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	20	0.65	0.17	0.63
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	20	0.65	0.17	0.63
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	20	0.61	0.38	0.51
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	20	0.61	0.38	0.51
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	20	0.61	0.38	0.51
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	20	0.43	0.1	0.46
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	20	0.39	0.18	0.34
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	20	0.39	0.18	0.34
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	20	0.35	0.02	0.36
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	20	0.25	0.05	0.26
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	20	0.25	0.05	0.26
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	20	0.25	0.05	0.26
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	20	0.22	0.05	0.23
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	19	2.85	0.69	2.8
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	19	2.85	0.69	2.8
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	19	2.85	0.69	2.8

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	19	2.39	0.68	2.21
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	19	2.19	1.12	1.9
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	19	2.19	1.12	1.9
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	19	2.19	1.12	1.9
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	19	2.19	1.12	1.9
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	19	2.19	1.12	1.9
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	19	2.19	1.12	1.9
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	19	1.77	1.0	1.76
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	19	1.63	0.76	1.51
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	19	1.63	0.76	1.51
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	19	1.63	0.76	1.51
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	19	1.55	0.82	1.54
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	19	1.55	0.66	1.77
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	19	1.55	0.66	1.77
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	19	1.55	0.66	1.77
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	19	1.33	0.59	1.27
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	19	1.25	0.45	1.24
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	19	1.25	0.45	1.24
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	19	1.25	0.45	1.24
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	19	1.23	0.69	1.14
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	19	1.23	0.69	1.14
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	19	1.23	0.69	1.14
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	19	1.23	0.69	1.14
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	19	1.23	0.69	1.14
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	19	1.23	0.69	1.14
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	19	1.23	0.69	1.14
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	19	1.23	0.69	1.14
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	19	1.23	0.69	1.14
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	19	1.23	0.69	1.14
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	19	1.23	0.69	1.14
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	19	1.23	0.69	1.14
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	19	1.23	0.69	1.14
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	19	1.23	0.69	1.14
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	19	1.23	0.69	1.14
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	19	1.23	0.69	1.14
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	19	1.23	0.69	1.14
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	19	1.23	0.69	1.14
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	19	1.21	1.16	1.04
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	19	1.17	0.57	1.08
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	19	0.99	0.35	1.02
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	19	0.99	0.35	1.02
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	19	0.99	0.35	1.02

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	19	0.99	0.35	1.02
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	19	0.99	0.35	1.02
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	19	0.99	0.35	1.02
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	19	0.93	0.58	0.81
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	19	0.82	0.24	0.88
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	19	0.82	0.24	0.88
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	19	0.82	0.24	0.88
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	19	0.79	0.42	0.73
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	19	0.79	0.42	0.73
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	19	0.79	0.42	0.73
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	19	0.79	0.42	0.73
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	19	0.79	0.42	0.73
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	19	0.79	0.42	0.73
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	19	0.79	0.29	0.75
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	19	0.79	0.29	0.75
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	19	0.79	0.29	0.75
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	19	0.78	0.21	0.86
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	19	0.76	0.3	0.75
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	19	0.76	0.3	0.75
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	19	0.76	0.3	0.75
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	19	0.76	0.3	0.75
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	19	0.76	0.3	0.75
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	19	0.76	0.3	0.75
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	19	0.75	0.25	0.72
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	19	0.65	0.38	0.53
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	19	0.58	0.25	0.64
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	19	0.42	0.26	0.38
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	19	0.29	0.09	0.27
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	19	0.21	0.04	0.22
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	18	3.18	0.75	3.3
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	18	2.44	0.66	2.28
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	18	2.31	0.92	2.7
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	18	2.19	0.83	1.99
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	18	2.19	0.83	1.99
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	18	2.19	0.83	1.99
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	18	2.18	1.22	2.2
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	18	2.18	1.22	2.2
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	18	2.18	1.22	2.2
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	18	2.12	0.49	1.98
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	18	2.01	0.31	1.92
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	18	2.01	0.31	1.92
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	18	1.5	0.73	1.59

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	18	1.35	0.2	1.32
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	18	1.35	0.2	1.32
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	18	1.35	0.2	1.32
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	18	1.31	0.5	1.28
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	18	1.09	0.74	1.0
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	18	1.09	0.74	1.0
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	18	1.09	0.74	1.0
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	18	1.09	0.74	1.0
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	18	1.09	0.74	1.0
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	18	1.09	0.74	1.0
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	18	0.96	0.53	0.93
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	18	0.88	0.43	0.84
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	18	0.88	0.43	0.84
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	18	0.88	0.43	0.84
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	18	0.8	0.47	0.67
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	18	0.8	0.47	0.67
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	18	0.8	0.47	0.67
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	18	0.72	0.38	0.7
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	18	0.62	0.36	0.56
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	18	0.62	0.36	0.56
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	18	0.62	0.36	0.56
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	18	0.59	0.21	0.5
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	18	0.58	0.26	0.62
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	18	0.58	0.26	0.62
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	18	0.58	0.26	0.62
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	18	0.53	0.21	0.5
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	18	0.53	0.21	0.5
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	18	0.53	0.21	0.5
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	18	0.49	0.21	0.5
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	18	0.47	0.19	0.48
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	18	0.44	0.21	0.38
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	18	0.44	0.21	0.38
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	18	0.44	0.21	0.38
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	18	0.44	0.21	0.38
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	18	0.44	0.21	0.38
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	18	0.44	0.21	0.38
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	18	0.35	0.15	0.32
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	18	0.33	0.13	0.36
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	18	0.33	0.13	0.36
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	18	0.33	0.13	0.36
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	18	0.33	0.13	0.36
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	18	0.33	0.13	0.36

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	18	0.33	0.13	0.36
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	18	0.29	0.12	0.34
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	18	0.25	0.1	0.22
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	18	0.25	0.1	0.22
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	18	0.21	0.07	0.22
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	18	0.21	0.07	0.22
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	18	0.21	0.07	0.22
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	18	0.17	0.02	0.18
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	17	1.62	0.88	1.65
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	17	1.62	0.88	1.65
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	17	1.62	0.88	1.65
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	17	1.57	0.82	1.29
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	17	1.57	0.82	1.29
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	17	1.57	0.82	1.29
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	17	1.31	0.53	1.41
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	17	1.31	0.53	1.41
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	17	1.31	0.53	1.41
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	17	1.11	0.57	1.13
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	17	1.11	0.57	1.13
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	17	1.11	0.57	1.13
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	17	1.04	0.7	0.84
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	17	0.96	0.75	0.6
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	17	0.96	0.75	0.6
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	17	0.66	0.39	0.56
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	17	0.66	0.39	0.56
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	17	0.66	0.39	0.56
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	17	0.63	0.29	0.61
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	17	0.56	0.31	0.6
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	17	0.56	0.31	0.6
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	17	0.56	0.31	0.6
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	17	0.56	0.31	0.6
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	17	0.56	0.31	0.6
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	17	0.56	0.31	0.6
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	17	0.48	0.3	0.46
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	17	0.48	0.3	0.46
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	17	0.48	0.3	0.46
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	17	0.46	0.13	0.49
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	17	0.46	0.13	0.49
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	17	0.36	0.11	0.39
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	17	0.36	0.11	0.39
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	17	0.36	0.11	0.39
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	17	0.23	0.1	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	17	0.23	0.1	0.2
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	17	0.23	0.1	0.2
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD21	16	1.61	0.96	1.59
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD22	16	1.61	0.96	1.59
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD23	16	1.61	0.96	1.59
(1,75)	1:38:A:THR:HB	1:40:A:PRO:HG3	16	1.56	0.93	1.62
(1,500)	1:81:A:LYS:HB2	1:104:A:LEU:HA	16	1.56	0.84	1.81
(1,953)	1:49:A:HIS:HE1	1:68:A:LYS:H	16	1.44	0.71	1.41
(1,1310)	1:81:A:LYS:HE2	1:85:A:GLN:HE22	16	1.4	0.68	1.38
(1,923)	1:71:A:GLN:HE21	1:72:A:PHE:H	16	0.85	0.4	1.04
(1,76)	1:38:A:THR:HB	1:40:A:PRO:HD3	16	0.82	0.46	0.76
(1,130)	1:48:A:VAL:HG11	1:50:A:TYR:HD1	16	0.76	0.65	0.7
(1,130)	1:48:A:VAL:HG12	1:50:A:TYR:HD1	16	0.76	0.65	0.7
(1,130)	1:48:A:VAL:HG13	1:50:A:TYR:HD1	16	0.76	0.65	0.7
(1,185)	1:53:A:ARG:HB3	1:57:A:GLY:HA2	16	0.64	0.36	0.61
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD21	16	0.52	0.22	0.54
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD22	16	0.52	0.22	0.54
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD23	16	0.52	0.22	0.54
(1,1594)	1:97:A:LEU:HD11	1:123:A:PHE:H	16	0.4	0.19	0.4
(1,1594)	1:97:A:LEU:HD12	1:123:A:PHE:H	16	0.4	0.19	0.4
(1,1594)	1:97:A:LEU:HD13	1:123:A:PHE:H	16	0.4	0.19	0.4
(1,1594)	1:97:A:LEU:HD21	1:123:A:PHE:H	16	0.4	0.19	0.4
(1,1594)	1:97:A:LEU:HD22	1:123:A:PHE:H	16	0.4	0.19	0.4
(1,1594)	1:97:A:LEU:HD23	1:123:A:PHE:H	16	0.4	0.19	0.4
(1,103)	1:45:A:LYS:HG2	1:46:A:VAL:H	16	0.32	0.08	0.32
(1,191)	1:54:A:PHE:HD1	1:58:A:LYS:HD3	15	2.49	1.31	2.33
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB2	15	2.17	0.95	2.3
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB3	15	2.17	0.95	2.3
(1,960)	1:50:A:TYR:HE2	1:70:A:PHE:H	15	1.94	1.64	0.98
(1,758)	1:28:A:LYS:HG2	1:30:A:VAL:H	15	1.22	0.32	1.26
(1,165)	1:53:A:ARG:HG2	1:60:A:PHE:H	15	1.08	0.51	1.14
(1,28)	1:27:A:GLU:HG2	1:99:A:THR:HB	15	0.96	0.44	0.9
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG21	15	0.96	0.57	0.83
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG22	15	0.96	0.57	0.83
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG23	15	0.96	0.57	0.83
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG11	15	0.95	0.46	0.94
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG12	15	0.95	0.46	0.94
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG13	15	0.95	0.46	0.94
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG21	15	0.95	0.46	0.94
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG22	15	0.95	0.46	0.94
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG23	15	0.95	0.46	0.94
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG11	15	0.95	0.46	0.94

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG12	15	0.95	0.46	0.94
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG13	15	0.95	0.46	0.94
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG21	15	0.95	0.46	0.94
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG22	15	0.95	0.46	0.94
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG23	15	0.95	0.46	0.94
(1,1300)	1:92:A:LEU:HD21	1:130:A:VAL:H	15	0.92	0.38	0.9
(1,1300)	1:92:A:LEU:HD22	1:130:A:VAL:H	15	0.92	0.38	0.9
(1,1300)	1:92:A:LEU:HD23	1:130:A:VAL:H	15	0.92	0.38	0.9
(1,857)	1:49:A:HIS:HD2	1:51:A:ASP:H	15	0.9	0.64	0.5
(1,1543)	1:85:A:GLN:HB2	1:98:A:PHE:HD2	15	0.89	0.52	0.73
(1,1543)	1:85:A:GLN:HB3	1:98:A:PHE:HD2	15	0.89	0.52	0.73
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG21	15	0.85	0.21	0.89
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG22	15	0.85	0.21	0.89
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG23	15	0.85	0.21	0.89
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG21	15	0.81	0.81	0.54
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG22	15	0.81	0.81	0.54
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG23	15	0.81	0.81	0.54
(1,146)	1:49:A:HIS:HD2	1:50:A:TYR:HA	15	0.81	0.56	0.49
(1,211)	1:49:A:HIS:HB3	1:64:A:ARG:HA	15	0.79	0.32	0.68
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD11	15	0.78	0.4	0.68
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD12	15	0.78	0.4	0.68
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD13	15	0.78	0.4	0.68
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG21	15	0.76	0.52	0.72
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG22	15	0.76	0.52	0.72
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG23	15	0.76	0.52	0.72
(1,422)	1:38:A:THR:HG21	1:91:A:THR:HA	15	0.74	0.62	0.48
(1,422)	1:38:A:THR:HG22	1:91:A:THR:HA	15	0.74	0.62	0.48
(1,422)	1:38:A:THR:HG23	1:91:A:THR:HA	15	0.74	0.62	0.48
(1,686)	1:102:A:TYR:HE2	1:118:A:LYS:HA	15	0.72	0.44	0.67
(1,1111)	1:38:A:THR:HG21	1:92:A:LEU:H	15	0.66	0.55	0.37
(1,1111)	1:38:A:THR:HG22	1:92:A:LEU:H	15	0.66	0.55	0.37
(1,1111)	1:38:A:THR:HG23	1:92:A:LEU:H	15	0.66	0.55	0.37
(1,632)	1:93:A:GLY:H	1:127:A:LEU:HG	15	0.64	0.28	0.61
(1,1599)	1:97:A:LEU:HD11	1:124:A:GLU:HB3	15	0.48	0.21	0.48
(1,1599)	1:97:A:LEU:HD12	1:124:A:GLU:HB3	15	0.48	0.21	0.48
(1,1599)	1:97:A:LEU:HD13	1:124:A:GLU:HB3	15	0.48	0.21	0.48
(1,1599)	1:97:A:LEU:HD21	1:124:A:GLU:HB3	15	0.48	0.21	0.48
(1,1599)	1:97:A:LEU:HD22	1:124:A:GLU:HB3	15	0.48	0.21	0.48
(1,1599)	1:97:A:LEU:HD23	1:124:A:GLU:HB3	15	0.48	0.21	0.48
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB2	15	0.41	0.17	0.46
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB3	15	0.41	0.17	0.46
(1,1006)	1:77:A:GLY:H	1:78:A:GLU:HB2	15	0.38	0.15	0.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,64)	1:38:A:THR:HG21	1:39:A:LYS:H	15	0.32	0.11	0.36
(1,64)	1:38:A:THR:HG22	1:39:A:LYS:H	15	0.32	0.11	0.36
(1,64)	1:38:A:THR:HG23	1:39:A:LYS:H	15	0.32	0.11	0.36
(1,1116)	1:92:A:LEU:HD11	1:93:A:GLY:H	15	0.25	0.1	0.22
(1,1116)	1:92:A:LEU:HD12	1:93:A:GLY:H	15	0.25	0.1	0.22
(1,1116)	1:92:A:LEU:HD13	1:93:A:GLY:H	15	0.25	0.1	0.22
(1,460)	1:97:A:LEU:HD11	1:98:A:PHE:H	15	0.2	0.06	0.19
(1,460)	1:97:A:LEU:HD12	1:98:A:PHE:H	15	0.2	0.06	0.19
(1,460)	1:97:A:LEU:HD13	1:98:A:PHE:H	15	0.2	0.06	0.19
(1,682)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	14	1.71	1.48	1.3
(1,134)	1:48:A:VAL:HG21	1:50:A:TYR:HD1	14	1.54	0.38	1.46
(1,134)	1:48:A:VAL:HG22	1:50:A:TYR:HD1	14	1.54	0.38	1.46
(1,134)	1:48:A:VAL:HG23	1:50:A:TYR:HD1	14	1.54	0.38	1.46
(1,1323)	1:19:A:PRO:HG2	1:55:A:PRO:HB2	14	1.09	0.65	0.9
(1,1323)	1:19:A:PRO:HG3	1:55:A:PRO:HB2	14	1.09	0.65	0.9
(1,582)	1:55:A:PRO:HG2	1:120:A:THR:HB	14	1.05	0.71	1.03
(1,547)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	14	0.92	0.61	0.73
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG21	14	0.8	0.54	0.78
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG22	14	0.8	0.54	0.78
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG23	14	0.8	0.54	0.78
(1,193)	1:53:A:ARG:HB3	1:59:A:GLN:HA	14	0.75	0.37	0.74
(1,1648)	1:121:A:LEU:HD11	1:123:A:PHE:HD1	14	0.73	0.64	0.59
(1,1648)	1:121:A:LEU:HD12	1:123:A:PHE:HD1	14	0.73	0.64	0.59
(1,1648)	1:121:A:LEU:HD13	1:123:A:PHE:HD1	14	0.73	0.64	0.59
(1,1648)	1:121:A:LEU:HD21	1:123:A:PHE:HD1	14	0.73	0.64	0.59
(1,1648)	1:121:A:LEU:HD22	1:123:A:PHE:HD1	14	0.73	0.64	0.59
(1,1648)	1:121:A:LEU:HD23	1:123:A:PHE:HD1	14	0.73	0.64	0.59
(1,602)	1:100:A:ILE:HD11	1:123:A:PHE:HB3	14	0.61	0.39	0.44
(1,602)	1:100:A:ILE:HD12	1:123:A:PHE:HB3	14	0.61	0.39	0.44
(1,602)	1:100:A:ILE:HD13	1:123:A:PHE:HB3	14	0.61	0.39	0.44
(1,68)	1:38:A:THR:HG21	1:92:A:LEU:HA	14	0.6	0.43	0.36
(1,68)	1:38:A:THR:HG22	1:92:A:LEU:HA	14	0.6	0.43	0.36
(1,68)	1:38:A:THR:HG23	1:92:A:LEU:HA	14	0.6	0.43	0.36
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG21	14	0.43	0.18	0.4
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG22	14	0.43	0.18	0.4
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG23	14	0.43	0.18	0.4
(1,105)	1:45:A:LYS:H	1:45:A:LYS:HE2	14	0.43	0.14	0.37
(1,630)	1:127:A:LEU:HG	1:129:A:ALA:HA	14	0.39	0.14	0.38
(1,859)	1:50:A:TYR:HD2	1:51:A:ASP:H	14	0.38	0.09	0.38
(1,578)	1:119:A:ALA:HB1	1:120:A:THR:HB	14	0.29	0.13	0.28
(1,578)	1:119:A:ALA:HB2	1:120:A:THR:HB	14	0.29	0.13	0.28
(1,578)	1:119:A:ALA:HB3	1:120:A:THR:HB	14	0.29	0.13	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1106)	1:37:A:VAL:H	1:92:A:LEU:H	14	0.28	0.16	0.25
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG11	14	0.22	0.05	0.24
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG12	14	0.22	0.05	0.24
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG13	14	0.22	0.05	0.24
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG21	14	0.22	0.05	0.24
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG22	14	0.22	0.05	0.24
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG23	14	0.22	0.05	0.24
(1,149)	1:50:A:TYR:HB2	1:123:A:PHE:HD2	13	2.62	1.09	2.94
(1,190)	1:54:A:PHE:HD1	1:58:A:LYS:HD2	13	2.38	1.14	2.65
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD11	13	1.73	0.49	1.86
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD12	13	1.73	0.49	1.86
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD13	13	1.73	0.49	1.86
(1,225)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	13	1.66	1.05	1.35
(1,539)	1:102:A:TYR:HE2	1:108:A:GLU:HA	13	1.15	0.7	1.05
(1,536)	1:102:A:TYR:HE2	1:108:A:GLU:HB2	13	1.07	1.11	0.43
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG21	13	1.06	0.59	1.11
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG22	13	1.06	0.59	1.11
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG23	13	1.06	0.59	1.11
(1,1219)	1:111:A:TYR:H	1:115:A:ILE:HB	13	0.87	0.61	0.9
(1,695)	1:83:A:TRP:HZ2	1:123:A:PHE:HD1	13	0.81	0.51	0.58
(1,194)	1:53:A:ARG:HG2	1:59:A:GLN:HA	13	0.78	0.42	0.84
(1,240)	1:47:A:THR:HG21	1:69:A:PRO:HG3	13	0.74	0.35	0.8
(1,240)	1:47:A:THR:HG22	1:69:A:PRO:HG3	13	0.74	0.35	0.8
(1,240)	1:47:A:THR:HG23	1:69:A:PRO:HG3	13	0.74	0.35	0.8
(1,1235)	1:55:A:PRO:HG3	1:120:A:THR:H	13	0.72	0.37	0.73
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG21	13	0.63	0.44	0.45
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG22	13	0.63	0.44	0.45
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG23	13	0.63	0.44	0.45
(1,415)	1:90:A:MET:HE1	1:94:A:GLU:HA	13	0.62	0.37	0.48
(1,415)	1:90:A:MET:HE2	1:94:A:GLU:HA	13	0.62	0.37	0.48
(1,415)	1:90:A:MET:HE3	1:94:A:GLU:HA	13	0.62	0.37	0.48
(1,385)	1:82:A:GLY:HA2	1:85:A:GLN:HB3	13	0.55	0.15	0.56
(1,346)	1:81:A:LYS:HB3	1:82:A:GLY:HA3	13	0.48	0.12	0.48
(1,89)	1:42:A:ALA:HB1	1:74:A:LEU:HA	13	0.46	0.23	0.39
(1,89)	1:42:A:ALA:HB2	1:74:A:LEU:HA	13	0.46	0.23	0.39
(1,89)	1:42:A:ALA:HB3	1:74:A:LEU:HA	13	0.46	0.23	0.39
(1,1346)	1:28:A:LYS:HG2	1:30:A:VAL:H	13	0.44	0.24	0.39
(1,1346)	1:28:A:LYS:HG3	1:30:A:VAL:H	13	0.44	0.24	0.39
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE21	13	0.43	0.32	0.4
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE22	13	0.43	0.32	0.4
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG21	13	0.43	0.23	0.39
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG22	13	0.43	0.23	0.39

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG23	13	0.43	0.23	0.39
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB1	13	0.42	0.2	0.43
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB2	13	0.42	0.2	0.43
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB3	13	0.42	0.2	0.43
(1,747)	1:27:A:GLU:H	1:98:A:PHE:HA	13	0.42	0.14	0.41
(1,265)	1:42:A:ALA:H	1:74:A:LEU:HB3	13	0.4	0.17	0.36
(1,781)	1:37:A:VAL:H	1:91:A:THR:HB	13	0.4	0.28	0.27
(1,820)	1:44:A:LYS:H	1:44:A:LYS:HG3	13	0.38	0.21	0.3
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB2	13	0.34	0.18	0.34
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB3	13	0.34	0.18	0.34
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD21	13	0.15	0.02	0.15
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD22	13	0.15	0.02	0.15
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD23	13	0.15	0.02	0.15
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG21	12	3.0	0.22	2.98
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG22	12	3.0	0.22	2.98
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG23	12	3.0	0.22	2.98
(1,856)	1:51:A:ASP:H	1:123:A:PHE:HD2	12	2.42	0.19	2.43
(1,148)	1:50:A:TYR:HB3	1:123:A:PHE:HD2	12	2.36	0.69	2.13
(1,685)	1:102:A:TYR:HE2	1:108:A:GLU:HG2	12	2.07	1.42	1.51
(1,688)	1:83:A:TRP:HD1	1:98:A:PHE:HD2	12	2.07	0.56	2.16
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG21	12	1.82	1.14	1.68
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG22	12	1.82	1.14	1.68
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG23	12	1.82	1.14	1.68
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG2	12	1.75	0.65	1.62
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG3	12	1.75	0.65	1.62
(1,167)	1:53:A:ARG:HG2	1:54:A:PHE:HD1	12	1.5	0.48	1.37
(1,594)	1:122:A:VAL:HA	1:123:A:PHE:HD1	12	1.4	0.13	1.4
(1,1311)	1:81:A:LYS:HE3	1:85:A:GLN:HE22	12	1.35	0.66	1.33
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	12	1.23	0.69	1.27
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	12	1.23	0.69	1.27
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	12	1.23	0.69	1.27
(1,1253)	1:123:A:PHE:HD2	1:124:A:GLU:H	12	1.18	0.04	1.17
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD21	12	1.1	0.69	1.11
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD22	12	1.1	0.69	1.11
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD23	12	1.1	0.69	1.11
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB2	12	1.07	0.99	0.5
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB3	12	1.07	0.99	0.5
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD11	12	0.94	0.21	0.91
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD12	12	0.94	0.21	0.91
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD13	12	0.94	0.21	0.91
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD21	12	0.94	0.21	0.91
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD22	12	0.94	0.21	0.91

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD23	12	0.94	0.21	0.91
(1,516)	1:81:A:LYS:H	1:105:A:ALA:HA	12	0.93	0.64	0.73
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD2	12	0.85	0.07	0.86
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD3	12	0.85	0.07	0.86
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD2	12	0.82	0.38	0.78
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD3	12	0.82	0.38	0.78
(1,1248)	1:123:A:PHE:H	1:123:A:PHE:HD1	12	0.81	0.07	0.78
(1,1069)	1:86:A:GLY:H	1:98:A:PHE:HD2	12	0.72	0.47	0.6
(1,198)	1:59:A:GLN:HG2	1:61:A:ASP:H	12	0.71	0.36	0.72
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG21	12	0.71	0.44	0.7
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG22	12	0.71	0.44	0.7
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG23	12	0.71	0.44	0.7
(1,518)	1:80:A:ILE:HA	1:105:A:ALA:HA	12	0.68	0.62	0.52
(1,1195)	1:80:A:ILE:HB	1:105:A:ALA:H	12	0.61	0.39	0.53
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG2	12	0.61	0.46	0.46
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG3	12	0.61	0.46	0.46
(1,26)	1:27:A:GLU:HG3	1:99:A:THR:H	12	0.51	0.3	0.48
(1,554)	1:106:A:TYR:HB2	1:110:A:GLY:HA2	12	0.44	0.24	0.44
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG11	12	0.39	0.22	0.36
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG12	12	0.39	0.22	0.36
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG13	12	0.39	0.22	0.36
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG21	12	0.38	0.17	0.4
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG22	12	0.38	0.17	0.4
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG23	12	0.38	0.17	0.4
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG2	12	0.38	0.2	0.3
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG3	12	0.38	0.2	0.3
(1,863)	1:50:A:TYR:HB2	1:51:A:ASP:H	12	0.22	0.1	0.2
(1,787)	1:37:A:VAL:HB	1:38:A:THR:H	12	0.22	0.09	0.2
(1,1506)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	12	0.2	0.08	0.18
(1,1506)	1:67:A:GLY:HA3	1:68:A:LYS:HB2	12	0.2	0.08	0.18
(1,1185)	1:24:A:ALA:HB1	1:103:A:GLN:H	11	1.26	0.71	1.29
(1,1185)	1:24:A:ALA:HB2	1:103:A:GLN:H	11	1.26	0.71	1.29
(1,1185)	1:24:A:ALA:HB3	1:103:A:GLN:H	11	1.26	0.71	1.29
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	11	1.07	0.76	0.93
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	11	1.07	0.76	0.93
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	11	1.07	0.76	0.93
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	11	1.07	0.76	0.93
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	11	1.07	0.76	0.93
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	11	1.07	0.76	0.93
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE2	11	0.94	0.55	1.01
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE3	11	0.94	0.55	1.01
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE2	11	0.94	0.55	1.01

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE3	11	0.94	0.55	1.01
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE2	11	0.92	0.61	0.69
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE3	11	0.92	0.61	0.69
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE2	11	0.92	0.61	0.69
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE3	11	0.92	0.61	0.69
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG11	11	0.89	0.71	0.87
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG12	11	0.89	0.71	0.87
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG13	11	0.89	0.71	0.87
(1,1440)	1:53:A:ARG:HD2	1:57:A:GLY:H	11	0.72	0.36	0.68
(1,1440)	1:53:A:ARG:HD3	1:57:A:GLY:H	11	0.72	0.36	0.68
(1,1309)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	11	0.71	0.69	0.32
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG21	11	0.67	0.42	0.67
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG22	11	0.67	0.42	0.67
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG23	11	0.67	0.42	0.67
(1,154)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	11	0.6	0.32	0.57
(1,152)	1:51:A:ASP:HB2	1:124:A:GLU:H	11	0.58	0.16	0.56
(1,881)	1:54:A:PHE:H	1:54:A:PHE:HD1	11	0.43	0.12	0.44
(1,121)	1:46:A:VAL:HG11	1:130:A:VAL:H	11	0.42	0.19	0.41
(1,121)	1:46:A:VAL:HG12	1:130:A:VAL:H	11	0.42	0.19	0.41
(1,121)	1:46:A:VAL:HG13	1:130:A:VAL:H	11	0.42	0.19	0.41
(1,197)	1:59:A:GLN:HG2	1:60:A:PHE:H	11	0.41	0.17	0.41
(1,42)	1:33:A:PRO:HA	1:94:A:GLU:HG2	11	0.35	0.15	0.35
(1,1003)	1:74:A:LEU:HB3	1:76:A:ALA:H	11	0.31	0.16	0.24
(1,459)	1:97:A:LEU:HG	1:99:A:THR:H	11	0.3	0.13	0.26
(1,369)	1:83:A:TRP:H	1:84:A:ASP:HB2	11	0.27	0.22	0.21
(1,1050)	1:80:A:ILE:HG12	1:84:A:ASP:H	11	0.26	0.11	0.23
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD11	11	0.24	0.07	0.24
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD12	11	0.24	0.07	0.24
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD13	11	0.24	0.07	0.24
(1,828)	1:46:A:VAL:H	1:71:A:GLN:HA	11	0.23	0.07	0.23
(1,413)	1:90:A:MET:HE1	1:91:A:THR:H	11	0.22	0.12	0.16
(1,413)	1:90:A:MET:HE2	1:91:A:THR:H	11	0.22	0.12	0.16
(1,413)	1:90:A:MET:HE3	1:91:A:THR:H	11	0.22	0.12	0.16
(1,1301)	1:71:A:GLN:HA	1:71:A:GLN:HE21	11	0.2	0.05	0.19
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	10	2.07	1.39	2.5
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	10	2.07	1.39	2.5
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG21	10	1.67	0.94	1.86
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG22	10	1.67	0.94	1.86
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG23	10	1.67	0.94	1.86
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG21	10	1.65	1.18	1.74
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG22	10	1.65	1.18	1.74
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG23	10	1.65	1.18	1.74

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1306)	1:81:A:LYS:HE2	1:85:A:GLN:HE21	10	0.97	0.29	0.94
(1,1324)	1:19:A:PRO:HG2	1:55:A:PRO:HG2	10	0.86	0.43	0.76
(1,1324)	1:19:A:PRO:HG3	1:55:A:PRO:HG2	10	0.86	0.43	0.76
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB2	10	0.8	0.41	0.68
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB3	10	0.8	0.41	0.68
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB2	10	0.8	0.41	0.68
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB3	10	0.8	0.41	0.68
(1,744)	1:26:A:LEU:H	1:27:A:GLU:HG3	10	0.79	0.7	0.42
(1,537)	1:108:A:GLU:HB2	1:118:A:LYS:HG2	10	0.78	0.45	0.66
(1,519)	1:80:A:ILE:HB	1:105:A:ALA:HA	10	0.76	0.72	0.47
(1,1625)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	10	0.76	0.44	0.74
(1,1625)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	10	0.76	0.44	0.74
(1,696)	1:83:A:TRP:HZ2	1:123:A:PHE:HB3	10	0.74	0.44	0.64
(1,912)	1:53:A:ARG:HD3	1:57:A:GLY:H	10	0.59	0.29	0.55
(1,557)	1:110:A:GLY:HA3	1:115:A:ILE:HB	10	0.52	0.3	0.46
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG11	10	0.52	0.2	0.54
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG12	10	0.52	0.2	0.54
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG13	10	0.52	0.2	0.54
(1,751)	1:27:A:GLU:HG2	1:28:A:LYS:H	10	0.51	0.31	0.42
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG21	10	0.48	0.55	0.22
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG22	10	0.48	0.55	0.22
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG23	10	0.48	0.55	0.22
(1,581)	1:55:A:PRO:HG3	1:120:A:THR:HB	10	0.47	0.22	0.48
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD11	10	0.46	0.22	0.52
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD12	10	0.46	0.22	0.52
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD13	10	0.46	0.22	0.52
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD11	10	0.46	0.22	0.52
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD12	10	0.46	0.22	0.52
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD13	10	0.46	0.22	0.52
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD11	10	0.46	0.22	0.52
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD12	10	0.46	0.22	0.52
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD13	10	0.46	0.22	0.52
(1,316)	1:80:A:ILE:HB	1:104:A:LEU:HB3	10	0.45	0.36	0.28
(1,364)	1:80:A:ILE:HD11	1:83:A:TRP:HA	10	0.45	0.43	0.29
(1,364)	1:80:A:ILE:HD12	1:83:A:TRP:HA	10	0.45	0.43	0.29
(1,364)	1:80:A:ILE:HD13	1:83:A:TRP:HA	10	0.45	0.43	0.29
(1,375)	1:74:A:LEU:HD11	1:84:A:ASP:HB3	10	0.44	0.34	0.24
(1,375)	1:74:A:LEU:HD12	1:84:A:ASP:HB3	10	0.44	0.34	0.24
(1,375)	1:74:A:LEU:HD13	1:84:A:ASP:HB3	10	0.44	0.34	0.24
(1,419)	1:34:A:GLY:HA3	1:91:A:THR:HA	10	0.44	0.18	0.42
(1,81)	1:42:A:ALA:HA	1:74:A:LEU:H	10	0.38	0.16	0.32
(1,1104)	1:91:A:THR:H	1:127:A:LEU:HG	10	0.37	0.24	0.29

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,806)	1:42:A:ALA:H	1:74:A:LEU:HG	10	0.35	0.22	0.26
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB1	10	0.33	0.13	0.32
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB2	10	0.33	0.13	0.32
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB3	10	0.33	0.13	0.32
(1,629)	1:92:A:LEU:HA	1:127:A:LEU:HG	10	0.3	0.11	0.3
(1,242)	1:68:A:LYS:H	1:69:A:PRO:HD2	10	0.3	0.08	0.32
(1,1041)	1:80:A:ILE:HG21	1:83:A:TRP:H	10	0.28	0.14	0.24
(1,1041)	1:80:A:ILE:HG22	1:83:A:TRP:H	10	0.28	0.14	0.24
(1,1041)	1:80:A:ILE:HG23	1:83:A:TRP:H	10	0.28	0.14	0.24
(1,1152)	1:98:A:PHE:H	1:123:A:PHE:HB3	10	0.18	0.05	0.22
(1,208)	1:63:A:SER:H	1:64:A:ARG:HA	10	0.18	0.06	0.17
(1,1147)	1:98:A:PHE:H	1:99:A:THR:H	10	0.15	0.04	0.14
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG11	9	1.3	0.56	1.15
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG12	9	1.3	0.56	1.15
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG13	9	1.3	0.56	1.15
(1,177)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	9	1.25	0.6	1.32
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA2	9	1.17	0.85	1.35
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	9	1.17	0.85	1.35
(1,176)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	9	1.15	0.44	1.16
(1,911)	1:53:A:ARG:HD2	1:57:A:GLY:H	9	0.92	0.51	1.07
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG11	9	0.91	0.72	0.65
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG12	9	0.91	0.72	0.65
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG13	9	0.91	0.72	0.65
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD11	9	0.91	0.44	0.87
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD12	9	0.91	0.44	0.87
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD13	9	0.91	0.44	0.87
(1,611)	1:123:A:PHE:H	1:124:A:GLU:HG3	9	0.8	0.61	0.41
(1,544)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	9	0.78	0.69	0.52
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG11	9	0.71	0.31	0.73
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG12	9	0.71	0.31	0.73
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG13	9	0.71	0.31	0.73
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG21	9	0.71	0.31	0.73
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG22	9	0.71	0.31	0.73
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG23	9	0.71	0.31	0.73
(1,310)	1:80:A:ILE:HA	1:81:A:LYS:HG2	9	0.63	0.19	0.66
(1,283)	1:73:A:THR:HG21	1:76:A:ALA:HA	9	0.47	0.17	0.48
(1,283)	1:73:A:THR:HG22	1:76:A:ALA:HA	9	0.47	0.17	0.48
(1,283)	1:73:A:THR:HG23	1:76:A:ALA:HA	9	0.47	0.17	0.48
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE21	9	0.45	0.35	0.28
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	9	0.45	0.35	0.28
(1,1023)	1:81:A:LYS:H	1:81:A:LYS:HG3	9	0.4	0.11	0.46
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB1	9	0.33	0.16	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB2	9	0.33	0.16	0.28
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB3	9	0.33	0.16	0.28
(1,2)	1:28:A:LYS:HB2	1:30:A:VAL:H	9	0.28	0.07	0.3
(1,231)	1:68:A:LYS:H	1:69:A:PRO:HA	9	0.23	0.07	0.26
(1,830)	1:46:A:VAL:H	1:72:A:PHE:HA	9	0.22	0.06	0.2
(1,1113)	1:91:A:THR:HG21	1:92:A:LEU:H	9	0.14	0.02	0.13
(1,1113)	1:91:A:THR:HG22	1:92:A:LEU:H	9	0.14	0.02	0.13
(1,1113)	1:91:A:THR:HG23	1:92:A:LEU:H	9	0.14	0.02	0.13
(1,548)	1:102:A:TYR:HE2	1:108:A:GLU:HG3	8	2.43	1.91	2.55
(1,673)	1:52:A:GLY:HA3	1:123:A:PHE:HD1	8	1.82	0.36	1.82
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG11	8	1.3	0.65	1.36
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG12	8	1.3	0.65	1.36
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG13	8	1.3	0.65	1.36
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG21	8	1.3	0.65	1.36
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG22	8	1.3	0.65	1.36
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG23	8	1.3	0.65	1.36
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	8	1.25	1.05	0.77
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	8	1.25	1.05	0.77
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	8	1.25	1.05	0.77
(1,1325)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	8	1.21	0.31	1.18
(1,1325)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	8	1.21	0.31	1.18
(1,1328)	1:19:A:PRO:HG2	1:56:A:ASP:HA	8	1.12	0.69	1.13
(1,1328)	1:19:A:PRO:HG3	1:56:A:ASP:HA	8	1.12	0.69	1.13
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB1	8	0.85	0.67	0.5
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB2	8	0.85	0.67	0.5
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB3	8	0.85	0.67	0.5
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB1	8	0.85	0.67	0.5
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB2	8	0.85	0.67	0.5
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB3	8	0.85	0.67	0.5
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB1	8	0.85	0.67	0.5
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB2	8	0.85	0.67	0.5
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB3	8	0.85	0.67	0.5
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD2	8	0.84	0.48	0.73
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD3	8	0.84	0.48	0.73
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD2	8	0.84	0.48	0.73
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD3	8	0.84	0.48	0.73
(1,546)	1:108:A:GLU:HG3	1:118:A:LYS:HG2	8	0.83	0.56	0.84
(1,694)	1:80:A:ILE:HD11	1:83:A:TRP:HD1	8	0.82	0.83	0.55
(1,694)	1:80:A:ILE:HD12	1:83:A:TRP:HD1	8	0.82	0.83	0.55
(1,694)	1:80:A:ILE:HD13	1:83:A:TRP:HD1	8	0.82	0.83	0.55
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD2	8	0.82	0.45	0.66
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD3	8	0.82	0.45	0.66

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD2	8	0.82	0.45	0.66
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD3	8	0.82	0.45	0.66
(1,897)	1:59:A:GLN:HE21	1:62:A:SER:HB3	8	0.8	0.66	0.52
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB1	8	0.79	0.39	0.94
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB2	8	0.79	0.39	0.94
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB3	8	0.79	0.39	0.94
(1,27)	1:27:A:GLU:HG3	1:99:A:THR:HB	8	0.68	0.23	0.7
(1,1298)	1:92:A:LEU:HG	1:130:A:VAL:H	8	0.67	0.4	0.65
(1,786)	1:38:A:THR:H	1:91:A:THR:HA	8	0.6	0.49	0.42
(1,1252)	1:100:A:ILE:HD11	1:123:A:PHE:H	8	0.58	0.26	0.58
(1,1252)	1:100:A:ILE:HD12	1:123:A:PHE:H	8	0.58	0.26	0.58
(1,1252)	1:100:A:ILE:HD13	1:123:A:PHE:H	8	0.58	0.26	0.58
(1,631)	1:92:A:LEU:H	1:127:A:LEU:HG	8	0.58	0.21	0.58
(1,1004)	1:73:A:THR:HG21	1:76:A:ALA:H	8	0.54	0.17	0.5
(1,1004)	1:73:A:THR:HG22	1:76:A:ALA:H	8	0.54	0.17	0.5
(1,1004)	1:73:A:THR:HG23	1:76:A:ALA:H	8	0.54	0.17	0.5
(1,1601)	1:97:A:LEU:HD11	1:124:A:GLU:HG3	8	0.5	0.23	0.54
(1,1601)	1:97:A:LEU:HD12	1:124:A:GLU:HG3	8	0.5	0.23	0.54
(1,1601)	1:97:A:LEU:HD13	1:124:A:GLU:HG3	8	0.5	0.23	0.54
(1,1601)	1:97:A:LEU:HD21	1:124:A:GLU:HG3	8	0.5	0.23	0.54
(1,1601)	1:97:A:LEU:HD22	1:124:A:GLU:HG3	8	0.5	0.23	0.54
(1,1601)	1:97:A:LEU:HD23	1:124:A:GLU:HG3	8	0.5	0.23	0.54
(1,1505)	1:66:A:ARG:HG2	1:68:A:LYS:H	8	0.38	0.16	0.43
(1,1505)	1:66:A:ARG:HG3	1:68:A:LYS:H	8	0.38	0.16	0.43
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD11	8	0.33	0.13	0.3
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD12	8	0.33	0.13	0.3
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD13	8	0.33	0.13	0.3
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD21	8	0.33	0.13	0.3
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD22	8	0.33	0.13	0.3
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD23	8	0.33	0.13	0.3
(1,1433)	1:51:A:ASP:HB2	1:124:A:GLU:HB3	8	0.3	0.1	0.32
(1,1433)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	8	0.3	0.1	0.32
(1,1474)	1:59:A:GLN:HG2	1:60:A:PHE:H	8	0.29	0.11	0.29
(1,1474)	1:59:A:GLN:HG3	1:60:A:PHE:H	8	0.29	0.11	0.29
(1,179)	1:54:A:PHE:HB2	1:55:A:PRO:HD3	8	0.25	0.07	0.24
(1,1172)	1:102:A:TYR:H	1:105:A:ALA:H	8	0.22	0.07	0.2
(1,224)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	8	0.18	0.07	0.14
(1,1193)	1:105:A:ALA:H	1:107:A:GLY:H	8	0.16	0.09	0.12
(1,16)	1:41:A:GLN:H	1:41:A:GLN:HB2	8	0.16	0.04	0.16
(1,127)	1:47:A:THR:HB	1:48:A:VAL:HA	8	0.14	0.03	0.13
(1,683)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	7	2.72	1.08	2.95
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG11	7	1.56	0.65	1.77

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG12	7	1.56	0.65	1.77
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG13	7	1.56	0.65	1.77
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG21	7	1.56	0.65	1.77
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG22	7	1.56	0.65	1.77
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG23	7	1.56	0.65	1.77
(1,1307)	1:81:A:LYS:HE3	1:85:A:GLN:HE21	7	0.9	0.42	0.99
(1,3)	1:28:A:LYS:HG3	1:30:A:VAL:H	7	0.71	0.46	0.68
(1,166)	1:53:A:ARG:HG3	1:60:A:PHE:H	7	0.63	0.41	0.55
(1,158)	1:52:A:GLY:HA2	1:123:A:PHE:HD1	7	0.62	0.31	0.61
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG21	7	0.58	0.32	0.59
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG22	7	0.58	0.32	0.59
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG23	7	0.58	0.32	0.59
(1,464)	1:27:A:GLU:HB2	1:99:A:THR:HB	7	0.58	0.22	0.55
(1,383)	1:66:A:ARG:HG2	1:68:A:LYS:H	7	0.55	0.27	0.46
(1,789)	1:38:A:THR:H	1:91:A:THR:HG21	7	0.54	0.58	0.22
(1,789)	1:38:A:THR:H	1:91:A:THR:HG22	7	0.54	0.58	0.22
(1,789)	1:38:A:THR:H	1:91:A:THR:HG23	7	0.54	0.58	0.22
(1,684)	1:48:A:VAL:HG21	1:50:A:TYR:HE1	7	0.53	0.79	0.2
(1,684)	1:48:A:VAL:HG22	1:50:A:TYR:HE1	7	0.53	0.79	0.2
(1,684)	1:48:A:VAL:HG23	1:50:A:TYR:HE1	7	0.53	0.79	0.2
(1,1442)	1:53:A:ARG:HD2	1:59:A:GLN:HA	7	0.49	0.22	0.42
(1,1442)	1:53:A:ARG:HD3	1:59:A:GLN:HA	7	0.49	0.22	0.42
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD21	7	0.45	0.39	0.27
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD22	7	0.45	0.39	0.27
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD23	7	0.45	0.39	0.27
(1,1118)	1:34:A:GLY:H	1:94:A:GLU:H	7	0.38	0.19	0.29
(1,542)	1:108:A:GLU:HA	1:118:A:LYS:HG3	7	0.33	0.14	0.28
(1,702)	1:80:A:ILE:HG21	1:83:A:TRP:HE3	7	0.33	0.19	0.26
(1,702)	1:80:A:ILE:HG22	1:83:A:TRP:HE3	7	0.33	0.19	0.26
(1,702)	1:80:A:ILE:HG23	1:83:A:TRP:HE3	7	0.33	0.19	0.26
(1,209)	1:64:A:ARG:HA	1:68:A:LYS:H	7	0.32	0.13	0.28
(1,1001)	1:73:A:THR:HB	1:76:A:ALA:H	7	0.32	0.19	0.26
(1,411)	1:90:A:MET:HE1	1:127:A:LEU:H	7	0.28	0.14	0.23
(1,411)	1:90:A:MET:HE2	1:127:A:LEU:H	7	0.28	0.14	0.23
(1,411)	1:90:A:MET:HE3	1:127:A:LEU:H	7	0.28	0.14	0.23
(1,564)	1:114:A:VAL:HB	1:115:A:ILE:H	7	0.28	0.05	0.3
(1,1097)	1:34:A:GLY:HA3	1:91:A:THR:H	7	0.27	0.11	0.23
(1,919)	1:60:A:PHE:HD1	1:61:A:ASP:H	7	0.25	0.07	0.26
(1,289)	1:76:A:ALA:HB1	1:78:A:GLU:HB2	7	0.25	0.09	0.25
(1,289)	1:76:A:ALA:HB2	1:78:A:GLU:HB2	7	0.25	0.09	0.25
(1,289)	1:76:A:ALA:HB3	1:78:A:GLU:HB2	7	0.25	0.09	0.25
(1,1236)	1:119:A:ALA:HB1	1:120:A:THR:H	7	0.17	0.07	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1236)	1:119:A:ALA:HB2	1:120:A:THR:H	7	0.17	0.07	0.12
(1,1236)	1:119:A:ALA:HB3	1:120:A:THR:H	7	0.17	0.07	0.12
(1,563)	1:114:A:VAL:H	1:114:A:VAL:HB	7	0.15	0.01	0.15
(1,1184)	1:103:A:GLN:H	1:104:A:LEU:HB2	7	0.14	0.03	0.14
(1,98)	1:45:A:LYS:HB3	1:46:A:VAL:H	7	0.13	0.02	0.13
(1,1647)	1:121:A:LEU:HD11	1:122:A:VAL:H	7	0.13	0.03	0.12
(1,1647)	1:121:A:LEU:HD12	1:122:A:VAL:H	7	0.13	0.03	0.12
(1,1647)	1:121:A:LEU:HD13	1:122:A:VAL:H	7	0.13	0.03	0.12
(1,1647)	1:121:A:LEU:HD21	1:122:A:VAL:H	7	0.13	0.03	0.12
(1,1647)	1:121:A:LEU:HD22	1:122:A:VAL:H	7	0.13	0.03	0.12
(1,1647)	1:121:A:LEU:HD23	1:122:A:VAL:H	7	0.13	0.03	0.12
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG21	7	0.11	0.0	0.11
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG22	7	0.11	0.0	0.11
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG23	7	0.11	0.0	0.11
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG11	6	1.35	0.72	1.13
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG12	6	1.35	0.72	1.13
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG13	6	1.35	0.72	1.13
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG21	6	1.35	0.72	1.13
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG22	6	1.35	0.72	1.13
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG23	6	1.35	0.72	1.13
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG11	6	1.29	0.81	1.12
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG12	6	1.29	0.81	1.12
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG13	6	1.29	0.81	1.12
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG21	6	1.29	0.81	1.12
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG22	6	1.29	0.81	1.12
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG23	6	1.29	0.81	1.12
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG11	6	1.29	0.81	1.12
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG12	6	1.29	0.81	1.12
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG13	6	1.29	0.81	1.12
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG21	6	1.29	0.81	1.12
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG22	6	1.29	0.81	1.12
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG23	6	1.29	0.81	1.12
(1,545)	1:108:A:GLU:HG2	1:118:A:LYS:HG2	6	0.98	0.67	0.82
(1,1333)	1:24:A:ALA:HB1	1:103:A:GLN:HG2	6	0.95	0.48	0.84
(1,1333)	1:24:A:ALA:HB1	1:103:A:GLN:HG3	6	0.95	0.48	0.84
(1,1333)	1:24:A:ALA:HB2	1:103:A:GLN:HG2	6	0.95	0.48	0.84
(1,1333)	1:24:A:ALA:HB2	1:103:A:GLN:HG3	6	0.95	0.48	0.84
(1,1333)	1:24:A:ALA:HB3	1:103:A:GLN:HG2	6	0.95	0.48	0.84
(1,1333)	1:24:A:ALA:HB3	1:103:A:GLN:HG3	6	0.95	0.48	0.84
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG11	6	0.85	0.67	0.52
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG12	6	0.85	0.67	0.52
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG13	6	0.85	0.67	0.52

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG21	6	0.85	0.67	0.52
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG22	6	0.85	0.67	0.52
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG23	6	0.85	0.67	0.52
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG11	6	0.85	0.67	0.52
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG12	6	0.85	0.67	0.52
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG13	6	0.85	0.67	0.52
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG21	6	0.85	0.67	0.52
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG22	6	0.85	0.67	0.52
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG23	6	0.85	0.67	0.52
(1,92)	1:41:A:GLN:HG2	1:44:A:LYS:HG2	6	0.83	0.58	0.66
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD21	6	0.79	0.37	0.78
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD22	6	0.79	0.37	0.78
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD23	6	0.79	0.37	0.78
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD21	6	0.73	0.39	0.75
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD22	6	0.73	0.39	0.75
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD23	6	0.73	0.39	0.75
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG21	6	0.7	0.33	0.76
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG22	6	0.7	0.33	0.76
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG23	6	0.7	0.33	0.76
(1,1624)	1:108:A:GLU:HG2	1:118:A:LYS:HG2	6	0.66	0.59	0.45
(1,1624)	1:108:A:GLU:HG3	1:118:A:LYS:HG2	6	0.66	0.59	0.45
(1,417)	1:90:A:MET:HE1	1:94:A:GLU:HG2	6	0.65	0.32	0.61
(1,417)	1:90:A:MET:HE2	1:94:A:GLU:HG2	6	0.65	0.32	0.61
(1,417)	1:90:A:MET:HE3	1:94:A:GLU:HG2	6	0.65	0.32	0.61
(1,1475)	1:59:A:GLN:HG2	1:61:A:ASP:H	6	0.65	0.49	0.47
(1,1475)	1:59:A:GLN:HG3	1:61:A:ASP:H	6	0.65	0.49	0.47
(1,183)	1:53:A:ARG:HD2	1:57:A:GLY:HA2	6	0.55	0.28	0.64
(1,278)	1:74:A:LEU:HD11	1:87:A:VAL:HB	6	0.52	0.25	0.61
(1,278)	1:74:A:LEU:HD12	1:87:A:VAL:HB	6	0.52	0.25	0.61
(1,278)	1:74:A:LEU:HD13	1:87:A:VAL:HB	6	0.52	0.25	0.61
(1,1199)	1:80:A:ILE:HG21	1:105:A:ALA:H	6	0.49	0.25	0.45
(1,1199)	1:80:A:ILE:HG22	1:105:A:ALA:H	6	0.49	0.25	0.45
(1,1199)	1:80:A:ILE:HG23	1:105:A:ALA:H	6	0.49	0.25	0.45
(1,444)	1:31:A:LEU:HG	1:95:A:LYS:HB3	6	0.49	0.46	0.24
(1,543)	1:108:A:GLU:HA	1:118:A:LYS:HG2	6	0.49	0.26	0.56
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG21	6	0.38	0.19	0.35
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG22	6	0.38	0.19	0.35
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG23	6	0.38	0.19	0.35
(1,1575)	1:92:A:LEU:HD11	1:130:A:VAL:H	6	0.36	0.19	0.29
(1,1575)	1:92:A:LEU:HD12	1:130:A:VAL:H	6	0.36	0.19	0.29
(1,1575)	1:92:A:LEU:HD13	1:130:A:VAL:H	6	0.36	0.19	0.29
(1,1575)	1:92:A:LEU:HD21	1:130:A:VAL:H	6	0.36	0.19	0.29

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1575)	1:92:A:LEU:HD22	1:130:A:VAL:H	6	0.36	0.19	0.29
(1,1575)	1:92:A:LEU:HD23	1:130:A:VAL:H	6	0.36	0.19	0.29
(1,192)	1:59:A:GLN:HA	1:61:A:ASP:H	6	0.35	0.25	0.3
(1,1619)	1:103:A:GLN:HG2	1:104:A:LEU:H	6	0.33	0.16	0.26
(1,1619)	1:103:A:GLN:HG3	1:104:A:LEU:H	6	0.33	0.16	0.26
(1,1308)	1:81:A:LYS:HD2	1:85:A:GLN:HE21	6	0.33	0.2	0.26
(1,343)	1:66:A:ARG:HG3	1:68:A:LYS:H	6	0.31	0.16	0.3
(1,952)	1:67:A:GLY:H	1:68:A:LYS:HB2	6	0.31	0.15	0.3
(1,457)	1:29:A:LYS:H	1:97:A:LEU:HB2	6	0.29	0.19	0.17
(1,481)	1:100:A:ILE:HG21	1:104:A:LEU:HA	6	0.27	0.15	0.2
(1,481)	1:100:A:ILE:HG22	1:104:A:LEU:HA	6	0.27	0.15	0.2
(1,481)	1:100:A:ILE:HG23	1:104:A:LEU:HA	6	0.27	0.15	0.2
(1,212)	1:64:A:ARG:HA	1:64:A:ARG:HD2	6	0.26	0.01	0.26
(1,1197)	1:100:A:ILE:HG21	1:105:A:ALA:H	6	0.25	0.05	0.26
(1,1197)	1:100:A:ILE:HG22	1:105:A:ALA:H	6	0.25	0.05	0.26
(1,1197)	1:100:A:ILE:HG23	1:105:A:ALA:H	6	0.25	0.05	0.26
(1,862)	1:50:A:TYR:HB3	1:51:A:ASP:H	6	0.25	0.08	0.24
(1,482)	1:100:A:ILE:HG21	1:104:A:LEU:HB2	6	0.24	0.08	0.24
(1,482)	1:100:A:ILE:HG22	1:104:A:LEU:HB2	6	0.24	0.08	0.24
(1,482)	1:100:A:ILE:HG23	1:104:A:LEU:HB2	6	0.24	0.08	0.24
(1,1204)	1:100:A:ILE:HG21	1:106:A:TYR:H	6	0.24	0.14	0.18
(1,1204)	1:100:A:ILE:HG22	1:106:A:TYR:H	6	0.24	0.14	0.18
(1,1204)	1:100:A:ILE:HG23	1:106:A:TYR:H	6	0.24	0.14	0.18
(1,858)	1:50:A:TYR:HD1	1:51:A:ASP:H	6	0.24	0.05	0.23
(1,1276)	1:96:A:ALA:H	1:127:A:LEU:H	6	0.21	0.12	0.15
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB1	6	0.2	0.05	0.2
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB2	6	0.2	0.05	0.2
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB3	6	0.2	0.05	0.2
(1,29)	1:27:A:GLU:H	1:27:A:GLU:HG2	6	0.19	0.04	0.18
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB1	6	0.16	0.04	0.16
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB2	6	0.16	0.04	0.16
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB3	6	0.16	0.04	0.16
(1,1065)	1:79:A:VAL:HG21	1:85:A:GLN:H	6	0.16	0.07	0.12
(1,1065)	1:79:A:VAL:HG22	1:85:A:GLN:H	6	0.16	0.07	0.12
(1,1065)	1:79:A:VAL:HG23	1:85:A:GLN:H	6	0.16	0.07	0.12
(1,530)	1:106:A:TYR:HB3	1:111:A:TYR:HD2	5	1.79	1.0	2.07
(1,226)	1:49:A:HIS:HE1	1:67:A:GLY:HA2	5	1.33	0.55	1.37
(1,1299)	1:92:A:LEU:HD11	1:130:A:VAL:H	5	1.23	0.34	1.3
(1,1299)	1:92:A:LEU:HD12	1:130:A:VAL:H	5	1.23	0.34	1.3
(1,1299)	1:92:A:LEU:HD13	1:130:A:VAL:H	5	1.23	0.34	1.3
(1,896)	1:59:A:GLN:HE21	1:62:A:SER:HB2	5	0.83	0.66	0.69
(1,403)	1:89:A:THR:HG21	1:98:A:PHE:HD2	5	0.71	0.16	0.74

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,403)	1:89:A:THR:HG22	1:98:A:PHE:HD2	5	0.71	0.16	0.74
(1,403)	1:89:A:THR:HG23	1:98:A:PHE:HD2	5	0.71	0.16	0.74
(1,689)	1:83:A:TRP:HD1	1:123:A:PHE:HD1	5	0.66	0.09	0.68
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD11	5	0.55	0.21	0.52
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD12	5	0.55	0.21	0.52
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD13	5	0.55	0.21	0.52
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD21	5	0.55	0.21	0.52
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD22	5	0.55	0.21	0.52
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD23	5	0.55	0.21	0.52
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD11	5	0.55	0.21	0.52
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD12	5	0.55	0.21	0.52
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD13	5	0.55	0.21	0.52
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD21	5	0.55	0.21	0.52
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD22	5	0.55	0.21	0.52
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD23	5	0.55	0.21	0.52
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD11	5	0.55	0.21	0.52
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD12	5	0.55	0.21	0.52
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD13	5	0.55	0.21	0.52
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD21	5	0.55	0.21	0.52
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD22	5	0.55	0.21	0.52
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD23	5	0.55	0.21	0.52
(1,449)	1:32:A:THR:HB	1:95:A:LYS:HE2	5	0.54	0.32	0.49
(1,528)	1:80:A:ILE:HG21	1:106:A:TYR:HA	5	0.49	0.49	0.28
(1,528)	1:80:A:ILE:HG22	1:106:A:TYR:HA	5	0.49	0.49	0.28
(1,528)	1:80:A:ILE:HG23	1:106:A:TYR:HA	5	0.49	0.49	0.28
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG21	5	0.49	0.4	0.24
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG22	5	0.49	0.4	0.24
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG23	5	0.49	0.4	0.24
(1,929)	1:63:A:SER:H	1:64:A:ARG:HG3	5	0.48	0.19	0.5
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG11	5	0.46	0.19	0.53
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG12	5	0.46	0.19	0.53
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG13	5	0.46	0.19	0.53
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG11	5	0.46	0.19	0.53
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG12	5	0.46	0.19	0.53
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG13	5	0.46	0.19	0.53
(1,681)	1:50:A:TYR:H	1:50:A:TYR:HD2	5	0.43	0.36	0.29
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG21	5	0.39	0.08	0.39
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG22	5	0.39	0.08	0.39
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG23	5	0.39	0.08	0.39
(1,910)	1:55:A:PRO:HA	1:57:A:GLY:H	5	0.38	0.24	0.38
(1,1613)	1:102:A:TYR:HE2	1:118:A:LYS:HB2	5	0.37	0.17	0.38
(1,1613)	1:102:A:TYR:HE2	1:118:A:LYS:HB3	5	0.37	0.17	0.38

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1405)	1:44:A:LYS:HE2	1:45:A:LYS:H	5	0.36	0.14	0.3
(1,1405)	1:44:A:LYS:HE3	1:45:A:LYS:H	5	0.36	0.14	0.3
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG21	5	0.35	0.11	0.35
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG22	5	0.35	0.11	0.35
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG23	5	0.35	0.11	0.35
(1,1612)	1:102:A:TYR:HB2	1:108:A:GLU:HG2	5	0.33	0.08	0.3
(1,1612)	1:102:A:TYR:HB2	1:108:A:GLU:HG3	5	0.33	0.08	0.3
(1,972)	1:70:A:PHE:HD2	1:71:A:GLN:H	5	0.32	0.06	0.29
(1,266)	1:74:A:LEU:HD21	1:75:A:GLY:H	5	0.31	0.15	0.26
(1,266)	1:74:A:LEU:HD22	1:75:A:GLY:H	5	0.31	0.15	0.26
(1,266)	1:74:A:LEU:HD23	1:75:A:GLY:H	5	0.31	0.15	0.26
(1,1441)	1:53:A:ARG:HD2	1:57:A:GLY:HA2	5	0.24	0.09	0.25
(1,1441)	1:53:A:ARG:HD3	1:57:A:GLY:HA2	5	0.24	0.09	0.25
(1,216)	1:64:A:ARG:HA	1:64:A:ARG:HD3	5	0.24	0.04	0.26
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD11	5	0.24	0.1	0.22
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD12	5	0.24	0.1	0.22
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD13	5	0.24	0.1	0.22
(1,866)	1:51:A:ASP:H	1:124:A:GLU:HB3	5	0.23	0.12	0.2
(1,1120)	1:34:A:GLY:HA2	1:94:A:GLU:H	5	0.22	0.1	0.18
(1,775)	1:34:A:GLY:H	1:94:A:GLU:HB3	5	0.21	0.05	0.21
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB1	5	0.2	0.09	0.15
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB2	5	0.2	0.09	0.15
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB3	5	0.2	0.09	0.15
(1,1384)	1:41:A:GLN:H	1:41:A:GLN:HB2	5	0.17	0.02	0.17
(1,1384)	1:41:A:GLN:H	1:41:A:GLN:HB3	5	0.17	0.02	0.17
(1,977)	1:47:A:THR:HG21	1:71:A:GLN:H	5	0.17	0.04	0.17
(1,977)	1:47:A:THR:HG22	1:71:A:GLN:H	5	0.17	0.04	0.17
(1,977)	1:47:A:THR:HG23	1:71:A:GLN:H	5	0.17	0.04	0.17
(1,1218)	1:111:A:TYR:H	1:111:A:TYR:HB3	5	0.15	0.01	0.15
(1,498)	1:103:A:GLN:HA	1:104:A:LEU:HG	5	0.14	0.03	0.13
(1,1173)	1:102:A:TYR:H	1:102:A:TYR:HE1	4	1.47	0.07	1.48
(1,959)	1:49:A:HIS:HD2	1:70:A:PHE:H	4	1.31	0.38	1.43
(1,902)	1:59:A:GLN:HE22	1:62:A:SER:HB3	4	1.17	0.88	1.01
(1,1085)	1:89:A:THR:H	1:90:A:MET:HE1	4	1.0	0.1	0.98
(1,1085)	1:89:A:THR:H	1:90:A:MET:HE2	4	1.0	0.1	0.98
(1,1085)	1:89:A:THR:H	1:90:A:MET:HE3	4	1.0	0.1	0.98
(1,395)	1:40:A:PRO:HG2	1:88:A:ALA:HA	4	0.99	0.79	0.89
(1,1386)	1:41:A:GLN:H	1:44:A:LYS:HG2	4	0.88	0.54	0.8
(1,1386)	1:41:A:GLN:H	1:44:A:LYS:HG3	4	0.88	0.54	0.8
(1,800)	1:41:A:GLN:H	1:44:A:LYS:HB2	4	0.82	0.27	0.74
(1,903)	1:59:A:GLN:HE22	1:62:A:SER:HB2	4	0.79	0.4	0.86
(1,494)	1:102:A:TYR:HB2	1:102:A:TYR:HE2	4	0.78	0.02	0.78

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,450)	1:32:A:THR:HB	1:95:A:LYS:HE3	4	0.68	0.32	0.7
(1,651)	1:92:A:LEU:HD11	1:129:A:ALA:HA	4	0.66	0.19	0.6
(1,651)	1:92:A:LEU:HD12	1:129:A:ALA:HA	4	0.66	0.19	0.6
(1,651)	1:92:A:LEU:HD13	1:129:A:ALA:HA	4	0.66	0.19	0.6
(1,106)	1:45:A:LYS:H	1:45:A:LYS:HE3	4	0.62	0.24	0.64
(1,1025)	1:82:A:GLY:H	1:104:A:LEU:HA	4	0.55	0.34	0.55
(1,315)	1:80:A:ILE:HD11	1:100:A:ILE:HG21	4	0.52	0.42	0.35
(1,315)	1:80:A:ILE:HD11	1:100:A:ILE:HG22	4	0.52	0.42	0.35
(1,315)	1:80:A:ILE:HD11	1:100:A:ILE:HG23	4	0.52	0.42	0.35
(1,315)	1:80:A:ILE:HD12	1:100:A:ILE:HG21	4	0.52	0.42	0.35
(1,315)	1:80:A:ILE:HD12	1:100:A:ILE:HG22	4	0.52	0.42	0.35
(1,315)	1:80:A:ILE:HD12	1:100:A:ILE:HG23	4	0.52	0.42	0.35
(1,315)	1:80:A:ILE:HD13	1:100:A:ILE:HG21	4	0.52	0.42	0.35
(1,315)	1:80:A:ILE:HD13	1:100:A:ILE:HG22	4	0.52	0.42	0.35
(1,315)	1:80:A:ILE:HD13	1:100:A:ILE:HG23	4	0.52	0.42	0.35
(1,155)	1:51:A:ASP:HB3	1:124:A:GLU:H	4	0.5	0.18	0.42
(1,78)	1:40:A:PRO:HD3	1:91:A:THR:HG21	4	0.48	0.32	0.42
(1,78)	1:40:A:PRO:HD3	1:91:A:THR:HG22	4	0.48	0.32	0.42
(1,78)	1:40:A:PRO:HD3	1:91:A:THR:HG23	4	0.48	0.32	0.42
(1,730)	1:35:A:ASP:H	1:37:A:VAL:HG21	4	0.44	0.16	0.53
(1,730)	1:35:A:ASP:H	1:37:A:VAL:HG22	4	0.44	0.16	0.53
(1,730)	1:35:A:ASP:H	1:37:A:VAL:HG23	4	0.44	0.16	0.53
(1,145)	1:49:A:HIS:HB2	1:126:A:GLU:HG2	4	0.42	0.09	0.4
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD11	4	0.38	0.04	0.4
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD12	4	0.38	0.04	0.4
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD13	4	0.38	0.04	0.4
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD21	4	0.38	0.04	0.4
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD22	4	0.38	0.04	0.4
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD23	4	0.38	0.04	0.4
(1,153)	1:51:A:ASP:HB2	1:124:A:GLU:HB3	4	0.38	0.16	0.38
(1,1162)	1:27:A:GLU:HB2	1:99:A:THR:H	4	0.37	0.12	0.4
(1,660)	1:72:A:PHE:HB2	1:79:A:VAL:HG11	4	0.36	0.12	0.4
(1,660)	1:72:A:PHE:HB2	1:79:A:VAL:HG12	4	0.36	0.12	0.4
(1,660)	1:72:A:PHE:HB2	1:79:A:VAL:HG13	4	0.36	0.12	0.4
(1,276)	1:74:A:LEU:HD11	1:88:A:ALA:H	4	0.36	0.29	0.24
(1,276)	1:74:A:LEU:HD12	1:88:A:ALA:H	4	0.36	0.29	0.24
(1,276)	1:74:A:LEU:HD13	1:88:A:ALA:H	4	0.36	0.29	0.24
(1,966)	1:69:A:PRO:HB3	1:70:A:PHE:H	4	0.36	0.23	0.33
(1,284)	1:73:A:THR:HG21	1:76:A:ALA:HB1	4	0.35	0.18	0.25
(1,284)	1:73:A:THR:HG21	1:76:A:ALA:HB2	4	0.35	0.18	0.25
(1,284)	1:73:A:THR:HG21	1:76:A:ALA:HB3	4	0.35	0.18	0.25
(1,284)	1:73:A:THR:HG22	1:76:A:ALA:HB1	4	0.35	0.18	0.25

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,284)	1:73:A:THR:HG22	1:76:A:ALA:HB2	4	0.35	0.18	0.25
(1,284)	1:73:A:THR:HG22	1:76:A:ALA:HB3	4	0.35	0.18	0.25
(1,284)	1:73:A:THR:HG23	1:76:A:ALA:HB1	4	0.35	0.18	0.25
(1,284)	1:73:A:THR:HG23	1:76:A:ALA:HB2	4	0.35	0.18	0.25
(1,284)	1:73:A:THR:HG23	1:76:A:ALA:HB3	4	0.35	0.18	0.25
(1,490)	1:102:A:TYR:HB3	1:102:A:TYR:HE1	4	0.34	0.01	0.34
(1,1105)	1:38:A:THR:H	1:92:A:LEU:H	4	0.34	0.31	0.2
(1,49)	1:35:A:ASP:HA	1:37:A:VAL:HG21	4	0.33	0.16	0.36
(1,49)	1:35:A:ASP:HA	1:37:A:VAL:HG22	4	0.33	0.16	0.36
(1,49)	1:35:A:ASP:HA	1:37:A:VAL:HG23	4	0.33	0.16	0.36
(1,824)	1:44:A:LYS:HB3	1:45:A:LYS:H	4	0.3	0.1	0.32
(1,491)	1:102:A:TYR:HB3	1:105:A:ALA:HB1	4	0.3	0.05	0.31
(1,491)	1:102:A:TYR:HB3	1:105:A:ALA:HB2	4	0.3	0.05	0.31
(1,491)	1:102:A:TYR:HB3	1:105:A:ALA:HB3	4	0.3	0.05	0.31
(1,797)	1:41:A:GLN:H	1:41:A:GLN:HG2	4	0.3	0.17	0.26
(1,229)	1:69:A:PRO:HA	1:128:A:LEU:HG	4	0.28	0.22	0.17
(1,350)	1:82:A:GLY:HA3	1:104:A:LEU:HD11	4	0.28	0.12	0.3
(1,350)	1:82:A:GLY:HA3	1:104:A:LEU:HD12	4	0.28	0.12	0.3
(1,350)	1:82:A:GLY:HA3	1:104:A:LEU:HD13	4	0.28	0.12	0.3
(1,661)	1:72:A:PHE:HB3	1:79:A:VAL:HG11	4	0.26	0.15	0.18
(1,661)	1:72:A:PHE:HB3	1:79:A:VAL:HG12	4	0.26	0.15	0.18
(1,661)	1:72:A:PHE:HB3	1:79:A:VAL:HG13	4	0.26	0.15	0.18
(1,48)	1:34:A:GLY:HA2	1:94:A:GLU:HB3	4	0.24	0.08	0.28
(1,813)	1:43:A:GLY:H	1:74:A:LEU:HG	4	0.23	0.11	0.21
(1,425)	1:92:A:LEU:HG	1:93:A:GLY:H	4	0.21	0.06	0.22
(1,616)	1:50:A:TYR:HA	1:125:A:VAL:HG11	4	0.2	0.07	0.18
(1,616)	1:50:A:TYR:HA	1:125:A:VAL:HG12	4	0.2	0.07	0.18
(1,616)	1:50:A:TYR:HA	1:125:A:VAL:HG13	4	0.2	0.07	0.18
(1,405)	1:85:A:GLN:HA	1:89:A:THR:HG21	4	0.2	0.05	0.22
(1,405)	1:85:A:GLN:HA	1:89:A:THR:HG22	4	0.2	0.05	0.22
(1,405)	1:85:A:GLN:HA	1:89:A:THR:HG23	4	0.2	0.05	0.22
(1,1380)	1:40:A:PRO:HB2	1:41:A:GLN:H	4	0.19	0.04	0.2
(1,1380)	1:40:A:PRO:HB3	1:41:A:GLN:H	4	0.19	0.04	0.2
(1,378)	1:81:A:LYS:HA	1:84:A:ASP:HB3	4	0.19	0.07	0.19
(1,579)	1:102:A:TYR:HB2	1:119:A:ALA:HB1	4	0.19	0.05	0.17
(1,579)	1:102:A:TYR:HB2	1:119:A:ALA:HB2	4	0.19	0.05	0.17
(1,579)	1:102:A:TYR:HB2	1:119:A:ALA:HB3	4	0.19	0.05	0.17
(1,220)	1:66:A:ARG:HA	1:66:A:ARG:HD2	4	0.18	0.07	0.16
(1,812)	1:43:A:GLY:H	1:44:A:LYS:HB2	4	0.18	0.06	0.16
(1,160)	1:53:A:ARG:HB2	1:59:A:GLN:HA	4	0.16	0.01	0.16
(1,603)	1:123:A:PHE:H	1:124:A:GLU:HA	4	0.15	0.03	0.16
(1,887)	1:53:A:ARG:HB3	1:54:A:PHE:H	4	0.15	0.03	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,328)	1:80:A:ILE:HG13	1:83:A:TRP:H	4	0.13	0.01	0.12
(1,1490)	1:64:A:ARG:H	1:64:A:ARG:HD2	4	0.13	0.03	0.12
(1,1490)	1:64:A:ARG:H	1:64:A:ARG:HD3	4	0.13	0.03	0.12
(1,836)	1:47:A:THR:H	1:128:A:LEU:H	4	0.12	0.02	0.12
(1,1284)	1:127:A:LEU:H	1:127:A:LEU:HG	4	0.12	0.0	0.12
(1,1600)	1:97:A:LEU:HD11	1:124:A:GLU:HG2	3	2.03	0.11	1.95
(1,1600)	1:97:A:LEU:HD12	1:124:A:GLU:HG2	3	2.03	0.11	1.95
(1,1600)	1:97:A:LEU:HD13	1:124:A:GLU:HG2	3	2.03	0.11	1.95
(1,1600)	1:97:A:LEU:HD21	1:124:A:GLU:HG2	3	2.03	0.11	1.95
(1,1600)	1:97:A:LEU:HD22	1:124:A:GLU:HG2	3	2.03	0.11	1.95
(1,1600)	1:97:A:LEU:HD23	1:124:A:GLU:HG2	3	2.03	0.11	1.95
(1,609)	1:123:A:PHE:HA	1:124:A:GLU:HG3	3	1.2	0.09	1.15
(1,534)	1:106:A:TYR:HB2	1:111:A:TYR:HD2	3	1.03	0.52	1.34
(1,400)	1:74:A:LEU:HD21	1:88:A:ALA:HB1	3	0.98	0.37	1.08
(1,400)	1:74:A:LEU:HD21	1:88:A:ALA:HB2	3	0.98	0.37	1.08
(1,400)	1:74:A:LEU:HD21	1:88:A:ALA:HB3	3	0.98	0.37	1.08
(1,400)	1:74:A:LEU:HD22	1:88:A:ALA:HB1	3	0.98	0.37	1.08
(1,400)	1:74:A:LEU:HD22	1:88:A:ALA:HB2	3	0.98	0.37	1.08
(1,400)	1:74:A:LEU:HD22	1:88:A:ALA:HB3	3	0.98	0.37	1.08
(1,400)	1:74:A:LEU:HD23	1:88:A:ALA:HB1	3	0.98	0.37	1.08
(1,400)	1:74:A:LEU:HD23	1:88:A:ALA:HB2	3	0.98	0.37	1.08
(1,400)	1:74:A:LEU:HD23	1:88:A:ALA:HB3	3	0.98	0.37	1.08
(1,587)	1:115:A:ILE:HD11	1:121:A:LEU:HG	3	0.78	0.22	0.67
(1,587)	1:115:A:ILE:HD12	1:121:A:LEU:HG	3	0.78	0.22	0.67
(1,587)	1:115:A:ILE:HD13	1:121:A:LEU:HG	3	0.78	0.22	0.67
(1,1130)	1:90:A:MET:HE1	1:95:A:LYS:H	3	0.75	0.29	0.79
(1,1130)	1:90:A:MET:HE2	1:95:A:LYS:H	3	0.75	0.29	0.79
(1,1130)	1:90:A:MET:HE3	1:95:A:LYS:H	3	0.75	0.29	0.79
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG11	3	0.69	0.2	0.83
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG12	3	0.69	0.2	0.83
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG13	3	0.69	0.2	0.83
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG21	3	0.69	0.2	0.83
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG22	3	0.69	0.2	0.83
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG23	3	0.69	0.2	0.83
(1,371)	1:81:A:LYS:HD3	1:84:A:ASP:HB2	3	0.64	0.46	0.4
(1,1476)	1:59:A:GLN:HE21	1:62:A:SER:HB2	3	0.6	0.04	0.59
(1,1476)	1:59:A:GLN:HE21	1:62:A:SER:HB3	3	0.6	0.04	0.59
(1,1476)	1:59:A:GLN:HE22	1:62:A:SER:HB2	3	0.6	0.04	0.59
(1,1476)	1:59:A:GLN:HE22	1:62:A:SER:HB3	3	0.6	0.04	0.59
(1,292)	1:76:A:ALA:HB1	1:78:A:GLU:HG2	3	0.52	0.22	0.6
(1,292)	1:76:A:ALA:HB2	1:78:A:GLU:HG2	3	0.52	0.22	0.6
(1,292)	1:76:A:ALA:HB3	1:78:A:GLU:HG2	3	0.52	0.22	0.6

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,85)	1:42:A:ALA:HA	1:74:A:LEU:HD21	3	0.52	0.37	0.38
(1,85)	1:42:A:ALA:HA	1:74:A:LEU:HD22	3	0.52	0.37	0.38
(1,85)	1:42:A:ALA:HA	1:74:A:LEU:HD23	3	0.52	0.37	0.38
(1,580)	1:115:A:ILE:HD11	1:119:A:ALA:HB1	3	0.5	0.33	0.31
(1,580)	1:115:A:ILE:HD11	1:119:A:ALA:HB2	3	0.5	0.33	0.31
(1,580)	1:115:A:ILE:HD11	1:119:A:ALA:HB3	3	0.5	0.33	0.31
(1,580)	1:115:A:ILE:HD12	1:119:A:ALA:HB1	3	0.5	0.33	0.31
(1,580)	1:115:A:ILE:HD12	1:119:A:ALA:HB2	3	0.5	0.33	0.31
(1,580)	1:115:A:ILE:HD12	1:119:A:ALA:HB3	3	0.5	0.33	0.31
(1,580)	1:115:A:ILE:HD13	1:119:A:ALA:HB1	3	0.5	0.33	0.31
(1,580)	1:115:A:ILE:HD13	1:119:A:ALA:HB2	3	0.5	0.33	0.31
(1,580)	1:115:A:ILE:HD13	1:119:A:ALA:HB3	3	0.5	0.33	0.31
(1,394)	1:74:A:LEU:HD11	1:88:A:ALA:HA	3	0.49	0.25	0.53
(1,394)	1:74:A:LEU:HD12	1:88:A:ALA:HA	3	0.49	0.25	0.53
(1,394)	1:74:A:LEU:HD13	1:88:A:ALA:HA	3	0.49	0.25	0.53
(1,983)	1:73:A:THR:H	1:78:A:GLU:HB2	3	0.47	0.34	0.27
(1,421)	1:91:A:THR:HA	1:127:A:LEU:HG	3	0.46	0.23	0.32
(1,93)	1:41:A:GLN:HG3	1:44:A:LYS:HG2	3	0.45	0.36	0.27
(1,1265)	1:124:A:GLU:HB3	1:125:A:VAL:H	3	0.44	0.05	0.46
(1,504)	1:82:A:GLY:H	1:104:A:LEU:HD11	3	0.4	0.19	0.29
(1,504)	1:82:A:GLY:H	1:104:A:LEU:HD12	3	0.4	0.19	0.29
(1,504)	1:82:A:GLY:H	1:104:A:LEU:HD13	3	0.4	0.19	0.29
(1,623)	1:95:A:LYS:HB2	1:126:A:GLU:HA	3	0.39	0.13	0.39
(1,802)	1:41:A:GLN:H	1:74:A:LEU:HB3	3	0.37	0.28	0.21
(1,1584)	1:95:A:LYS:HG2	1:124:A:GLU:HB3	3	0.36	0.14	0.43
(1,1584)	1:95:A:LYS:HG3	1:124:A:GLU:HB3	3	0.36	0.14	0.43
(1,608)	1:97:A:LEU:HG	1:124:A:GLU:HG3	3	0.35	0.14	0.36
(1,950)	1:64:A:ARG:HA	1:67:A:GLY:H	3	0.34	0.12	0.39
(1,749)	1:27:A:GLU:H	1:27:A:GLU:HG3	3	0.33	0.05	0.31
(1,1281)	1:95:A:LYS:HB2	1:127:A:LEU:H	3	0.32	0.13	0.38
(1,161)	1:53:A:ARG:HA	1:60:A:PHE:H	3	0.28	0.14	0.28
(1,1029)	1:82:A:GLY:H	1:104:A:LEU:HB3	3	0.26	0.1	0.21
(1,1215)	1:110:A:GLY:HA3	1:111:A:TYR:H	3	0.26	0.02	0.27
(1,1036)	1:79:A:VAL:HB	1:83:A:TRP:H	3	0.24	0.08	0.24
(1,520)	1:100:A:ILE:HG21	1:105:A:ALA:HA	3	0.23	0.09	0.29
(1,520)	1:100:A:ILE:HG22	1:105:A:ALA:HA	3	0.23	0.09	0.29
(1,520)	1:100:A:ILE:HG23	1:105:A:ALA:HA	3	0.23	0.09	0.29
(1,541)	1:108:A:GLU:HA	1:118:A:LYS:HA	3	0.23	0.04	0.22
(1,1461)	1:55:A:PRO:HD2	1:120:A:THR:HG21	3	0.23	0.04	0.24
(1,1461)	1:55:A:PRO:HD2	1:120:A:THR:HG22	3	0.23	0.04	0.24
(1,1461)	1:55:A:PRO:HD2	1:120:A:THR:HG23	3	0.23	0.04	0.24
(1,1461)	1:55:A:PRO:HD3	1:120:A:THR:HG21	3	0.23	0.04	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1461)	1:55:A:PRO:HD3	1:120:A:THR:HG22	3	0.23	0.04	0.24
(1,1461)	1:55:A:PRO:HD3	1:120:A:THR:HG23	3	0.23	0.04	0.24
(1,227)	1:67:A:GLY:HA3	1:68:A:LYS:HB2	3	0.21	0.07	0.23
(1,1093)	1:87:A:VAL:HG11	1:90:A:MET:H	3	0.21	0.04	0.18
(1,1093)	1:87:A:VAL:HG12	1:90:A:MET:H	3	0.21	0.04	0.18
(1,1093)	1:87:A:VAL:HG13	1:90:A:MET:H	3	0.21	0.04	0.18
(1,309)	1:80:A:ILE:HA	1:81:A:LYS:HB2	3	0.2	0.06	0.22
(1,72)	1:40:A:PRO:HB3	1:41:A:GLN:H	3	0.2	0.07	0.17
(1,109)	1:46:A:VAL:HB	1:129:A:ALA:H	3	0.19	0.1	0.12
(1,119)	1:46:A:VAL:HG21	1:74:A:LEU:HD11	3	0.19	0.07	0.14
(1,119)	1:46:A:VAL:HG21	1:74:A:LEU:HD12	3	0.19	0.07	0.14
(1,119)	1:46:A:VAL:HG21	1:74:A:LEU:HD13	3	0.19	0.07	0.14
(1,119)	1:46:A:VAL:HG22	1:74:A:LEU:HD11	3	0.19	0.07	0.14
(1,119)	1:46:A:VAL:HG22	1:74:A:LEU:HD12	3	0.19	0.07	0.14
(1,119)	1:46:A:VAL:HG22	1:74:A:LEU:HD13	3	0.19	0.07	0.14
(1,119)	1:46:A:VAL:HG23	1:74:A:LEU:HD11	3	0.19	0.07	0.14
(1,119)	1:46:A:VAL:HG23	1:74:A:LEU:HD12	3	0.19	0.07	0.14
(1,119)	1:46:A:VAL:HG23	1:74:A:LEU:HD13	3	0.19	0.07	0.14
(1,1005)	1:77:A:GLY:H	1:78:A:GLU:H	3	0.18	0.02	0.17
(1,1627)	1:109:A:ARG:HA	1:109:A:ARG:HG2	3	0.17	0.01	0.18
(1,1627)	1:109:A:ARG:HA	1:109:A:ARG:HG3	3	0.17	0.01	0.18
(1,470)	1:100:A:ILE:HB	1:121:A:LEU:HB2	3	0.16	0.04	0.14
(1,123)	1:46:A:VAL:HG11	1:130:A:VAL:HB	3	0.16	0.03	0.17
(1,123)	1:46:A:VAL:HG12	1:130:A:VAL:HB	3	0.16	0.03	0.17
(1,123)	1:46:A:VAL:HG13	1:130:A:VAL:HB	3	0.16	0.03	0.17
(1,1037)	1:80:A:ILE:HG12	1:83:A:TRP:H	3	0.15	0.03	0.15
(1,868)	1:51:A:ASP:H	1:125:A:VAL:HG11	3	0.15	0.05	0.13
(1,868)	1:51:A:ASP:H	1:125:A:VAL:HG12	3	0.15	0.05	0.13
(1,868)	1:51:A:ASP:H	1:125:A:VAL:HG13	3	0.15	0.05	0.13
(1,355)	1:81:A:LYS:HB3	1:82:A:GLY:HA2	3	0.15	0.03	0.15
(1,638)	1:127:A:LEU:HD11	1:129:A:ALA:HB1	3	0.15	0.04	0.17
(1,638)	1:127:A:LEU:HD11	1:129:A:ALA:HB2	3	0.15	0.04	0.17
(1,638)	1:127:A:LEU:HD11	1:129:A:ALA:HB3	3	0.15	0.04	0.17
(1,638)	1:127:A:LEU:HD12	1:129:A:ALA:HB1	3	0.15	0.04	0.17
(1,638)	1:127:A:LEU:HD12	1:129:A:ALA:HB2	3	0.15	0.04	0.17
(1,638)	1:127:A:LEU:HD12	1:129:A:ALA:HB3	3	0.15	0.04	0.17
(1,638)	1:127:A:LEU:HD13	1:129:A:ALA:HB1	3	0.15	0.04	0.17
(1,638)	1:127:A:LEU:HD13	1:129:A:ALA:HB2	3	0.15	0.04	0.17
(1,638)	1:127:A:LEU:HD13	1:129:A:ALA:HB3	3	0.15	0.04	0.17
(1,1491)	1:64:A:ARG:HA	1:64:A:ARG:HD2	3	0.13	0.02	0.13
(1,1491)	1:64:A:ARG:HA	1:64:A:ARG:HD3	3	0.13	0.02	0.13
(1,199)	1:59:A:GLN:HG3	1:61:A:ASP:H	2	1.36	0.5	1.36

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,163)	1:53:A:ARG:HG3	1:59:A:GLN:H	2	1.03	0.84	1.03
(1,393)	1:74:A:LEU:HD21	1:88:A:ALA:HA	2	0.98	0.1	0.98
(1,393)	1:74:A:LEU:HD22	1:88:A:ALA:HA	2	0.98	0.1	0.98
(1,393)	1:74:A:LEU:HD23	1:88:A:ALA:HA	2	0.98	0.1	0.98
(1,1064)	1:81:A:LYS:HD3	1:85:A:GLN:H	2	0.98	0.04	0.98
(1,522)	1:80:A:ILE:HG21	1:105:A:ALA:HA	2	0.94	0.53	0.94
(1,522)	1:80:A:ILE:HG22	1:105:A:ALA:HA	2	0.94	0.53	0.94
(1,522)	1:80:A:ILE:HG23	1:105:A:ALA:HA	2	0.94	0.53	0.94
(1,705)	1:49:A:HIS:HE1	1:64:A:ARG:HA	2	0.9	0.68	0.9
(1,94)	1:41:A:GLN:HG2	1:44:A:LYS:HG3	2	0.88	0.66	0.88
(1,462)	1:97:A:LEU:HD21	1:123:A:PHE:H	2	0.87	0.64	0.87
(1,462)	1:97:A:LEU:HD22	1:123:A:PHE:H	2	0.87	0.64	0.87
(1,462)	1:97:A:LEU:HD23	1:123:A:PHE:H	2	0.87	0.64	0.87
(1,39)	1:32:A:THR:HB	1:95:A:LYS:HB2	2	0.7	0.36	0.7
(1,271)	1:74:A:LEU:HD21	1:88:A:ALA:H	2	0.57	0.02	0.57
(1,271)	1:74:A:LEU:HD22	1:88:A:ALA:H	2	0.57	0.02	0.57
(1,271)	1:74:A:LEU:HD23	1:88:A:ALA:H	2	0.57	0.02	0.57
(1,329)	1:72:A:PHE:HD2	1:79:A:VAL:HG21	2	0.57	0.23	0.57
(1,329)	1:72:A:PHE:HD2	1:79:A:VAL:HG22	2	0.57	0.23	0.57
(1,329)	1:72:A:PHE:HD2	1:79:A:VAL:HG23	2	0.57	0.23	0.57
(1,200)	1:59:A:GLN:HG3	1:60:A:PHE:H	2	0.56	0.05	0.56
(1,1096)	1:91:A:THR:H	1:94:A:GLU:H	2	0.55	0.22	0.55
(1,1049)	1:81:A:LYS:HD3	1:84:A:ASP:H	2	0.54	0.06	0.54
(1,575)	1:102:A:TYR:HE2	1:118:A:LYS:HG2	2	0.5	0.06	0.5
(1,201)	1:59:A:GLN:H	1:59:A:GLN:HG3	2	0.49	0.06	0.49
(1,644)	1:49:A:HIS:HB2	1:128:A:LEU:HG	2	0.47	0.16	0.47
(1,1332)	1:24:A:ALA:HA	1:103:A:GLN:HG2	2	0.43	0.22	0.43
(1,1332)	1:24:A:ALA:HA	1:103:A:GLN:HG3	2	0.43	0.22	0.43
(1,305)	1:79:A:VAL:HB	1:80:A:ILE:HD11	2	0.41	0.18	0.41
(1,305)	1:79:A:VAL:HB	1:80:A:ILE:HD12	2	0.41	0.18	0.41
(1,305)	1:79:A:VAL:HB	1:80:A:ILE:HD13	2	0.41	0.18	0.41
(1,71)	1:38:A:THR:HG21	1:92:A:LEU:HD21	2	0.4	0.1	0.4
(1,71)	1:38:A:THR:HG21	1:92:A:LEU:HD22	2	0.4	0.1	0.4
(1,71)	1:38:A:THR:HG21	1:92:A:LEU:HD23	2	0.4	0.1	0.4
(1,71)	1:38:A:THR:HG22	1:92:A:LEU:HD21	2	0.4	0.1	0.4
(1,71)	1:38:A:THR:HG22	1:92:A:LEU:HD22	2	0.4	0.1	0.4
(1,71)	1:38:A:THR:HG22	1:92:A:LEU:HD23	2	0.4	0.1	0.4
(1,71)	1:38:A:THR:HG23	1:92:A:LEU:HD21	2	0.4	0.1	0.4
(1,71)	1:38:A:THR:HG23	1:92:A:LEU:HD22	2	0.4	0.1	0.4
(1,71)	1:38:A:THR:HG23	1:92:A:LEU:HD23	2	0.4	0.1	0.4
(1,354)	1:82:A:GLY:HA2	1:104:A:LEU:HB3	2	0.4	0.16	0.4
(1,349)	1:82:A:GLY:HA3	1:100:A:ILE:HG21	2	0.39	0.24	0.39

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,349)	1:82:A:GLY:HA3	1:100:A:ILE:HG22	2	0.39	0.24	0.39
(1,349)	1:82:A:GLY:HA3	1:100:A:ILE:HG23	2	0.39	0.24	0.39
(1,1397)	1:43:A:GLY:HA2	1:44:A:LYS:HG2	2	0.38	0.01	0.38
(1,1397)	1:43:A:GLY:HA2	1:44:A:LYS:HG3	2	0.38	0.01	0.38
(1,1397)	1:43:A:GLY:HA3	1:44:A:LYS:HG2	2	0.38	0.01	0.38
(1,1397)	1:43:A:GLY:HA3	1:44:A:LYS:HG3	2	0.38	0.01	0.38
(1,38)	1:31:A:LEU:HG	1:32:A:THR:H	2	0.36	0.1	0.36
(1,443)	1:32:A:THR:HG21	1:95:A:LYS:HB3	2	0.36	0.16	0.36
(1,443)	1:32:A:THR:HG22	1:95:A:LYS:HB3	2	0.36	0.16	0.36
(1,443)	1:32:A:THR:HG23	1:95:A:LYS:HB3	2	0.36	0.16	0.36
(1,1470)	1:59:A:GLN:H	1:59:A:GLN:HG2	2	0.36	0.06	0.36
(1,1470)	1:59:A:GLN:H	1:59:A:GLN:HG3	2	0.36	0.06	0.36
(1,1314)	1:13:A:GLU:H	1:13:A:GLU:HB2	2	0.36	0.08	0.36
(1,1314)	1:13:A:GLU:H	1:13:A:GLU:HB3	2	0.36	0.08	0.36
(1,465)	1:99:A:THR:HB	1:122:A:VAL:HG11	2	0.35	0.07	0.35
(1,465)	1:99:A:THR:HB	1:122:A:VAL:HG12	2	0.35	0.07	0.35
(1,465)	1:99:A:THR:HB	1:122:A:VAL:HG13	2	0.35	0.07	0.35
(1,232)	1:48:A:VAL:H	1:69:A:PRO:HB3	2	0.34	0.08	0.34
(1,601)	1:100:A:ILE:HD11	1:123:A:PHE:HB2	2	0.34	0.18	0.34
(1,601)	1:100:A:ILE:HD12	1:123:A:PHE:HB2	2	0.34	0.18	0.34
(1,601)	1:100:A:ILE:HD13	1:123:A:PHE:HB2	2	0.34	0.18	0.34
(1,424)	1:34:A:GLY:HA3	1:91:A:THR:HB	2	0.33	0.0	0.33
(1,228)	1:47:A:THR:HG21	1:69:A:PRO:HA	2	0.31	0.16	0.31
(1,228)	1:47:A:THR:HG22	1:69:A:PRO:HA	2	0.31	0.16	0.31
(1,228)	1:47:A:THR:HG23	1:69:A:PRO:HA	2	0.31	0.16	0.31
(1,708)	1:11:A:THR:HA	1:12:A:LEU:H	2	0.31	0.07	0.31
(1,336)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	2	0.29	0.0	0.29
(1,418)	1:90:A:MET:HE1	1:96:A:ALA:HB1	2	0.27	0.07	0.27
(1,418)	1:90:A:MET:HE1	1:96:A:ALA:HB2	2	0.27	0.07	0.27
(1,418)	1:90:A:MET:HE1	1:96:A:ALA:HB3	2	0.27	0.07	0.27
(1,418)	1:90:A:MET:HE2	1:96:A:ALA:HB1	2	0.27	0.07	0.27
(1,418)	1:90:A:MET:HE2	1:96:A:ALA:HB2	2	0.27	0.07	0.27
(1,418)	1:90:A:MET:HE2	1:96:A:ALA:HB3	2	0.27	0.07	0.27
(1,418)	1:90:A:MET:HE3	1:96:A:ALA:HB1	2	0.27	0.07	0.27
(1,418)	1:90:A:MET:HE3	1:96:A:ALA:HB2	2	0.27	0.07	0.27
(1,418)	1:90:A:MET:HE3	1:96:A:ALA:HB3	2	0.27	0.07	0.27
(1,654)	1:47:A:THR:H	1:130:A:VAL:HG11	2	0.26	0.08	0.26
(1,654)	1:47:A:THR:H	1:130:A:VAL:HG12	2	0.26	0.08	0.26
(1,654)	1:47:A:THR:H	1:130:A:VAL:HG13	2	0.26	0.08	0.26
(1,1213)	1:109:A:ARG:HB3	1:110:A:GLY:H	2	0.26	0.02	0.26
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG11	2	0.26	0.04	0.26
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG12	2	0.26	0.04	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG13	2	0.26	0.04	0.26
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG21	2	0.26	0.04	0.26
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG22	2	0.26	0.04	0.26
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG23	2	0.26	0.04	0.26
(1,819)	1:44:A:LYS:H	1:44:A:LYS:HG2	2	0.26	0.05	0.26
(1,391)	1:46:A:VAL:HG21	1:87:A:VAL:HB	2	0.26	0.02	0.26
(1,391)	1:46:A:VAL:HG22	1:87:A:VAL:HB	2	0.26	0.02	0.26
(1,391)	1:46:A:VAL:HG23	1:87:A:VAL:HB	2	0.26	0.02	0.26
(1,700)	1:79:A:VAL:HB	1:83:A:TRP:HE3	2	0.25	0.08	0.25
(1,965)	1:69:A:PRO:HG3	1:70:A:PHE:H	2	0.24	0.1	0.24
(1,430)	1:92:A:LEU:HD21	1:129:A:ALA:HA	2	0.24	0.05	0.24
(1,430)	1:92:A:LEU:HD22	1:129:A:ALA:HA	2	0.24	0.05	0.24
(1,430)	1:92:A:LEU:HD23	1:129:A:ALA:HA	2	0.24	0.05	0.24
(1,274)	1:74:A:LEU:HD11	1:87:A:VAL:H	2	0.23	0.12	0.23
(1,274)	1:74:A:LEU:HD12	1:87:A:VAL:H	2	0.23	0.12	0.23
(1,274)	1:74:A:LEU:HD13	1:87:A:VAL:H	2	0.23	0.12	0.23
(1,1399)	1:44:A:LYS:HB2	1:44:A:LYS:HE2	2	0.23	0.02	0.23
(1,1399)	1:44:A:LYS:HB2	1:44:A:LYS:HE3	2	0.23	0.02	0.23
(1,147)	1:50:A:TYR:HA	1:124:A:GLU:HB3	2	0.22	0.04	0.22
(1,690)	1:83:A:TRP:HD1	1:123:A:PHE:HD2	2	0.22	0.07	0.22
(1,1631)	1:109:A:ARG:HB2	1:110:A:GLY:H	2	0.2	0.06	0.2
(1,1631)	1:109:A:ARG:HB3	1:110:A:GLY:H	2	0.2	0.06	0.2
(1,416)	1:87:A:VAL:HA	1:90:A:MET:HE1	2	0.2	0.01	0.2
(1,416)	1:87:A:VAL:HA	1:90:A:MET:HE2	2	0.2	0.01	0.2
(1,416)	1:87:A:VAL:HA	1:90:A:MET:HE3	2	0.2	0.01	0.2
(1,1606)	1:98:A:PHE:HB2	1:100:A:ILE:HD11	2	0.2	0.06	0.2
(1,1606)	1:98:A:PHE:HB2	1:100:A:ILE:HD12	2	0.2	0.06	0.2
(1,1606)	1:98:A:PHE:HB2	1:100:A:ILE:HD13	2	0.2	0.06	0.2
(1,1606)	1:98:A:PHE:HB3	1:100:A:ILE:HD11	2	0.2	0.06	0.2
(1,1606)	1:98:A:PHE:HB3	1:100:A:ILE:HD12	2	0.2	0.06	0.2
(1,1606)	1:98:A:PHE:HB3	1:100:A:ILE:HD13	2	0.2	0.06	0.2
(1,709)	1:11:A:THR:HG21	1:12:A:LEU:H	2	0.2	0.02	0.2
(1,709)	1:11:A:THR:HG22	1:12:A:LEU:H	2	0.2	0.02	0.2
(1,709)	1:11:A:THR:HG23	1:12:A:LEU:H	2	0.2	0.02	0.2
(1,412)	1:90:A:MET:H	1:90:A:MET:HE1	2	0.19	0.05	0.19
(1,412)	1:90:A:MET:H	1:90:A:MET:HE2	2	0.19	0.05	0.19
(1,412)	1:90:A:MET:H	1:90:A:MET:HE3	2	0.19	0.05	0.19
(1,388)	1:86:A:GLY:HA2	1:98:A:PHE:HD2	2	0.18	0.02	0.18
(1,487)	1:102:A:TYR:HA	1:105:A:ALA:HB1	2	0.18	0.08	0.18
(1,487)	1:102:A:TYR:HA	1:105:A:ALA:HB2	2	0.18	0.08	0.18
(1,487)	1:102:A:TYR:HA	1:105:A:ALA:HB3	2	0.18	0.08	0.18
(1,1425)	1:49:A:HIS:HB3	1:126:A:GLU:HB2	2	0.18	0.02	0.18

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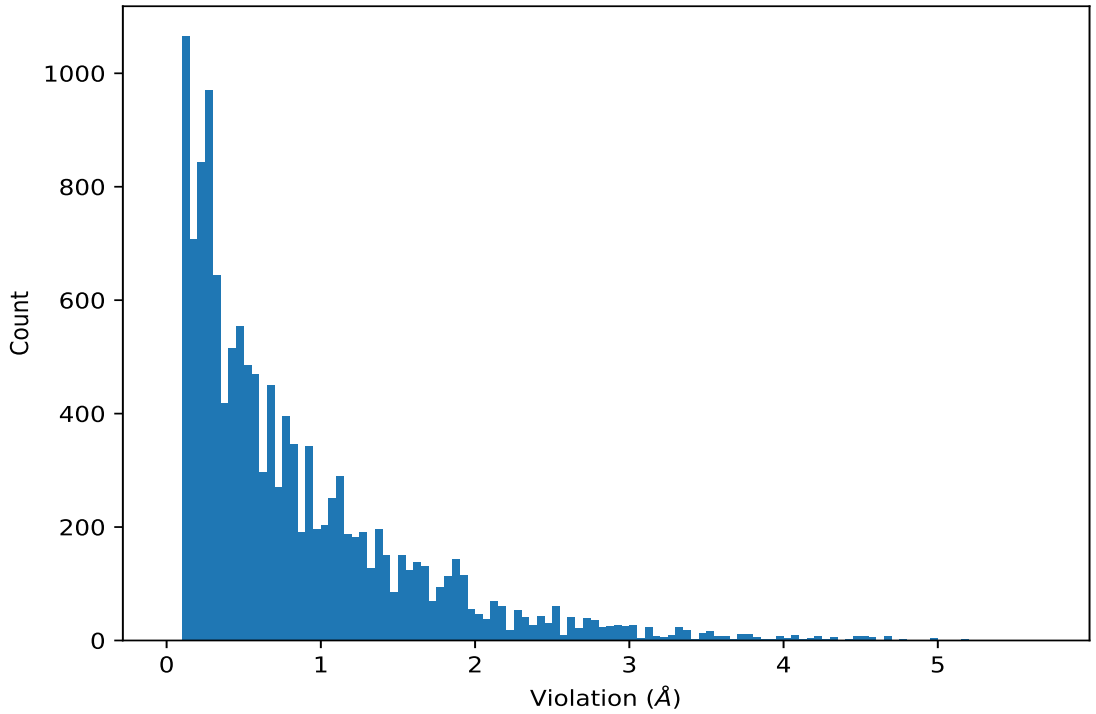
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1425)	1:49:A:HIS:HB3	1:126:A:GLU:HB3	2	0.18	0.02	0.18
(1,1605)	1:98:A:PHE:HB2	1:100:A:ILE:H	2	0.18	0.02	0.18
(1,1605)	1:98:A:PHE:HB3	1:100:A:ILE:H	2	0.18	0.02	0.18
(1,157)	1:52:A:GLY:HA2	1:124:A:GLU:H	2	0.18	0.04	0.18
(1,624)	1:49:A:HIS:HB3	1:126:A:GLU:HB3	2	0.18	0.02	0.18
(1,808)	1:43:A:GLY:H	1:74:A:LEU:H	2	0.17	0.0	0.17
(1,799)	1:40:A:PRO:HB2	1:41:A:GLN:H	2	0.16	0.04	0.16
(1,1511)	1:70:A:PHE:HB2	1:71:A:GLN:H	2	0.16	0.01	0.16
(1,1511)	1:70:A:PHE:HB3	1:71:A:GLN:H	2	0.16	0.01	0.16
(1,1009)	1:76:A:ALA:H	1:78:A:GLU:H	2	0.16	0.05	0.16
(1,428)	1:38:A:THR:HG21	1:92:A:LEU:HD11	2	0.16	0.02	0.16
(1,428)	1:38:A:THR:HG21	1:92:A:LEU:HD12	2	0.16	0.02	0.16
(1,428)	1:38:A:THR:HG21	1:92:A:LEU:HD13	2	0.16	0.02	0.16
(1,428)	1:38:A:THR:HG22	1:92:A:LEU:HD11	2	0.16	0.02	0.16
(1,428)	1:38:A:THR:HG22	1:92:A:LEU:HD12	2	0.16	0.02	0.16
(1,428)	1:38:A:THR:HG22	1:92:A:LEU:HD13	2	0.16	0.02	0.16
(1,428)	1:38:A:THR:HG23	1:92:A:LEU:HD11	2	0.16	0.02	0.16
(1,428)	1:38:A:THR:HG23	1:92:A:LEU:HD12	2	0.16	0.02	0.16
(1,428)	1:38:A:THR:HG23	1:92:A:LEU:HD13	2	0.16	0.02	0.16
(1,680)	1:50:A:TYR:HB3	1:50:A:TYR:HD1	2	0.16	0.02	0.16
(1,679)	1:50:A:TYR:HB2	1:50:A:TYR:HD2	2	0.16	0.02	0.16
(1,333)	1:81:A:LYS:HA	1:81:A:LYS:HD3	2	0.15	0.02	0.15
(1,1525)	1:78:A:GLU:HG2	1:79:A:VAL:HG11	2	0.15	0.03	0.15
(1,1525)	1:78:A:GLU:HG2	1:79:A:VAL:HG12	2	0.15	0.03	0.15
(1,1525)	1:78:A:GLU:HG2	1:79:A:VAL:HG13	2	0.15	0.03	0.15
(1,1525)	1:78:A:GLU:HG3	1:79:A:VAL:HG11	2	0.15	0.03	0.15
(1,1525)	1:78:A:GLU:HG3	1:79:A:VAL:HG12	2	0.15	0.03	0.15
(1,1525)	1:78:A:GLU:HG3	1:79:A:VAL:HG13	2	0.15	0.03	0.15
(1,100)	1:45:A:LYS:HB3	1:46:A:VAL:HA	2	0.13	0.02	0.13
(1,1259)	1:124:A:GLU:H	1:125:A:VAL:HG11	2	0.13	0.02	0.13
(1,1259)	1:124:A:GLU:H	1:125:A:VAL:HG12	2	0.13	0.02	0.13
(1,1259)	1:124:A:GLU:H	1:125:A:VAL:HG13	2	0.13	0.02	0.13
(1,114)	1:46:A:VAL:HG21	1:47:A:THR:H	2	0.12	0.02	0.12
(1,114)	1:46:A:VAL:HG22	1:47:A:THR:H	2	0.12	0.02	0.12
(1,114)	1:46:A:VAL:HG23	1:47:A:THR:H	2	0.12	0.02	0.12
(1,909)	1:56:A:ASP:HA	1:57:A:GLY:H	2	0.12	0.01	0.12
(1,748)	1:27:A:GLU:H	1:99:A:THR:HB	2	0.12	0.0	0.12
(1,45)	1:34:A:GLY:HA3	1:94:A:GLU:HB2	2	0.11	0.0	0.11

[1]Number of violated models, [2]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)
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	20	5.69
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	9	5.47
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	8	5.4
(1,548)	1:102:A:TYR:HE2	1:108:A:GLU:HG3	7	5.38
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	20	5.31
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	20	5.23
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	14	5.18
(1,685)	1:102:A:TYR:HE2	1:108:A:GLU:HG2	7	5.16
(1,682)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	5	5.15
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	8	5.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	4	4.98
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	12	4.97
(1,191)	1:54:A:PHE:HD1	1:58:A:LYS:HD3	8	4.96
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	2	4.95
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	13	4.91
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	12	4.78
(1,960)	1:50:A:TYR:HE2	1:70:A:PHE:H	5	4.75
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	5	4.68
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	5	4.68
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	5	4.68
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	5	4.68
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	5	4.68
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	5	4.68
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	3	4.66
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	17	4.6
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	9	4.58
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	9	4.58
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	9	4.58
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	6	4.56
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	13	4.55
(1,960)	1:50:A:TYR:HE2	1:70:A:PHE:H	3	4.54
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	2	4.51
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	2	4.51
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	2	4.51
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	2	4.51
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	2	4.51
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	2	4.51
(1,548)	1:102:A:TYR:HE2	1:108:A:GLU:HG3	18	4.49
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	12	4.48
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	19	4.47
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	19	4.47
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	19	4.47
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	4	4.46
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	4	4.46
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	4	4.46
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	2	4.44
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	2	4.44
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	8	4.43
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	3	4.33
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	5	4.31
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	5	4.31
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	14	4.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	14	4.31
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	15	4.3
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	6	4.27
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	19	4.25
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	16	4.24
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	3	4.22
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	3	4.22
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	15	4.22
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	13	4.22
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	18	4.21
(1,190)	1:54:A:PHE:HD1	1:58:A:LYS:HD2	5	4.21
(1,191)	1:54:A:PHE:HD1	1:58:A:LYS:HD3	10	4.2
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	9	4.19
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	8	4.17
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	3	4.15
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	3	4.15
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	3	4.15
(1,685)	1:102:A:TYR:HE2	1:108:A:GLU:HG2	17	4.14
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	12	4.11
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	9	4.11
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	3	4.1
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	15	4.1
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	19	4.09
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	12	4.07
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	15	4.06
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	15	4.06
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG21	15	4.06
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG22	15	4.06
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG23	15	4.06
(1,191)	1:54:A:PHE:HD1	1:58:A:LYS:HD3	9	4.02
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	6	4.01
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	20	4.01
(1,683)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	5	4.0
(1,149)	1:50:A:TYR:HB2	1:123:A:PHE:HD2	13	3.99
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	14	3.98
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	10	3.98
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	10	3.98
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	10	3.98
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	3	3.96
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	15	3.95
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	6	3.95
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	10	3.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	2	3.91
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	9	3.91
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	3	3.9
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	17	3.89
(1,960)	1:50:A:TYR:HE2	1:70:A:PHE:H	16	3.88
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	12	3.83
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	12	3.83
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	18	3.83
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	20	3.83
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	14	3.81
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	16	3.81
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	4	3.79
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	7	3.79
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	7	3.79
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	7	3.79
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG21	15	3.78
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG22	15	3.78
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG23	15	3.78
(1,960)	1:50:A:TYR:HE2	1:70:A:PHE:H	20	3.77
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	17	3.77
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	3	3.76
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	7	3.75
(1,548)	1:102:A:TYR:HE2	1:108:A:GLU:HG3	4	3.74
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	5	3.73
(1,190)	1:54:A:PHE:HD1	1:58:A:LYS:HD2	8	3.73
(1,148)	1:50:A:TYR:HB3	1:123:A:PHE:HD2	17	3.73
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	10	3.71
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	10	3.71
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	10	3.71
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	10	3.71
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	10	3.71
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	10	3.71
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	9	3.7
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	18	3.68
(1,149)	1:50:A:TYR:HB2	1:123:A:PHE:HD2	7	3.66
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	20	3.64
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	20	3.64
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	10	3.64
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	10	3.63
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	19	3.62
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	19	3.62
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	19	3.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	4	3.58
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	4	3.58
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	4	3.58
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	6	3.57
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	17	3.57
(1,960)	1:50:A:TYR:HE2	1:70:A:PHE:H	10	3.56
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	15	3.56
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	2	3.55
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	6	3.55
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	6	3.55
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	6	3.55
(1,149)	1:50:A:TYR:HB2	1:123:A:PHE:HD2	4	3.54
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB2	8	3.53
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB3	8	3.53
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	6	3.52
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	6	3.52
(1,149)	1:50:A:TYR:HB2	1:123:A:PHE:HD2	12	3.52
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	1	3.51
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	18	3.51
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	8	3.5
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD21	19	3.5
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD22	19	3.5
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD23	19	3.5
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	5	3.49
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	14	3.49
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	15	3.48
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	9	3.48
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	4	3.47
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	4	3.47
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	4	3.47
(1,685)	1:102:A:TYR:HE2	1:108:A:GLU:HG2	18	3.46
(1,682)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	3	3.46
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	16	3.46
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	16	3.46
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	16	3.46
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	7	3.46
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	4	3.43
(1,191)	1:54:A:PHE:HD1	1:58:A:LYS:HD3	1	3.43
(1,683)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	3	3.41
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	3	3.4
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	3	3.4
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	1	3.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	5	3.4
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	5	3.4
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	5	3.4
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG21	4	3.4
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG22	4	3.4
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG23	4	3.4
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	17	3.39
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	3	3.39
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	14	3.38
(1,149)	1:50:A:TYR:HB2	1:123:A:PHE:HD2	1	3.38
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	17	3.37
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	17	3.37
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG21	14	3.36
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG22	14	3.36
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG23	14	3.36
(1,75)	1:38:A:THR:HB	1:40:A:PRO:HG3	8	3.36
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	2	3.34
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	2	3.34
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	2	3.34
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB2	13	3.33
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB3	13	3.33
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB2	9	3.33
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB3	9	3.33
(1,190)	1:54:A:PHE:HD1	1:58:A:LYS:HD2	1	3.33
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	4	3.32
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	4	3.32
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	4	3.32
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	4	3.32
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	4	3.32
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	4	3.32
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	19	3.32
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	19	3.32
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD21	4	3.32
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD22	4	3.32
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD23	4	3.32
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG21	7	3.32
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG22	7	3.32
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG23	7	3.32
(1,149)	1:50:A:TYR:HB2	1:123:A:PHE:HD2	14	3.31
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	7	3.3
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	8	3.3
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	5	3.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	7	3.26
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	7	3.26
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	12	3.26
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	17	3.26
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	17	3.26
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	17	3.26
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	19	3.25
(1,191)	1:54:A:PHE:HD1	1:58:A:LYS:HD3	4	3.23
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG21	15	3.22
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG22	15	3.22
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG23	15	3.22
(1,148)	1:50:A:TYR:HB3	1:123:A:PHE:HD2	3	3.21
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	16	3.2
(1,190)	1:54:A:PHE:HD1	1:58:A:LYS:HD2	9	3.19
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	1	3.18
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	1	3.18
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	1	3.18
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	4	3.18
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	2	3.17
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	14	3.17
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	11	3.16
(1,536)	1:102:A:TYR:HE2	1:108:A:GLU:HB2	18	3.15
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB2	5	3.14
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB3	5	3.14
(1,953)	1:49:A:HIS:HE1	1:68:A:LYS:H	2	3.14
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG21	5	3.14
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG22	5	3.14
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG23	5	3.14
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	4	3.13
(1,190)	1:54:A:PHE:HD1	1:58:A:LYS:HD2	20	3.13
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG21	9	3.12
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG22	9	3.12
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG23	9	3.12
(1,130)	1:48:A:VAL:HG11	1:50:A:TYR:HD1	17	3.11
(1,130)	1:48:A:VAL:HG12	1:50:A:TYR:HD1	17	3.11
(1,130)	1:48:A:VAL:HG13	1:50:A:TYR:HD1	17	3.11
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB2	10	3.1
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB3	10	3.1
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	9	3.1
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	11	3.1
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	11	3.1
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	11	3.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	4	3.1
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	4	3.1
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	4	3.1
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	2	3.09
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	15	3.07
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	15	3.07
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	15	3.07
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	6	3.07
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	18	3.05
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	18	3.05
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	18	3.05
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	12	3.05
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	17	3.04
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG21	16	3.04
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG22	16	3.04
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG23	16	3.04
(1,148)	1:50:A:TYR:HB3	1:123:A:PHE:HD2	9	3.03
(1,148)	1:50:A:TYR:HB3	1:123:A:PHE:HD2	20	3.03
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	13	3.02
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	13	3.02
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	13	3.02
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	19	3.02
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG21	1	3.02
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG22	1	3.02
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG23	1	3.02
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	19	3.01
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	19	3.01
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	2	3.01
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	9	3.0
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD21	3	3.0
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD22	3	3.0
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD23	3	3.0
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	6	3.0
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	6	3.0
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	6	3.0
(1,683)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	10	2.99
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	14	2.99
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG21	3	2.99
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG22	3	2.99
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG23	3	2.99
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	4	2.99
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	10	2.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	10	2.98
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	16	2.97
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	16	2.97
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	13	2.97
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG21	12	2.97
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG22	12	2.97
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG23	12	2.97
(1,75)	1:38:A:THR:HB	1:40:A:PRO:HG3	15	2.97
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	9	2.96
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	9	2.96
(1,694)	1:80:A:ILE:HD11	1:83:A:TRP:HD1	9	2.96
(1,694)	1:80:A:ILE:HD12	1:83:A:TRP:HD1	9	2.96
(1,694)	1:80:A:ILE:HD13	1:83:A:TRP:HD1	9	2.96
(1,191)	1:54:A:PHE:HD1	1:58:A:LYS:HD3	19	2.96
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	6	2.95
(1,683)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	16	2.95
(1,683)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	20	2.95
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	5	2.95
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	11	2.95
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	20	2.94
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	2	2.94
(1,682)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	16	2.94
(1,500)	1:81:A:LYS:HB2	1:104:A:LEU:HA	1	2.94
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG21	10	2.94
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG22	10	2.94
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG23	10	2.94
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	4	2.94
(1,149)	1:50:A:TYR:HB2	1:123:A:PHE:HD2	6	2.94
(1,682)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	10	2.93
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	16	2.93
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	16	2.93
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	16	2.93
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG21	17	2.93
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG22	17	2.93
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG23	17	2.93
(1,167)	1:53:A:ARG:HG2	1:54:A:PHE:HD1	12	2.93
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	1	2.92
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	19	2.92
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	19	2.92
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	19	2.92
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	14	2.92
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG11	15	2.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG12	15	2.91
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG13	15	2.91
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG21	15	2.91
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG22	15	2.91
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG23	15	2.91
(1,191)	1:54:A:PHE:HD1	1:58:A:LYS:HD3	5	2.9
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	20	2.89
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	20	2.89
(1,688)	1:83:A:TRP:HD1	1:98:A:PHE:HD2	5	2.89
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	13	2.89
(1,1648)	1:121:A:LEU:HD11	1:123:A:PHE:HD1	17	2.88
(1,1648)	1:121:A:LEU:HD12	1:123:A:PHE:HD1	17	2.88
(1,1648)	1:121:A:LEU:HD13	1:123:A:PHE:HD1	17	2.88
(1,1648)	1:121:A:LEU:HD21	1:123:A:PHE:HD1	17	2.88
(1,1648)	1:121:A:LEU:HD22	1:123:A:PHE:HD1	17	2.88
(1,1648)	1:121:A:LEU:HD23	1:123:A:PHE:HD1	17	2.88
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	16	2.88
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	16	2.88
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	16	2.88
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	16	2.88
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	16	2.88
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	16	2.88
(1,225)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	20	2.88
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	8	2.87
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	8	2.87
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	11	2.87
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	4	2.87
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	4	2.87
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	4	2.87
(1,530)	1:106:A:TYR:HB3	1:111:A:TYR:HD2	8	2.85
(1,1323)	1:19:A:PRO:HG2	1:55:A:PRO:HB2	18	2.84
(1,1323)	1:19:A:PRO:HG3	1:55:A:PRO:HB2	18	2.84
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	8	2.84
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	8	2.84
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	8	2.84
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	17	2.84
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	17	2.84
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	9	2.83
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	11	2.83
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	7	2.83
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	7	2.83
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	7	2.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	8	2.82
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	7	2.81
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	2	2.81
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	4	2.81
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	8	2.81
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	8	2.81
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	8	2.81
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG21	7	2.81
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG22	7	2.81
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG23	7	2.81
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	4	2.81
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG2	8	2.8
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG3	8	2.8
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	12	2.8
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	12	2.8
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	12	2.8
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	18	2.79
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	18	2.79
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	3	2.79
(1,682)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	20	2.79
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	7	2.79
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	4	2.78
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	4	2.78
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	4	2.78
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	4	2.78
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	4	2.78
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	4	2.78
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	2	2.78
(1,688)	1:83:A:TRP:HD1	1:98:A:PHE:HD2	16	2.78
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG21	8	2.78
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG22	8	2.78
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG23	8	2.78
(1,536)	1:102:A:TYR:HE2	1:108:A:GLU:HB2	4	2.78
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	2	2.77
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	10	2.76
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA2	2	2.75
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	2	2.75
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	11	2.75
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	15	2.75
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	15	2.75
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	15	2.75
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	16	2.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	16	2.75
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	16	2.75
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	16	2.75
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	16	2.75
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	16	2.75
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	15	2.74
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	16	2.74
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	20	2.73
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG21	8	2.73
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG22	8	2.73
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG23	8	2.73
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	12	2.73
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG11	3	2.72
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG12	3	2.72
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG13	3	2.72
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG21	3	2.72
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG22	3	2.72
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG23	3	2.72
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG11	3	2.72
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG12	3	2.72
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG13	3	2.72
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG21	3	2.72
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG22	3	2.72
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG23	3	2.72
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	7	2.72
(1,530)	1:106:A:TYR:HB3	1:111:A:TYR:HD2	7	2.72
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	3	2.72
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	3	2.72
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	3	2.72
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB2	20	2.71
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB3	20	2.71
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	20	2.71
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	20	2.71
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	20	2.71
(1,519)	1:80:A:ILE:HB	1:105:A:ALA:HA	9	2.71
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	2	2.71
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	8	2.71
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	9	2.7
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	9	2.7
(1,1185)	1:24:A:ALA:HB1	1:103:A:GLN:H	8	2.7
(1,1185)	1:24:A:ALA:HB2	1:103:A:GLN:H	8	2.7
(1,1185)	1:24:A:ALA:HB3	1:103:A:GLN:H	8	2.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	17	2.7
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	10	2.7
(1,856)	1:51:A:ASP:H	1:123:A:PHE:HD2	20	2.69
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	1	2.69
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	3	2.69
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG21	7	2.68
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG22	7	2.68
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG23	7	2.68
(1,134)	1:48:A:VAL:HG21	1:50:A:TYR:HD1	17	2.68
(1,134)	1:48:A:VAL:HG22	1:50:A:TYR:HD1	17	2.68
(1,134)	1:48:A:VAL:HG23	1:50:A:TYR:HD1	17	2.68
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	13	2.67
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	13	2.67
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	13	2.67
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	13	2.67
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	13	2.67
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	13	2.67
(1,688)	1:83:A:TRP:HD1	1:98:A:PHE:HD2	17	2.67
(1,856)	1:51:A:ASP:H	1:123:A:PHE:HD2	17	2.66
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG21	7	2.66
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG22	7	2.66
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG23	7	2.66
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	10	2.66
(1,190)	1:54:A:PHE:HD1	1:58:A:LYS:HD2	15	2.66
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	13	2.65
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	7	2.65
(1,548)	1:102:A:TYR:HE2	1:108:A:GLU:HG3	11	2.65
(1,190)	1:54:A:PHE:HD1	1:58:A:LYS:HD2	10	2.65
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG21	7	2.64
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG22	7	2.64
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG23	7	2.64
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	4	2.63
(1,685)	1:102:A:TYR:HE2	1:108:A:GLU:HG2	4	2.63
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	7	2.63
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	1	2.63
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	1	2.63
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	1	2.63
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG11	15	2.63
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG12	15	2.63
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG13	15	2.63
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG11	15	2.62
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG12	15	2.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG13	15	2.62
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG21	15	2.62
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG22	15	2.62
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG23	15	2.62
(1,856)	1:51:A:ASP:H	1:123:A:PHE:HD2	3	2.62
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	7	2.62
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	20	2.62
(1,190)	1:54:A:PHE:HD1	1:58:A:LYS:HD2	19	2.62
(1,149)	1:50:A:TYR:HB2	1:123:A:PHE:HD2	17	2.62
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	6	2.61
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	6	2.61
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	6	2.61
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	6	2.61
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	6	2.61
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	6	2.61
(1,1310)	1:81:A:LYS:HE2	1:85:A:GLN:HE22	3	2.61
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB2	8	2.6
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB3	8	2.6
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG21	1	2.6
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG22	1	2.6
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG23	1	2.6
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG21	20	2.6
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG22	20	2.6
(1,480)	1:98:A:PHE:HD2	1:100:A:ILE:HG23	20	2.6
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG11	15	2.59
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG12	15	2.59
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG13	15	2.59
(1,225)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	15	2.59
(1,960)	1:50:A:TYR:HE2	1:70:A:PHE:H	9	2.58
(1,953)	1:49:A:HIS:HE1	1:68:A:LYS:H	15	2.57
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	6	2.57
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	6	2.57
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	6	2.57
(1,75)	1:38:A:THR:HB	1:40:A:PRO:HG3	2	2.57
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	18	2.55
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	3	2.55
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	3	2.55
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	3	2.55
(1,544)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	7	2.54
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	16	2.54
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	16	2.54
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	16	2.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD21	19	2.54
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD22	19	2.54
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD23	19	2.54
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG21	3	2.54
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG22	3	2.54
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG23	3	2.54
(1,856)	1:51:A:ASP:H	1:123:A:PHE:HD2	4	2.53
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	7	2.53
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	4	2.53
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	4	2.53
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	4	2.53
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG11	15	2.52
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG12	15	2.52
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG13	15	2.52
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG21	15	2.52
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG22	15	2.52
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG23	15	2.52
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	6	2.52
(1,536)	1:102:A:TYR:HE2	1:108:A:GLU:HB2	7	2.52
(1,500)	1:81:A:LYS:HB2	1:104:A:LEU:HA	13	2.52
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	3	2.51
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	3	2.51
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	7	2.51
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	7	2.51
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	7	2.51
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	7	2.51
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	7	2.51
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	7	2.51
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	7	2.51
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	7	2.51
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	7	2.51
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	7	2.51
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	7	2.51
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	7	2.51
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	7	2.51
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	7	2.51
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	7	2.51
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	7	2.51
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	7	2.51
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	7	2.51
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	18	2.51
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	6	2.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,902)	1:59:A:GLN:HE22	1:62:A:SER:HB3	16	2.5
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	3	2.5
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	3	2.5
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	3	2.5
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	3	2.5
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	3	2.5
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	3	2.5
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	1	2.5
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	1	2.5
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	1	2.5
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	2	2.49
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	2	2.49
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	2	2.49
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	1	2.49
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG2	5	2.48
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG3	5	2.48
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	14	2.48
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	14	2.48
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	14	2.48
(1,225)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	3	2.48
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	9	2.48
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	9	2.47
(1,516)	1:81:A:LYS:H	1:105:A:ALA:HA	9	2.47
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	1	2.47
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	1	2.47
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	1	2.47
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	9	2.47
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	9	2.47
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	9	2.47
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG11	15	2.46
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG12	15	2.46
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG13	15	2.46
(1,684)	1:48:A:VAL:HG21	1:50:A:TYR:HE1	17	2.45
(1,684)	1:48:A:VAL:HG22	1:50:A:TYR:HE1	17	2.45
(1,684)	1:48:A:VAL:HG23	1:50:A:TYR:HE1	17	2.45
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	17	2.45
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	1	2.45
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	1	2.45
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	1	2.45
(1,548)	1:102:A:TYR:HE2	1:108:A:GLU:HG3	17	2.45
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	2	2.45
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	20	2.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	20	2.44
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	20	2.44
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	20	2.44
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	20	2.44
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	20	2.44
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG2	10	2.44
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG3	10	2.44
(1,856)	1:51:A:ASP:H	1:123:A:PHE:HD2	1	2.44
(1,856)	1:51:A:ASP:H	1:123:A:PHE:HD2	13	2.44
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	9	2.44
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	9	2.44
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	9	2.44
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	15	2.44
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	10	2.44
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB2	1	2.43
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB3	1	2.43
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE2	19	2.43
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE3	19	2.43
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE2	19	2.43
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE3	19	2.43
(1,1311)	1:81:A:LYS:HE3	1:85:A:GLN:HE22	12	2.43
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	8	2.43
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	8	2.43
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	8	2.43
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	7	2.43
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	7	2.43
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	7	2.43
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB2	4	2.42
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB3	4	2.42
(1,856)	1:51:A:ASP:H	1:123:A:PHE:HD2	12	2.42
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	10	2.42
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG21	9	2.42
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG22	9	2.42
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG23	9	2.42
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	7	2.42
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	13	2.42
(1,75)	1:38:A:THR:HB	1:40:A:PRO:HG3	10	2.42
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	4	2.41
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	4	2.41
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	4	2.41
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG21	11	2.41
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG22	11	2.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG23	11	2.41
(1,683)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	9	2.4
(1,225)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	10	2.4
(1,856)	1:51:A:ASP:H	1:123:A:PHE:HD2	7	2.39
(1,536)	1:102:A:TYR:HE2	1:108:A:GLU:HB2	17	2.39
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	7	2.39
(1,673)	1:52:A:GLY:HA3	1:123:A:PHE:HD1	5	2.38
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	12	2.38
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	12	2.38
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	12	2.38
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	9	2.38
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	9	2.38
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	9	2.38
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	9	2.38
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	9	2.38
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	9	2.38
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	9	2.38
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	9	2.38
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	9	2.38
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	11	2.37
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	11	2.37
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	11	2.37
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	11	2.37
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	11	2.37
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	11	2.37
(1,856)	1:51:A:ASP:H	1:123:A:PHE:HD2	9	2.37
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	12	2.35
(1,545)	1:108:A:GLU:HG2	1:118:A:LYS:HG2	7	2.35
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	9	2.35
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	5	2.34
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	5	2.34
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	17	2.34
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	17	2.34
(1,1328)	1:19:A:PRO:HG2	1:56:A:ASP:HA	12	2.34
(1,1328)	1:19:A:PRO:HG3	1:56:A:ASP:HA	12	2.34
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	5	2.34
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	5	2.34
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	5	2.34
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	16	2.34
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	17	2.34
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	10	2.33
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	10	2.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	10	2.33
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	20	2.33
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	17	2.33
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	17	2.33
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	17	2.33
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	18	2.33
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	18	2.33
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	18	2.33
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	18	2.33
(1,191)	1:54:A:PHE:HD1	1:58:A:LYS:HD3	13	2.33
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	5	2.32
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	5	2.32
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	5	2.32
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	12	2.32
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	18	2.32
(1,500)	1:81:A:LYS:HB2	1:104:A:LEU:HA	9	2.32
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	13	2.32
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	13	2.32
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	13	2.32
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	12	2.31
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	12	2.31
(1,1310)	1:81:A:LYS:HE2	1:85:A:GLN:HE22	12	2.31
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	4	2.31
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	9	2.31
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	9	2.31
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	9	2.31
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	19	2.31
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	19	2.31
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	19	2.31
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB2	19	2.3
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB3	19	2.3
(1,518)	1:80:A:ILE:HA	1:105:A:ALA:HA	9	2.3
(1,422)	1:38:A:THR:HG21	1:91:A:THR:HA	7	2.3
(1,422)	1:38:A:THR:HG22	1:91:A:THR:HA	7	2.3
(1,422)	1:38:A:THR:HG23	1:91:A:THR:HA	7	2.3
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	14	2.3
(1,191)	1:54:A:PHE:HD1	1:58:A:LYS:HD3	11	2.3
(1,539)	1:102:A:TYR:HE2	1:108:A:GLU:HA	4	2.29
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	19	2.29
(1,856)	1:51:A:ASP:H	1:123:A:PHE:HD2	6	2.28
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	7	2.28
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	7	2.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	7	2.28
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	7	2.28
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	9	2.28
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	9	2.28
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	9	2.28
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD11	4	2.28
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD12	4	2.28
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD13	4	2.28
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	9	2.28
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	17	2.28
(1,226)	1:49:A:HIS:HE1	1:67:A:GLY:HA2	2	2.28
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	18	2.28
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	2	2.27
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	2	2.27
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	2	2.27
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	2	2.27
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	2	2.27
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	2	2.27
(1,688)	1:83:A:TRP:HD1	1:98:A:PHE:HD2	7	2.27
(1,148)	1:50:A:TYR:HB3	1:123:A:PHE:HD2	10	2.27
(1,148)	1:50:A:TYR:HB3	1:123:A:PHE:HD2	13	2.27
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG2	20	2.26
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG3	20	2.26
(1,1310)	1:81:A:LYS:HE2	1:85:A:GLN:HE22	19	2.26
(1,897)	1:59:A:GLN:HE21	1:62:A:SER:HB3	20	2.26
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB1	9	2.26
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB2	9	2.26
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB3	9	2.26
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB1	9	2.26
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB2	9	2.26
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB3	9	2.26
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB1	9	2.26
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB2	9	2.26
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB3	9	2.26
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	11	2.26
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	10	2.25
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	11	2.25
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	11	2.25
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	11	2.25
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	7	2.25
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	11	2.24
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	11	2.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	14	2.24
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	14	2.24
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	14	2.24
(1,539)	1:102:A:TYR:HE2	1:108:A:GLU:HA	18	2.24
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	13	2.24
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	3	2.23
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	14	2.22
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	17	2.21
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	20	2.21
(1,857)	1:49:A:HIS:HD2	1:51:A:ASP:H	13	2.21
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	17	2.21
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	1	2.21
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG21	11	2.2
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG22	11	2.2
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG23	11	2.2
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	19	2.2
(1,75)	1:38:A:THR:HB	1:40:A:PRO:HG3	5	2.2
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	1	2.19
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	1	2.19
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	1	2.19
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	1	2.19
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	1	2.19
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	1	2.19
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	1	2.19
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	1	2.19
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	1	2.19
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	1	2.19
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	1	2.19
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	1	2.19
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	1	2.19
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	1	2.19
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	1	2.19
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	1	2.19
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	1	2.19
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	1	2.19
(1,953)	1:49:A:HIS:HE1	1:68:A:LYS:H	14	2.19
(1,856)	1:51:A:ASP:H	1:123:A:PHE:HD2	14	2.19
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	4	2.19
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	4	2.19
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	4	2.19
(1,500)	1:81:A:LYS:HB2	1:104:A:LEU:HA	4	2.19
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	18	2.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	15	2.19
(1,1600)	1:97:A:LEU:HD11	1:124:A:GLU:HG2	9	2.18
(1,1600)	1:97:A:LEU:HD12	1:124:A:GLU:HG2	9	2.18
(1,1600)	1:97:A:LEU:HD13	1:124:A:GLU:HG2	9	2.18
(1,1600)	1:97:A:LEU:HD21	1:124:A:GLU:HG2	9	2.18
(1,1600)	1:97:A:LEU:HD22	1:124:A:GLU:HG2	9	2.18
(1,1600)	1:97:A:LEU:HD23	1:124:A:GLU:HG2	9	2.18
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	1	2.18
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG21	3	2.18
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG22	3	2.18
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG23	3	2.18
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	18	2.18
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	13	2.18
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	4	2.17
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	4	2.17
(1,688)	1:83:A:TRP:HD1	1:98:A:PHE:HD2	12	2.17
(1,673)	1:52:A:GLY:HA3	1:123:A:PHE:HD1	11	2.17
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	1	2.17
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD11	14	2.17
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD12	14	2.17
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD13	14	2.17
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	7	2.17
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	10	2.17
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB2	15	2.16
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB3	15	2.16
(1,1311)	1:81:A:LYS:HE3	1:85:A:GLN:HE22	3	2.16
(1,688)	1:83:A:TRP:HD1	1:98:A:PHE:HD2	8	2.16
(1,688)	1:83:A:TRP:HD1	1:98:A:PHE:HD2	14	2.16
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	6	2.15
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	9	2.15
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	9	2.15
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	9	2.15
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	18	2.15
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	18	2.15
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	18	2.15
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	13	2.15
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	2	2.14
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	2	2.14
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	20	2.13
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	20	2.13
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	4	2.13
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	4	2.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	1	2.13
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	1	2.13
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	1	2.13
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	2	2.13
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	2	2.13
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	2	2.13
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	8	2.12
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	8	2.12
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	8	2.12
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	8	2.12
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	8	2.12
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	8	2.12
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	16	2.12
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	16	2.12
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	9	2.12
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	9	2.12
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	10	2.12
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	9	2.12
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	7	2.12
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG21	7	2.12
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG22	7	2.12
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG23	7	2.12
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB2	11	2.11
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB3	11	2.11
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	20	2.11
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	17	2.11
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	17	2.11
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	17	2.11
(1,500)	1:81:A:LYS:HB2	1:104:A:LEU:HA	19	2.11
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	2	2.11
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	10	2.11
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	10	2.11
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	10	2.11
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	16	2.1
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	16	2.1
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	16	2.1
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	16	2.1
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	16	2.1
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	16	2.1
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	16	2.1
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	16	2.1
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	16	2.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	16	2.1
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	16	2.1
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	16	2.1
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	16	2.1
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	16	2.1
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	16	2.1
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	16	2.1
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	16	2.1
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	16	2.1
(1,1309)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	19	2.1
(1,1185)	1:24:A:ALA:HB1	1:103:A:GLN:H	18	2.1
(1,1185)	1:24:A:ALA:HB2	1:103:A:GLN:H	18	2.1
(1,1185)	1:24:A:ALA:HB3	1:103:A:GLN:H	18	2.1
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	4	2.1
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	4	2.1
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	4	2.1
(1,539)	1:102:A:TYR:HE2	1:108:A:GLU:HA	17	2.1
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	12	2.1
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	12	2.1
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	12	2.1
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	18	2.1
(1,896)	1:59:A:GLN:HE21	1:62:A:SER:HB2	2	2.09
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG21	15	2.09
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG22	15	2.09
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG23	15	2.09
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG21	16	2.09
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG22	16	2.09
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG23	16	2.09
(1,673)	1:52:A:GLY:HA3	1:123:A:PHE:HD1	15	2.08
(1,582)	1:55:A:PRO:HG2	1:120:A:THR:HB	13	2.08
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	18	2.08
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	18	2.08
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	18	2.08
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	20	2.08
(1,149)	1:50:A:TYR:HB2	1:123:A:PHE:HD2	9	2.08
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG21	4	2.08
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG22	4	2.08
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG23	4	2.08
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	1	2.07
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	1	2.07
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	1	2.07
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	1	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	1	2.07
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	1	2.07
(1,857)	1:49:A:HIS:HD2	1:51:A:ASP:H	5	2.07
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	7	2.07
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	7	2.07
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	7	2.07
(1,530)	1:106:A:TYR:HB3	1:111:A:TYR:HD2	4	2.07
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD21	16	2.07
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD22	16	2.07
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD23	16	2.07
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	12	2.07
(1,92)	1:41:A:GLN:HG2	1:44:A:LYS:HG2	19	2.07
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	2	2.07
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	2	2.06
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	20	2.06
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	2	2.06
(1,1543)	1:85:A:GLN:HB2	1:98:A:PHE:HD2	17	2.05
(1,1543)	1:85:A:GLN:HB3	1:98:A:PHE:HD2	17	2.05
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	3	2.05
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	13	2.05
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	13	2.05
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	13	2.05
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	5	2.05
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	19	2.04
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	4	2.04
(1,582)	1:55:A:PRO:HG2	1:120:A:THR:HB	7	2.04
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	17	2.04
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	17	2.04
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	17	2.04
(1,856)	1:51:A:ASP:H	1:123:A:PHE:HD2	10	2.03
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	7	2.03
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	7	2.03
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	7	2.03
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	13	2.03
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	13	2.03
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	13	2.03
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	16	2.03
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG2	9	2.02
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG3	9	2.02
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	17	2.02
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	16	2.02
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	16	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	16	2.02
(1,395)	1:40:A:PRO:HG2	1:88:A:ALA:HA	7	2.02
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	3	2.02
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	3	2.02
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	3	2.02
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	16	2.02
(1,1310)	1:81:A:LYS:HE2	1:85:A:GLN:HE22	15	2.01
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	14	2.01
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG21	7	2.01
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG22	7	2.01
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG23	7	2.01
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	13	2.0
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	16	2.0
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	16	2.0
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	16	2.0
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	19	2.0
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	19	2.0
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	19	2.0
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	13	2.0
(1,148)	1:50:A:TYR:HB3	1:123:A:PHE:HD2	7	2.0
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	5	2.0
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	3	1.99
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	3	1.99
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	3	1.99
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	3	1.99
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	3	1.99
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	3	1.99
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	4	1.99
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	4	1.99
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	4	1.99
(1,1310)	1:81:A:LYS:HE2	1:85:A:GLN:HE22	4	1.98
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	15	1.98
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	10	1.98
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	3	1.98
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	1	1.98
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	1	1.98
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	1	1.98
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	1	1.98
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	19	1.98
(1,165)	1:53:A:ARG:HG2	1:60:A:PHE:H	13	1.98
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	1	1.98
(1,76)	1:38:A:THR:HB	1:40:A:PRO:HD3	8	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	2	1.98
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	2	1.98
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	2	1.98
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	16	1.97
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	16	1.97
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	16	1.97
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	16	1.97
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	16	1.97
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	16	1.97
(1,1309)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	8	1.97
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	3	1.97
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	3	1.97
(1,582)	1:55:A:PRO:HG2	1:120:A:THR:HB	15	1.97
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD11	5	1.97
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD12	5	1.97
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD13	5	1.97
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	9	1.97
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	9	1.97
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	9	1.97
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	5	1.97
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	17	1.96
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	17	1.96
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	17	1.96
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	17	1.96
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	17	1.96
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	17	1.96
(1,1111)	1:38:A:THR:HG21	1:92:A:LEU:H	7	1.96
(1,1111)	1:38:A:THR:HG22	1:92:A:LEU:H	7	1.96
(1,1111)	1:38:A:THR:HG23	1:92:A:LEU:H	7	1.96
(1,953)	1:49:A:HIS:HE1	1:68:A:LYS:H	3	1.96
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	4	1.96
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	4	1.96
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	4	1.96
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	3	1.96
(1,1624)	1:108:A:GLU:HG2	1:118:A:LYS:HG2	7	1.95
(1,1624)	1:108:A:GLU:HG3	1:118:A:LYS:HG2	7	1.95
(1,1600)	1:97:A:LEU:HD11	1:124:A:GLU:HG2	8	1.95
(1,1600)	1:97:A:LEU:HD12	1:124:A:GLU:HG2	8	1.95
(1,1600)	1:97:A:LEU:HD13	1:124:A:GLU:HG2	8	1.95
(1,1600)	1:97:A:LEU:HD21	1:124:A:GLU:HG2	8	1.95
(1,1600)	1:97:A:LEU:HD22	1:124:A:GLU:HG2	8	1.95
(1,1600)	1:97:A:LEU:HD23	1:124:A:GLU:HG2	8	1.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1600)	1:97:A:LEU:HD11	1:124:A:GLU:HG2	19	1.95
(1,1600)	1:97:A:LEU:HD12	1:124:A:GLU:HG2	19	1.95
(1,1600)	1:97:A:LEU:HD13	1:124:A:GLU:HG2	19	1.95
(1,1600)	1:97:A:LEU:HD21	1:124:A:GLU:HG2	19	1.95
(1,1600)	1:97:A:LEU:HD22	1:124:A:GLU:HG2	19	1.95
(1,1600)	1:97:A:LEU:HD23	1:124:A:GLU:HG2	19	1.95
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	20	1.95
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	20	1.95
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	20	1.95
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	20	1.95
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	20	1.95
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	20	1.95
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG21	16	1.95
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG22	16	1.95
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG23	16	1.95
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	10	1.95
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	10	1.95
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	10	1.95
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	11	1.95
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	13	1.95
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	13	1.95
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	13	1.95
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD11	9	1.95
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD12	9	1.95
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD13	9	1.95
(1,177)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	20	1.95
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	12	1.95
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	12	1.95
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	12	1.95
(1,1625)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	7	1.94
(1,1625)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	7	1.94
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB2	7	1.94
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB3	7	1.94
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB2	7	1.94
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB3	7	1.94
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	10	1.94
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	10	1.94
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG11	13	1.94
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG12	13	1.94
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG13	13	1.94
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG21	13	1.94
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG22	13	1.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG23	13	1.94
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG11	13	1.94
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG12	13	1.94
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG13	13	1.94
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG21	13	1.94
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG22	13	1.94
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG23	13	1.94
(1,673)	1:52:A:GLY:HA3	1:123:A:PHE:HD1	16	1.94
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG21	3	1.94
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG22	3	1.94
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG23	3	1.94
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	7	1.94
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	2	1.94
(1,547)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	18	1.94
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	9	1.94
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	9	1.94
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	9	1.94
(1,149)	1:50:A:TYR:HB2	1:123:A:PHE:HD2	3	1.94
(1,148)	1:50:A:TYR:HB3	1:123:A:PHE:HD2	12	1.94
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG2	12	1.93
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG3	12	1.93
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	11	1.93
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	15	1.93
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	12	1.93
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	4	1.93
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	4	1.93
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	4	1.93
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	5	1.93
(1,177)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	16	1.93
(1,75)	1:38:A:THR:HB	1:40:A:PRO:HG3	18	1.93
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	6	1.93
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	6	1.93
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	6	1.93
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE2	11	1.92
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE3	11	1.92
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE2	11	1.92
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE3	11	1.92
(1,688)	1:83:A:TRP:HD1	1:98:A:PHE:HD2	9	1.92
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	1	1.92
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	2	1.91
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	2	1.91
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	2	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	2	1.91
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	2	1.91
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	2	1.91
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	7	1.91
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	7	1.91
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	7	1.91
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	7	1.91
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	7	1.91
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	7	1.91
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB2	13	1.91
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB3	13	1.91
(1,1311)	1:81:A:LYS:HE3	1:85:A:GLN:HE22	2	1.91
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	13	1.91
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	13	1.91
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	13	1.91
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	1	1.91
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	1	1.91
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	1	1.91
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	6	1.91
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	4	1.91
(1,547)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	14	1.91
(1,176)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	10	1.91
(1,165)	1:53:A:ARG:HG2	1:60:A:PHE:H	4	1.91
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	12	1.9
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	12	1.9
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	12	1.9
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	12	1.9
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	12	1.9
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	12	1.9
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	14	1.9
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	14	1.9
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	16	1.9
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	16	1.9
(1,1219)	1:111:A:TYR:H	1:115:A:ILE:HB	15	1.9
(1,857)	1:49:A:HIS:HD2	1:51:A:ASP:H	20	1.9
(1,744)	1:26:A:LEU:H	1:27:A:GLU:HG3	15	1.9
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	3	1.9
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	9	1.9
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD11	16	1.9
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD12	16	1.9
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD13	16	1.9
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	12	1.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	1	1.9
(1,148)	1:50:A:TYR:HB3	1:123:A:PHE:HD2	4	1.9
(1,134)	1:48:A:VAL:HG21	1:50:A:TYR:HD1	1	1.9
(1,134)	1:48:A:VAL:HG22	1:50:A:TYR:HD1	1	1.9
(1,134)	1:48:A:VAL:HG23	1:50:A:TYR:HD1	1	1.9
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	7	1.9
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	7	1.9
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	7	1.9
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	8	1.89
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	8	1.89
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	8	1.89
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	8	1.89
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	8	1.89
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	8	1.89
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA2	20	1.89
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	20	1.89
(1,688)	1:83:A:TRP:HD1	1:98:A:PHE:HD2	10	1.89
(1,685)	1:102:A:TYR:HE2	1:108:A:GLU:HG2	19	1.89
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	4	1.89
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	14	1.89
(1,500)	1:81:A:LYS:HB2	1:104:A:LEU:HA	3	1.89
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD21	4	1.89
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD22	4	1.89
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD23	4	1.89
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	4	1.89
(1,146)	1:49:A:HIS:HD2	1:50:A:TYR:HA	13	1.89
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	9	1.89
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	13	1.89
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	13	1.89
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	13	1.89
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	1	1.88
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	1	1.88
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	19	1.88
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	19	1.88
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB2	10	1.88
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB3	10	1.88
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	9	1.88
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	17	1.88
(1,1185)	1:24:A:ALA:HB1	1:103:A:GLN:H	14	1.88
(1,1185)	1:24:A:ALA:HB2	1:103:A:GLN:H	14	1.88
(1,1185)	1:24:A:ALA:HB3	1:103:A:GLN:H	14	1.88
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	11	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	14	1.88
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	14	1.88
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	14	1.88
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD21	17	1.88
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD22	17	1.88
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD23	17	1.88
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD11	3	1.88
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD12	3	1.88
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD13	3	1.88
(1,177)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	14	1.88
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG11	2	1.87
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG12	2	1.87
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG13	2	1.87
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG21	2	1.87
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG22	2	1.87
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG23	2	1.87
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG11	2	1.87
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG12	2	1.87
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG13	2	1.87
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG21	2	1.87
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG22	2	1.87
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG23	2	1.87
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	15	1.87
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	15	1.87
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	15	1.87
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	15	1.87
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	15	1.87
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	15	1.87
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	15	1.87
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	15	1.87
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	15	1.87
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	15	1.87
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	15	1.87
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	15	1.87
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	15	1.87
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	15	1.87
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	15	1.87
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	15	1.87
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	15	1.87
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	15	1.87
(1,744)	1:26:A:LEU:H	1:27:A:GLU:HG3	3	1.87
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	9	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	9	1.87
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	9	1.87
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	5	1.87
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	5	1.87
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	5	1.87
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	9	1.87
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	14	1.87
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	10	1.87
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	10	1.87
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	10	1.87
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	1	1.87
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	10	1.87
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	14	1.87
(1,199)	1:59:A:GLN:HG3	1:61:A:ASP:H	20	1.87
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG11	1	1.86
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG12	1	1.86
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG13	1	1.86
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG21	1	1.86
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG22	1	1.86
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG23	1	1.86
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	6	1.86
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	6	1.86
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	6	1.86
(1,500)	1:81:A:LYS:HB2	1:104:A:LEU:HA	16	1.86
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD11	10	1.86
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD12	10	1.86
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD13	10	1.86
(1,163)	1:53:A:ARG:HG3	1:59:A:GLN:H	12	1.86
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	2	1.86
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	15	1.86
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG21	20	1.86
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG22	20	1.86
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG23	20	1.86
(1,695)	1:83:A:TRP:HZ2	1:123:A:PHE:HD1	9	1.85
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	13	1.85
(1,611)	1:123:A:PHE:H	1:124:A:GLU:HG3	9	1.85
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	13	1.85
(1,582)	1:55:A:PRO:HG2	1:120:A:THR:HB	18	1.85
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	19	1.85
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	6	1.85
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	3	1.84
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	3	1.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	3	1.84
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	3	1.84
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	3	1.84
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	3	1.84
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	17	1.84
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	17	1.84
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	17	1.84
(1,546)	1:108:A:GLU:HG3	1:118:A:LYS:HG2	7	1.84
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD21	8	1.84
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD22	8	1.84
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD23	8	1.84
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	8	1.84
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	8	1.84
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	8	1.84
(1,500)	1:81:A:LYS:HB2	1:104:A:LEU:HA	5	1.84
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG21	7	1.84
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG22	7	1.84
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG23	7	1.84
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	18	1.84
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	12	1.83
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	12	1.83
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	2	1.83
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	2	1.83
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	2	1.83
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	2	1.83
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	2	1.83
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	2	1.83
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	2	1.83
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	2	1.83
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	2	1.83
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	2	1.83
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	2	1.83
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	2	1.83
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	2	1.83
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	2	1.83
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	2	1.83
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	2	1.83
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	2	1.83
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	2	1.83
(1,682)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	2	1.83
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	3	1.83
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	11	1.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	11	1.83
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	11	1.83
(1,149)	1:50:A:TYR:HB2	1:123:A:PHE:HD2	20	1.83
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	17	1.82
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	17	1.82
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	17	1.82
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	17	1.82
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	17	1.82
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	17	1.82
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	13	1.82
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	13	1.82
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA2	10	1.82
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	10	1.82
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG21	16	1.82
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG22	16	1.82
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG23	16	1.82
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	10	1.82
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	13	1.82
(1,148)	1:50:A:TYR:HB3	1:123:A:PHE:HD2	1	1.82
(1,146)	1:49:A:HIS:HD2	1:50:A:TYR:HA	5	1.82
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	13	1.81
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	13	1.81
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	13	1.81
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	13	1.81
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	13	1.81
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	13	1.81
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG11	16	1.81
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG12	16	1.81
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG13	16	1.81
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG21	16	1.81
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG22	16	1.81
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG23	16	1.81
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	15	1.81
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	15	1.81
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	15	1.81
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	15	1.81
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	15	1.81
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	15	1.81
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	1	1.81
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	15	1.81
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	15	1.81
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	15	1.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	9	1.81
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	2	1.81
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	2	1.81
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	2	1.81
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	4	1.81
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	10	1.81
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	10	1.81
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	10	1.81
(1,422)	1:38:A:THR:HG21	1:91:A:THR:HA	2	1.81
(1,422)	1:38:A:THR:HG22	1:91:A:THR:HA	2	1.81
(1,422)	1:38:A:THR:HG23	1:91:A:THR:HA	2	1.81
(1,191)	1:54:A:PHE:HD1	1:58:A:LYS:HD3	12	1.81
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	4	1.8
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	4	1.8
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	4	1.8
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	4	1.8
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	4	1.8
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	4	1.8
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	16	1.8
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	16	1.8
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	16	1.8
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	4	1.8
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG21	13	1.8
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG22	13	1.8
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG23	13	1.8
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	8	1.8
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	8	1.8
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	8	1.8
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD2	19	1.79
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD3	19	1.79
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD2	19	1.79
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD3	19	1.79
(1,1311)	1:81:A:LYS:HE3	1:85:A:GLN:HE22	10	1.79
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	19	1.79
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	19	1.79
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	19	1.79
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	6	1.79
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG21	6	1.79
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG22	6	1.79
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG23	6	1.79
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	18	1.78
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	18	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	7	1.78
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	16	1.78
(1,500)	1:81:A:LYS:HB2	1:104:A:LEU:HA	20	1.78
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	7	1.77
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	7	1.77
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	7	1.77
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	7	1.77
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	7	1.77
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	7	1.77
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG11	3	1.77
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG12	3	1.77
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG13	3	1.77
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG21	3	1.77
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG22	3	1.77
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG23	3	1.77
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	1	1.77
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	1	1.77
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	1	1.77
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	1	1.77
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	1	1.77
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	1	1.77
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	8	1.77
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	8	1.77
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	8	1.77
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	8	1.77
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	8	1.77
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	8	1.77
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	8	1.77
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	8	1.77
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	8	1.77
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	8	1.77
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	8	1.77
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	8	1.77
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	8	1.77
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	8	1.77
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	8	1.77
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	8	1.77
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	8	1.77
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	8	1.77
(1,1069)	1:86:A:GLY:H	1:98:A:PHE:HD2	17	1.77
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG21	1	1.77
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG22	1	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG23	1	1.77
(1,789)	1:38:A:THR:H	1:91:A:THR:HG21	7	1.77
(1,789)	1:38:A:THR:H	1:91:A:THR:HG22	7	1.77
(1,789)	1:38:A:THR:H	1:91:A:THR:HG23	7	1.77
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	15	1.77
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	15	1.77
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	15	1.77
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	16	1.77
(1,539)	1:102:A:TYR:HE2	1:108:A:GLU:HA	7	1.77
(1,500)	1:81:A:LYS:HB2	1:104:A:LEU:HA	14	1.77
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG21	4	1.77
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG22	4	1.77
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG23	4	1.77
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	4	1.77
(1,688)	1:83:A:TRP:HD1	1:98:A:PHE:HD2	3	1.76
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	18	1.76
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	6	1.76
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	15	1.76
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	15	1.76
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	15	1.76
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	9	1.76
(1,190)	1:54:A:PHE:HD1	1:58:A:LYS:HD2	4	1.76
(1,75)	1:38:A:THR:HB	1:40:A:PRO:HG3	1	1.76
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	13	1.76
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	13	1.76
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	13	1.76
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	14	1.76
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	14	1.76
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	14	1.76
(1,1299)	1:92:A:LEU:HD11	1:130:A:VAL:H	18	1.75
(1,1299)	1:92:A:LEU:HD12	1:130:A:VAL:H	18	1.75
(1,1299)	1:92:A:LEU:HD13	1:130:A:VAL:H	18	1.75
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	14	1.75
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	11	1.75
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	17	1.75
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	17	1.75
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	17	1.75
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	19	1.75
(1,245)	1:71:A:GLN:HA	1:72:A:PHE:HD1	20	1.75
(1,1323)	1:19:A:PRO:HG2	1:55:A:PRO:HB2	19	1.74
(1,1323)	1:19:A:PRO:HG3	1:55:A:PRO:HB2	19	1.74
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	14	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1195)	1:80:A:ILE:HB	1:105:A:ALA:H	9	1.74
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	20	1.74
(1,696)	1:83:A:TRP:HZ2	1:123:A:PHE:HB3	9	1.74
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	20	1.74
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	20	1.74
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	20	1.74
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	6	1.74
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD21	9	1.74
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD22	9	1.74
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD23	9	1.74
(1,191)	1:54:A:PHE:HD1	1:58:A:LYS:HD3	20	1.74
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	14	1.73
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	14	1.73
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	14	1.73
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	14	1.73
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	14	1.73
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	14	1.73
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG11	1	1.73
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG12	1	1.73
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG13	1	1.73
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG21	1	1.73
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG22	1	1.73
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG23	1	1.73
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG11	1	1.73
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG12	1	1.73
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG13	1	1.73
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG21	1	1.73
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG22	1	1.73
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG23	1	1.73
(1,786)	1:38:A:THR:H	1:91:A:THR:HA	7	1.73
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	12	1.73
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD11	12	1.73
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD12	12	1.73
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD13	12	1.73
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD11	17	1.73
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD12	17	1.73
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD13	17	1.73
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	3	1.73
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	7	1.73
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	16	1.73
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	16	1.73
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	16	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	7	1.72
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	7	1.72
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	7	1.72
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	7	1.72
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	7	1.72
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	7	1.72
(1,685)	1:102:A:TYR:HE2	1:108:A:GLU:HG2	11	1.72
(1,682)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	9	1.72
(1,675)	1:106:A:TYR:HE1	1:111:A:TYR:HB3	19	1.72
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD11	7	1.72
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD12	7	1.72
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD13	7	1.72
(1,176)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	14	1.72
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	11	1.71
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	11	1.71
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB2	12	1.71
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB3	12	1.71
(1,1300)	1:92:A:LEU:HD21	1:130:A:VAL:H	3	1.71
(1,1300)	1:92:A:LEU:HD22	1:130:A:VAL:H	3	1.71
(1,1300)	1:92:A:LEU:HD23	1:130:A:VAL:H	3	1.71
(1,673)	1:52:A:GLY:HA3	1:123:A:PHE:HD1	18	1.71
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	12	1.71
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	12	1.71
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	12	1.71
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	17	1.7
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	17	1.7
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	17	1.7
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	17	1.7
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	17	1.7
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	17	1.7
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD2	19	1.7
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD3	19	1.7
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD2	19	1.7
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD3	19	1.7
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	9	1.7
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG11	16	1.7
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG12	16	1.7
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG13	16	1.7
(1,758)	1:28:A:LYS:HG2	1:30:A:VAL:H	10	1.7
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	16	1.7
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	1	1.7
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	1	1.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	1	1.7
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	9	1.7
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	9	1.7
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	9	1.7
(1,516)	1:81:A:LYS:H	1:105:A:ALA:HA	16	1.7
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD11	8	1.7
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD12	8	1.7
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD13	8	1.7
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD21	3	1.7
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD22	3	1.7
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD23	3	1.7
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	10	1.7
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	5	1.7
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	12	1.7
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	17	1.7
(1,75)	1:38:A:THR:HB	1:40:A:PRO:HG3	12	1.7
(1,28)	1:27:A:GLU:HG2	1:99:A:THR:HB	18	1.7
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	5	1.69
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	5	1.69
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	5	1.69
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	5	1.69
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	5	1.69
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	5	1.69
(1,1386)	1:41:A:GLN:H	1:44:A:LYS:HG2	3	1.69
(1,1386)	1:41:A:GLN:H	1:44:A:LYS:HG3	3	1.69
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG11	16	1.69
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG12	16	1.69
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG13	16	1.69
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG21	16	1.69
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG22	16	1.69
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG23	16	1.69
(1,1325)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	14	1.69
(1,1325)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	14	1.69
(1,1310)	1:81:A:LYS:HE2	1:85:A:GLN:HE22	8	1.69
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	11	1.69
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	11	1.69
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	11	1.69
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	9	1.69
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	9	1.69
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	9	1.69
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	2	1.69
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	2	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	2	1.69
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD11	3	1.69
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD12	3	1.69
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD13	3	1.69
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	7	1.69
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	7	1.69
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	7	1.69
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	2	1.69
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	8	1.69
(1,1111)	1:38:A:THR:HG21	1:92:A:LEU:H	2	1.68
(1,1111)	1:38:A:THR:HG22	1:92:A:LEU:H	2	1.68
(1,1111)	1:38:A:THR:HG23	1:92:A:LEU:H	2	1.68
(1,959)	1:49:A:HIS:HD2	1:70:A:PHE:H	4	1.68
(1,611)	1:123:A:PHE:H	1:124:A:GLU:HG3	19	1.68
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	12	1.68
(1,205)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	8	1.68
(1,146)	1:49:A:HIS:HD2	1:50:A:TYR:HA	20	1.68
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	10	1.68
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	10	1.68
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	10	1.68
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG11	13	1.68
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG12	13	1.68
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG13	13	1.68
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	4	1.67
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	4	1.67
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	4	1.67
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	4	1.67
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	4	1.67
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	4	1.67
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	7	1.67
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	7	1.67
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	7	1.67
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	7	1.67
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	7	1.67
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	7	1.67
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	5	1.67
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	10	1.67
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	10	1.67
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	10	1.67
(1,364)	1:80:A:ILE:HD11	1:83:A:TRP:HA	9	1.67
(1,364)	1:80:A:ILE:HD12	1:83:A:TRP:HA	9	1.67
(1,364)	1:80:A:ILE:HD13	1:83:A:TRP:HA	9	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	20	1.67
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	20	1.67
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	20	1.67
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	13	1.67
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG11	5	1.66
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG12	5	1.66
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG13	5	1.66
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG21	5	1.66
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG22	5	1.66
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG23	5	1.66
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG11	5	1.66
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG12	5	1.66
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG13	5	1.66
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG21	5	1.66
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG22	5	1.66
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG23	5	1.66
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG21	11	1.66
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG22	11	1.66
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG23	11	1.66
(1,547)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	7	1.66
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD21	6	1.66
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD22	6	1.66
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD23	6	1.66
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	18	1.66
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	13	1.66
(1,167)	1:53:A:ARG:HG2	1:54:A:PHE:HD1	1	1.66
(1,134)	1:48:A:VAL:HG21	1:50:A:TYR:HD1	4	1.66
(1,134)	1:48:A:VAL:HG22	1:50:A:TYR:HD1	4	1.66
(1,134)	1:48:A:VAL:HG23	1:50:A:TYR:HD1	4	1.66
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	7	1.66
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	11	1.65
(1,953)	1:49:A:HIS:HE1	1:68:A:LYS:H	20	1.65
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	4	1.65
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	4	1.65
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	4	1.65
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	16	1.65
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	1	1.65
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	1	1.65
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	1	1.65
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	1	1.65
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	1	1.65
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	1	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	6	1.65
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG21	11	1.65
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG22	11	1.65
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG23	11	1.65
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	3	1.64
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	3	1.64
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	3	1.64
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	3	1.64
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	3	1.64
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	3	1.64
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	4	1.64
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	4	1.64
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	4	1.64
(1,706)	1:49:A:HIS:HE1	1:69:A:PRO:HB3	1	1.64
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	12	1.64
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	12	1.64
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	12	1.64
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	17	1.64
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	17	1.64
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	17	1.64
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	2	1.64
(1,594)	1:122:A:VAL:HA	1:123:A:PHE:HD1	10	1.64
(1,500)	1:81:A:LYS:HB2	1:104:A:LEU:HA	11	1.64
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	17	1.64
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	17	1.64
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	17	1.64
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	19	1.64
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	18	1.64
(1,167)	1:53:A:ARG:HG2	1:54:A:PHE:HD1	8	1.64
(1,148)	1:50:A:TYR:HB3	1:123:A:PHE:HD2	14	1.64
(1,134)	1:48:A:VAL:HG21	1:50:A:TYR:HD1	6	1.64
(1,134)	1:48:A:VAL:HG22	1:50:A:TYR:HD1	6	1.64
(1,134)	1:48:A:VAL:HG23	1:50:A:TYR:HD1	6	1.64
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	4	1.64
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	7	1.63
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	7	1.63
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE2	11	1.63
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE3	11	1.63
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE2	11	1.63
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE3	11	1.63
(1,1333)	1:24:A:ALA:HB1	1:103:A:GLN:HG2	8	1.63
(1,1333)	1:24:A:ALA:HB1	1:103:A:GLN:HG3	8	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1333)	1:24:A:ALA:HB2	1:103:A:GLN:HG2	8	1.63
(1,1333)	1:24:A:ALA:HB2	1:103:A:GLN:HG3	8	1.63
(1,1333)	1:24:A:ALA:HB3	1:103:A:GLN:HG2	8	1.63
(1,1333)	1:24:A:ALA:HB3	1:103:A:GLN:HG3	8	1.63
(1,1328)	1:19:A:PRO:HG2	1:56:A:ASP:HA	19	1.63
(1,1328)	1:19:A:PRO:HG3	1:56:A:ASP:HA	19	1.63
(1,1311)	1:81:A:LYS:HE3	1:85:A:GLN:HE22	18	1.63
(1,1310)	1:81:A:LYS:HE2	1:85:A:GLN:HE22	2	1.63
(1,1219)	1:111:A:TYR:H	1:115:A:ILE:HB	13	1.63
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	17	1.63
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	6	1.63
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	4	1.63
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	4	1.63
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	4	1.63
(1,547)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	12	1.63
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	3	1.63
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	11	1.62
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	11	1.62
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	11	1.62
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	11	1.62
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	11	1.62
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	11	1.62
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG2	4	1.62
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG3	4	1.62
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	3	1.62
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	3	1.62
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	3	1.62
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	14	1.62
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	14	1.62
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	14	1.62
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	13	1.62
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	13	1.62
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	13	1.62
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	8	1.62
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	8	1.62
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	8	1.62
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD11	19	1.62
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD12	19	1.62
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD13	19	1.62
(1,191)	1:54:A:PHE:HD1	1:58:A:LYS:HD3	3	1.62
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	18	1.62
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	16	1.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	16	1.62
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	16	1.62
(1,1475)	1:59:A:GLN:HG2	1:61:A:ASP:H	20	1.61
(1,1475)	1:59:A:GLN:HG3	1:61:A:ASP:H	20	1.61
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG2	1	1.61
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG3	1	1.61
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG11	15	1.61
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG12	15	1.61
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG13	15	1.61
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG21	15	1.61
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG22	15	1.61
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG23	15	1.61
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG11	15	1.61
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG12	15	1.61
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG13	15	1.61
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG21	15	1.61
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG22	15	1.61
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG23	15	1.61
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	14	1.61
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	14	1.61
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	14	1.61
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	14	1.61
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	14	1.61
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	14	1.61
(1,1324)	1:19:A:PRO:HG2	1:55:A:PRO:HG2	19	1.61
(1,1324)	1:19:A:PRO:HG3	1:55:A:PRO:HG2	19	1.61
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	13	1.61
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	8	1.61
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	6	1.6
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	6	1.6
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	6	1.6
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	7	1.6
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	7	1.6
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	7	1.6
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	12	1.6
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	12	1.6
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	12	1.6
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	4	1.6
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	4	1.6
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	4	1.6
(1,134)	1:48:A:VAL:HG21	1:50:A:TYR:HD1	15	1.6
(1,134)	1:48:A:VAL:HG22	1:50:A:TYR:HD1	15	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	1:48:A:VAL:HG23	1:50:A:TYR:HD1	15	1.6
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB2	5	1.59
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB3	5	1.59
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	7	1.59
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	7	1.59
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	7	1.59
(1,758)	1:28:A:LYS:HG2	1:30:A:VAL:H	11	1.59
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG21	15	1.59
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG22	15	1.59
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG23	15	1.59
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	2	1.59
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	2	1.59
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	2	1.59
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	7	1.59
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	5	1.59
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	10	1.58
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	10	1.58
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	10	1.58
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	10	1.58
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	10	1.58
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	10	1.58
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	3	1.58
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	3	1.58
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	3	1.58
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	3	1.58
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	3	1.58
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	3	1.58
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	3	1.58
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	3	1.58
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	3	1.58
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	3	1.58
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	3	1.58
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	3	1.58
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	3	1.58
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	3	1.58
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	3	1.58
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	3	1.58
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	3	1.58
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	3	1.58
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	13	1.58
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	13	1.58
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	13	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	13	1.58
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	13	1.58
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	13	1.58
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	13	1.58
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	13	1.58
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	13	1.58
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	13	1.58
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	13	1.58
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	13	1.58
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	13	1.58
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	13	1.58
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	13	1.58
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	13	1.58
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	13	1.58
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	13	1.58
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	9	1.58
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	9	1.58
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	9	1.58
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	9	1.58
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	9	1.58
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	9	1.58
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	18	1.58
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	18	1.58
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	18	1.58
(1,167)	1:53:A:ARG:HG2	1:54:A:PHE:HD1	9	1.58
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	3	1.58
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	12	1.58
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	12	1.58
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	12	1.58
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	1	1.58
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	1	1.58
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	1	1.58
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	1	1.57
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	1	1.57
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	1	1.57
(1,758)	1:28:A:LYS:HG2	1:30:A:VAL:H	19	1.57
(1,705)	1:49:A:HIS:HE1	1:64:A:ARG:HA	13	1.57
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	5	1.57
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	5	1.57
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	5	1.57
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	12	1.57
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	10	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	15	1.57
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	6	1.57
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	3	1.56
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	3	1.56
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	3	1.56
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	3	1.56
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	3	1.56
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	3	1.56
(1,744)	1:26:A:LEU:H	1:27:A:GLU:HG3	1	1.56
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	16	1.56
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	16	1.56
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	16	1.56
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	20	1.56
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	20	1.56
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	20	1.56
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	19	1.56
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	19	1.56
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	19	1.56
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	15	1.56
(1,225)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	14	1.56
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	11	1.56
(1,165)	1:53:A:ARG:HG2	1:60:A:PHE:H	10	1.56
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	18	1.56
(1,134)	1:48:A:VAL:HG21	1:50:A:TYR:HD1	2	1.56
(1,134)	1:48:A:VAL:HG22	1:50:A:TYR:HD1	2	1.56
(1,134)	1:48:A:VAL:HG23	1:50:A:TYR:HD1	2	1.56
(1,1543)	1:85:A:GLN:HB2	1:98:A:PHE:HD2	3	1.55
(1,1543)	1:85:A:GLN:HB3	1:98:A:PHE:HD2	3	1.55
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	1	1.55
(1,673)	1:52:A:GLY:HA3	1:123:A:PHE:HD1	19	1.55
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	8	1.55
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	8	1.55
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	8	1.55
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	3	1.55
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	3	1.55
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	3	1.55
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	3	1.55
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	4	1.55
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	3	1.55
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	3	1.55
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	3	1.55
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	17	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	12	1.54
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	12	1.54
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	12	1.54
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	12	1.54
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	12	1.54
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	12	1.54
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	18	1.54
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	18	1.54
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	18	1.54
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	18	1.54
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	18	1.54
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	18	1.54
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	1	1.54
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	1	1.54
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	1	1.54
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	1	1.54
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	1	1.54
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	1	1.54
(1,1173)	1:102:A:TYR:H	1:102:A:TYR:HE1	4	1.54
(1,1173)	1:102:A:TYR:H	1:102:A:TYR:HE1	17	1.54
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	11	1.54
(1,673)	1:52:A:GLY:HA3	1:123:A:PHE:HD1	8	1.54
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	10	1.54
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	10	1.54
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	10	1.54
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	14	1.54
(1,582)	1:55:A:PRO:HG2	1:120:A:THR:HB	6	1.54
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	16	1.54
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	20	1.54
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	9	1.54
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	9	1.54
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	9	1.54
(1,94)	1:41:A:GLN:HG2	1:44:A:LYS:HG3	19	1.54
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	10	1.54
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	15	1.54
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	15	1.54
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	15	1.54
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	12	1.53
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	12	1.53
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	12	1.53
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	12	1.53
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	12	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	12	1.53
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG2	11	1.53
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG3	11	1.53
(1,1219)	1:111:A:TYR:H	1:115:A:ILE:HB	1	1.53
(1,959)	1:49:A:HIS:HD2	1:70:A:PHE:H	16	1.53
(1,594)	1:122:A:VAL:HA	1:123:A:PHE:HD1	20	1.53
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	16	1.53
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	16	1.53
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	16	1.53
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	16	1.53
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	16	1.53
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	16	1.53
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	16	1.53
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	16	1.53
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	16	1.53
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	8	1.53
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	13	1.53
(1,194)	1:53:A:ARG:HG2	1:59:A:GLN:HA	13	1.53
(1,75)	1:38:A:THR:HB	1:40:A:PRO:HG3	17	1.53
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	15	1.52
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	15	1.52
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	15	1.52
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	15	1.52
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	15	1.52
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	15	1.52
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	1	1.52
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	1	1.52
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG11	19	1.52
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG12	19	1.52
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG13	19	1.52
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG21	19	1.52
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG22	19	1.52
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG23	19	1.52
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG11	19	1.52
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG12	19	1.52
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG13	19	1.52
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG21	19	1.52
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG22	19	1.52
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG23	19	1.52
(1,1235)	1:55:A:PRO:HG3	1:120:A:THR:H	12	1.52
(1,911)	1:53:A:ARG:HD2	1:57:A:GLY:H	2	1.52
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	20	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	20	1.52
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	20	1.52
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG11	13	1.52
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG12	13	1.52
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG13	13	1.52
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	4	1.52
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD21	1	1.52
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD22	1	1.52
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD23	1	1.52
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	12	1.52
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	12	1.52
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	12	1.52
(1,415)	1:90:A:MET:HE1	1:94:A:GLU:HA	4	1.52
(1,415)	1:90:A:MET:HE2	1:94:A:GLU:HA	4	1.52
(1,415)	1:90:A:MET:HE3	1:94:A:GLU:HA	4	1.52
(1,185)	1:53:A:ARG:HB3	1:57:A:GLY:HA2	3	1.52
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	6	1.52
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	6	1.52
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	6	1.52
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	6	1.52
(1,134)	1:48:A:VAL:HG21	1:50:A:TYR:HD1	8	1.52
(1,134)	1:48:A:VAL:HG22	1:50:A:TYR:HD1	8	1.52
(1,134)	1:48:A:VAL:HG23	1:50:A:TYR:HD1	8	1.52
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	16	1.52
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	16	1.52
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	16	1.52
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG11	2	1.52
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG12	2	1.52
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG13	2	1.52
(1,28)	1:27:A:GLU:HG2	1:99:A:THR:HB	4	1.52
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	11	1.52
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG11	11	1.51
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG12	11	1.51
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG13	11	1.51
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG21	11	1.51
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG22	11	1.51
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG23	11	1.51
(1,1328)	1:19:A:PRO:HG2	1:56:A:ASP:HA	13	1.51
(1,1328)	1:19:A:PRO:HG3	1:56:A:ASP:HA	13	1.51
(1,1325)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	20	1.51
(1,1325)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	20	1.51
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	14	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	14	1.51
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	14	1.51
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	14	1.51
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG11	2	1.51
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG12	2	1.51
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG13	2	1.51
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	15	1.51
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	15	1.51
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	15	1.51
(1,518)	1:80:A:ILE:HA	1:105:A:ALA:HA	16	1.51
(1,462)	1:97:A:LEU:HD21	1:123:A:PHE:H	14	1.51
(1,462)	1:97:A:LEU:HD22	1:123:A:PHE:H	14	1.51
(1,462)	1:97:A:LEU:HD23	1:123:A:PHE:H	14	1.51
(1,194)	1:53:A:ARG:HG2	1:59:A:GLN:HA	4	1.51
(1,167)	1:53:A:ARG:HG2	1:54:A:PHE:HD1	10	1.51
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	11	1.51
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	11	1.51
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	11	1.51
(1,3)	1:28:A:LYS:HG3	1:30:A:VAL:H	3	1.51
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	8	1.5
(1,594)	1:122:A:VAL:HA	1:123:A:PHE:HD1	4	1.5
(1,594)	1:122:A:VAL:HA	1:123:A:PHE:HD1	12	1.5
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	8	1.5
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	11	1.5
(1,1333)	1:24:A:ALA:HB1	1:103:A:GLN:HG2	18	1.49
(1,1333)	1:24:A:ALA:HB1	1:103:A:GLN:HG3	18	1.49
(1,1333)	1:24:A:ALA:HB2	1:103:A:GLN:HG2	18	1.49
(1,1333)	1:24:A:ALA:HB2	1:103:A:GLN:HG3	18	1.49
(1,1333)	1:24:A:ALA:HB3	1:103:A:GLN:HG2	18	1.49
(1,1333)	1:24:A:ALA:HB3	1:103:A:GLN:HG3	18	1.49
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	17	1.49
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	17	1.49
(1,1306)	1:81:A:LYS:HE2	1:85:A:GLN:HE21	3	1.49
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	1	1.49
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	15	1.49
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	15	1.49
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	15	1.49
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	8	1.49
(1,594)	1:122:A:VAL:HA	1:123:A:PHE:HD1	7	1.49
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	1	1.49
(1,395)	1:40:A:PRO:HG2	1:88:A:ALA:HA	11	1.49
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	3	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	11	1.48
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	11	1.48
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	11	1.48
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	11	1.48
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	11	1.48
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	11	1.48
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	11	1.48
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	11	1.48
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	11	1.48
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	11	1.48
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	11	1.48
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	11	1.48
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	11	1.48
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	11	1.48
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	11	1.48
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	11	1.48
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	11	1.48
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	11	1.48
(1,1310)	1:81:A:LYS:HE2	1:85:A:GLN:HE22	10	1.48
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	15	1.48
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	17	1.48
(1,211)	1:49:A:HIS:HB3	1:64:A:ARG:HA	16	1.48
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	1	1.48
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	1	1.47
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	1	1.47
(1,758)	1:28:A:LYS:HG2	1:30:A:VAL:H	18	1.47
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	19	1.47
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	19	1.47
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	19	1.47
(1,602)	1:100:A:ILE:HD11	1:123:A:PHE:HB3	9	1.47
(1,602)	1:100:A:ILE:HD12	1:123:A:PHE:HB3	9	1.47
(1,602)	1:100:A:ILE:HD13	1:123:A:PHE:HB3	9	1.47
(1,528)	1:80:A:ILE:HG21	1:106:A:TYR:HA	9	1.47
(1,528)	1:80:A:ILE:HG22	1:106:A:TYR:HA	9	1.47
(1,528)	1:80:A:ILE:HG23	1:106:A:TYR:HA	9	1.47
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB1	16	1.47
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB2	16	1.47
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB3	16	1.47
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB1	16	1.47
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB2	16	1.47
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB3	16	1.47
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB1	16	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB2	16	1.47
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB3	16	1.47
(1,522)	1:80:A:ILE:HG21	1:105:A:ALA:HA	9	1.47
(1,522)	1:80:A:ILE:HG22	1:105:A:ALA:HA	9	1.47
(1,522)	1:80:A:ILE:HG23	1:105:A:ALA:HA	9	1.47
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	13	1.47
(1,165)	1:53:A:ARG:HG2	1:60:A:PHE:H	8	1.47
(1,28)	1:27:A:GLU:HG2	1:99:A:THR:HB	10	1.47
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	10	1.47
(1,1655)	1:126:A:GLU:HA	1:128:A:LEU:HD11	9	1.46
(1,1655)	1:126:A:GLU:HA	1:128:A:LEU:HD12	9	1.46
(1,1655)	1:126:A:GLU:HA	1:128:A:LEU:HD13	9	1.46
(1,1655)	1:126:A:GLU:HA	1:128:A:LEU:HD21	9	1.46
(1,1655)	1:126:A:GLU:HA	1:128:A:LEU:HD22	9	1.46
(1,1655)	1:126:A:GLU:HA	1:128:A:LEU:HD23	9	1.46
(1,1543)	1:85:A:GLN:HB2	1:98:A:PHE:HD2	5	1.46
(1,1543)	1:85:A:GLN:HB3	1:98:A:PHE:HD2	5	1.46
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE2	17	1.46
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE3	17	1.46
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE2	17	1.46
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE3	17	1.46
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	14	1.46
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	18	1.46
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	2	1.46
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	2	1.46
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	2	1.46
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA2	15	1.45
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	15	1.45
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE2	19	1.45
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE3	19	1.45
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE2	19	1.45
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE3	19	1.45
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG11	3	1.45
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG12	3	1.45
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG13	3	1.45
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG21	3	1.45
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG22	3	1.45
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG23	3	1.45
(1,1323)	1:19:A:PRO:HG2	1:55:A:PRO:HB2	12	1.45
(1,1323)	1:19:A:PRO:HG3	1:55:A:PRO:HB2	12	1.45
(1,1298)	1:92:A:LEU:HG	1:130:A:VAL:H	15	1.45
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	13	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	13	1.45
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	13	1.45
(1,911)	1:53:A:ARG:HD2	1:57:A:GLY:H	16	1.45
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	18	1.45
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	18	1.45
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	18	1.45
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	19	1.45
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	9	1.45
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	7	1.45
(1,546)	1:108:A:GLU:HG3	1:118:A:LYS:HG2	14	1.45
(1,534)	1:106:A:TYR:HB2	1:111:A:TYR:HD2	8	1.45
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	7	1.45
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	15	1.45
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	15	1.45
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	15	1.45
(1,166)	1:53:A:ARG:HG3	1:60:A:PHE:H	12	1.45
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	5	1.45
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	5	1.45
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	5	1.45
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	17	1.45
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	17	1.45
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	17	1.45
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	3	1.45
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	3	1.45
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	3	1.45
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	19	1.45
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	19	1.45
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	19	1.45
(1,1185)	1:24:A:ALA:HB1	1:103:A:GLN:H	5	1.44
(1,1185)	1:24:A:ALA:HB2	1:103:A:GLN:H	5	1.44
(1,1185)	1:24:A:ALA:HB3	1:103:A:GLN:H	5	1.44
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	4	1.44
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	4	1.44
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	4	1.44
(1,953)	1:49:A:HIS:HE1	1:68:A:LYS:H	7	1.44
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	20	1.44
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	4	1.44
(1,148)	1:50:A:TYR:HB3	1:123:A:PHE:HD2	6	1.44
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG21	7	1.44
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG22	7	1.44
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG23	7	1.44
(1,28)	1:27:A:GLU:HG2	1:99:A:THR:HB	11	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	4	1.43
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	4	1.43
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	4	1.43
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	4	1.43
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	4	1.43
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	4	1.43
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	13	1.43
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	13	1.43
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	13	1.43
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	13	1.43
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	13	1.43
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	13	1.43
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB2	8	1.43
(1,1479)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	8	1.43
(1,1307)	1:81:A:LYS:HE3	1:85:A:GLN:HE21	12	1.43
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	8	1.43
(1,953)	1:49:A:HIS:HE1	1:68:A:LYS:H	12	1.43
(1,953)	1:49:A:HIS:HE1	1:68:A:LYS:H	18	1.43
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	3	1.43
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	15	1.43
(1,686)	1:102:A:TYR:HE2	1:118:A:LYS:HA	4	1.43
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	17	1.43
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	17	1.43
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	17	1.43
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	6	1.43
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	6	1.43
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	6	1.43
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	14	1.43
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	14	1.43
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	14	1.43
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD11	19	1.43
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD12	19	1.43
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD13	19	1.43
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	6	1.43
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	9	1.43
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	13	1.43
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	5	1.43
(1,76)	1:38:A:THR:HB	1:40:A:PRO:HD3	15	1.43
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD11	4	1.42
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD12	4	1.42
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD13	4	1.42
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD21	4	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD22	4	1.42
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD23	4	1.42
(1,911)	1:53:A:ARG:HD2	1:57:A:GLY:H	1	1.42
(1,686)	1:102:A:TYR:HE2	1:118:A:LYS:HA	17	1.42
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	13	1.42
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	13	1.42
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	13	1.42
(1,226)	1:49:A:HIS:HE1	1:67:A:GLY:HA2	10	1.42
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	12	1.42
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD2	9	1.41
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD3	9	1.41
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	6	1.41
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	6	1.41
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	6	1.41
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	6	1.41
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	6	1.41
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	6	1.41
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE2	16	1.41
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE3	16	1.41
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE2	16	1.41
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE3	16	1.41
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	8	1.41
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	8	1.41
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	8	1.41
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	8	1.41
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	8	1.41
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	8	1.41
(1,1219)	1:111:A:TYR:H	1:115:A:ILE:HB	5	1.41
(1,1173)	1:102:A:TYR:H	1:102:A:TYR:HE1	18	1.41
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	13	1.41
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	13	1.41
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	13	1.41
(1,758)	1:28:A:LYS:HG2	1:30:A:VAL:H	16	1.41
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	10	1.41
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	10	1.41
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	10	1.41
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	20	1.41
(1,594)	1:122:A:VAL:HA	1:123:A:PHE:HD1	6	1.41
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	8	1.41
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	8	1.41
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	8	1.41
(1,444)	1:31:A:LEU:HG	1:95:A:LYS:HB3	1	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	5	1.41
(1,206)	1:60:A:PHE:HD1	1:61:A:ASP:HB3	8	1.41
(1,134)	1:48:A:VAL:HG21	1:50:A:TYR:HD1	11	1.41
(1,134)	1:48:A:VAL:HG22	1:50:A:TYR:HD1	11	1.41
(1,134)	1:48:A:VAL:HG23	1:50:A:TYR:HD1	11	1.41
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	9	1.41
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	9	1.41
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	9	1.41
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	19	1.4
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	19	1.4
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	19	1.4
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	19	1.4
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	19	1.4
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	19	1.4
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG11	11	1.4
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG12	11	1.4
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG13	11	1.4
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG21	11	1.4
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG22	11	1.4
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG23	11	1.4
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	1	1.4
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	1	1.4
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	1	1.4
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	5	1.4
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	5	1.4
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	5	1.4
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	20	1.4
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	20	1.4
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	20	1.4
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	3	1.4
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	3	1.4
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	3	1.4
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	16	1.4
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	16	1.4
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	16	1.4
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	4	1.4
(1,611)	1:123:A:PHE:H	1:124:A:GLU:HG3	8	1.4
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	17	1.4
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	17	1.4
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	17	1.4
(1,537)	1:108:A:GLU:HB2	1:118:A:LYS:HG2	6	1.4
(1,516)	1:81:A:LYS:H	1:105:A:ALA:HA	1	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,193)	1:53:A:ARG:HB3	1:59:A:GLN:HA	13	1.4
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	19	1.4
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG2	13	1.39
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG3	13	1.39
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG2	15	1.39
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG3	15	1.39
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG11	7	1.39
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG12	7	1.39
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG13	7	1.39
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG21	7	1.39
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG22	7	1.39
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG23	7	1.39
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG11	7	1.39
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG12	7	1.39
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG13	7	1.39
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG21	7	1.39
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG22	7	1.39
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG23	7	1.39
(1,1323)	1:19:A:PRO:HG2	1:55:A:PRO:HB2	14	1.39
(1,1323)	1:19:A:PRO:HG3	1:55:A:PRO:HB2	14	1.39
(1,1323)	1:19:A:PRO:HG2	1:55:A:PRO:HB2	16	1.39
(1,1323)	1:19:A:PRO:HG3	1:55:A:PRO:HB2	16	1.39
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	1	1.39
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	1	1.39
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	1	1.39
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG21	15	1.39
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG22	15	1.39
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG23	15	1.39
(1,1185)	1:24:A:ALA:HB1	1:103:A:GLN:H	17	1.39
(1,1185)	1:24:A:ALA:HB2	1:103:A:GLN:H	17	1.39
(1,1185)	1:24:A:ALA:HB3	1:103:A:GLN:H	17	1.39
(1,1173)	1:102:A:TYR:H	1:102:A:TYR:HE1	7	1.39
(1,953)	1:49:A:HIS:HE1	1:68:A:LYS:H	6	1.39
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	14	1.39
(1,758)	1:28:A:LYS:HG2	1:30:A:VAL:H	15	1.39
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	2	1.39
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	2	1.39
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	2	1.39
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	3	1.39
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	3	1.39
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	3	1.39
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	2	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	2	1.39
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	2	1.39
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD11	9	1.39
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD12	9	1.39
(1,567)	1:106:A:TYR:HE1	1:115:A:ILE:HD13	9	1.39
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	17	1.39
(1,240)	1:47:A:THR:HG21	1:69:A:PRO:HG3	3	1.39
(1,240)	1:47:A:THR:HG22	1:69:A:PRO:HG3	3	1.39
(1,240)	1:47:A:THR:HG23	1:69:A:PRO:HG3	3	1.39
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	3	1.39
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	3	1.39
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	3	1.39
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	17	1.39
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	17	1.39
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	17	1.39
(1,154)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	20	1.39
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	13	1.39
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	13	1.39
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	13	1.39
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	18	1.38
(1,902)	1:59:A:GLN:HE22	1:62:A:SER:HB3	20	1.38
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG21	9	1.38
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG22	9	1.38
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG23	9	1.38
(1,695)	1:83:A:TRP:HZ2	1:123:A:PHE:HD1	18	1.38
(1,594)	1:122:A:VAL:HA	1:123:A:PHE:HD1	1	1.38
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	4	1.38
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	4	1.38
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	4	1.38
(1,167)	1:53:A:ARG:HG2	1:54:A:PHE:HD1	13	1.38
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	14	1.37
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	14	1.37
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	14	1.37
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	14	1.37
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	14	1.37
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	14	1.37
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE21	17	1.37
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE22	17	1.37
(1,1328)	1:19:A:PRO:HG2	1:56:A:ASP:HA	1	1.37
(1,1328)	1:19:A:PRO:HG3	1:56:A:ASP:HA	1	1.37
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	5	1.37
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	10	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	10	1.37
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	10	1.37
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	4	1.37
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	8	1.37
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD11	20	1.37
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD12	20	1.37
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD13	20	1.37
(1,400)	1:74:A:LEU:HD21	1:88:A:ALA:HB1	4	1.37
(1,400)	1:74:A:LEU:HD21	1:88:A:ALA:HB2	4	1.37
(1,400)	1:74:A:LEU:HD21	1:88:A:ALA:HB3	4	1.37
(1,400)	1:74:A:LEU:HD22	1:88:A:ALA:HB1	4	1.37
(1,400)	1:74:A:LEU:HD22	1:88:A:ALA:HB2	4	1.37
(1,400)	1:74:A:LEU:HD22	1:88:A:ALA:HB3	4	1.37
(1,400)	1:74:A:LEU:HD23	1:88:A:ALA:HB1	4	1.37
(1,400)	1:74:A:LEU:HD23	1:88:A:ALA:HB2	4	1.37
(1,400)	1:74:A:LEU:HD23	1:88:A:ALA:HB3	4	1.37
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	12	1.37
(1,226)	1:49:A:HIS:HE1	1:67:A:GLY:HA2	20	1.37
(1,165)	1:53:A:ARG:HG2	1:60:A:PHE:H	5	1.37
(1,134)	1:48:A:VAL:HG21	1:50:A:TYR:HD1	19	1.37
(1,134)	1:48:A:VAL:HG22	1:50:A:TYR:HD1	19	1.37
(1,134)	1:48:A:VAL:HG23	1:50:A:TYR:HD1	19	1.37
(1,68)	1:38:A:THR:HG21	1:92:A:LEU:HA	7	1.37
(1,68)	1:38:A:THR:HG22	1:92:A:LEU:HA	7	1.37
(1,68)	1:38:A:THR:HG23	1:92:A:LEU:HA	7	1.37
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	10	1.36
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	10	1.36
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	10	1.36
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	10	1.36
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	10	1.36
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	10	1.36
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	1	1.36
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	1	1.36
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	1	1.36
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	1	1.36
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	1	1.36
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	1	1.36
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	15	1.36
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	15	1.36
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	15	1.36
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	3	1.36
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	3	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	3	1.36
(1,695)	1:83:A:TRP:HZ2	1:123:A:PHE:HD1	16	1.36
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	10	1.36
(1,594)	1:122:A:VAL:HA	1:123:A:PHE:HD1	14	1.36
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD21	4	1.36
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD22	4	1.36
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD23	4	1.36
(1,167)	1:53:A:ARG:HG2	1:54:A:PHE:HD1	20	1.36
(1,134)	1:48:A:VAL:HG21	1:50:A:TYR:HD1	14	1.36
(1,134)	1:48:A:VAL:HG22	1:50:A:TYR:HD1	14	1.36
(1,134)	1:48:A:VAL:HG23	1:50:A:TYR:HD1	14	1.36
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	1	1.36
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	8	1.36
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	8	1.36
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	8	1.36
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA2	3	1.35
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	3	1.35
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	9	1.35
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	9	1.35
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	9	1.35
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	2	1.35
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	2	1.35
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	2	1.35
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	2	1.35
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	2	1.35
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	2	1.35
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	2	1.35
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	2	1.35
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	2	1.35
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	17	1.35
(1,225)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	7	1.35
(1,176)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	20	1.35
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	11	1.35
(1,68)	1:38:A:THR:HG21	1:92:A:LEU:HA	2	1.35
(1,68)	1:38:A:THR:HG22	1:92:A:LEU:HA	2	1.35
(1,68)	1:38:A:THR:HG23	1:92:A:LEU:HA	2	1.35
(1,1324)	1:19:A:PRO:HG2	1:55:A:PRO:HG2	20	1.34
(1,1324)	1:19:A:PRO:HG3	1:55:A:PRO:HG2	20	1.34
(1,1311)	1:81:A:LYS:HE3	1:85:A:GLN:HE22	6	1.34
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	6	1.34
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	6	1.34
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	6	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	17	1.34
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	17	1.34
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	17	1.34
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	18	1.34
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	18	1.34
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	18	1.34
(1,534)	1:106:A:TYR:HB2	1:111:A:TYR:HD2	7	1.34
(1,198)	1:59:A:GLN:HG2	1:61:A:ASP:H	3	1.34
(1,177)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	18	1.34
(1,167)	1:53:A:ARG:HG2	1:54:A:PHE:HD1	5	1.34
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	5	1.33
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	5	1.33
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	5	1.33
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	5	1.33
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	5	1.33
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	5	1.33
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	16	1.33
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	16	1.33
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	16	1.33
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	16	1.33
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	16	1.33
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	16	1.33
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG11	7	1.33
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG12	7	1.33
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG13	7	1.33
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG21	7	1.33
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG22	7	1.33
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG23	7	1.33
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG11	17	1.33
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG12	17	1.33
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG13	17	1.33
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG21	17	1.33
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG22	17	1.33
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG23	17	1.33
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG11	17	1.33
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG12	17	1.33
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG13	17	1.33
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG21	17	1.33
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG22	17	1.33
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG23	17	1.33
(1,1323)	1:19:A:PRO:HG2	1:55:A:PRO:HB2	9	1.33
(1,1323)	1:19:A:PRO:HG3	1:55:A:PRO:HB2	9	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	6	1.33
(1,959)	1:49:A:HIS:HD2	1:70:A:PHE:H	10	1.33
(1,609)	1:123:A:PHE:HA	1:124:A:GLU:HG3	9	1.33
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	7	1.33
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	7	1.33
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	7	1.33
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	13	1.33
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	13	1.33
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	13	1.33
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	8	1.33
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	1	1.33
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	1	1.33
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	1	1.33
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	15	1.33
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	15	1.33
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	15	1.33
(1,1311)	1:81:A:LYS:HE3	1:85:A:GLN:HE22	15	1.32
(1,923)	1:71:A:GLN:HE21	1:72:A:PHE:H	18	1.32
(1,185)	1:53:A:ARG:HB3	1:57:A:GLY:HA2	19	1.32
(1,177)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	11	1.32
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	12	1.32
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	12	1.32
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	12	1.32
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	6	1.31
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	6	1.31
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	6	1.31
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	6	1.31
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	6	1.31
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	6	1.31
(1,1325)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	16	1.31
(1,1325)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	16	1.31
(1,1307)	1:81:A:LYS:HE3	1:85:A:GLN:HE21	3	1.31
(1,1300)	1:92:A:LEU:HD21	1:130:A:VAL:H	7	1.31
(1,1300)	1:92:A:LEU:HD22	1:130:A:VAL:H	7	1.31
(1,1300)	1:92:A:LEU:HD23	1:130:A:VAL:H	7	1.31
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	12	1.31
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	19	1.31
(1,912)	1:53:A:ARG:HD3	1:57:A:GLY:H	17	1.31
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD21	18	1.31
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD22	18	1.31
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD23	18	1.31
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	8	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	8	1.31
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	8	1.31
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	5	1.31
(1,558)	1:106:A:TYR:HD1	1:111:A:TYR:HB2	4	1.31
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	5	1.31
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	5	1.31
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	5	1.31
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD11	13	1.31
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD12	13	1.31
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD13	13	1.31
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	1	1.31
(1,279)	1:75:A:GLY:HA3	1:84:A:ASP:HB3	11	1.31
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	19	1.31
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	8	1.31
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	8	1.31
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	8	1.31
(1,1299)	1:92:A:LEU:HD11	1:130:A:VAL:H	4	1.3
(1,1299)	1:92:A:LEU:HD12	1:130:A:VAL:H	4	1.3
(1,1299)	1:92:A:LEU:HD13	1:130:A:VAL:H	4	1.3
(1,1299)	1:92:A:LEU:HD11	1:130:A:VAL:H	10	1.3
(1,1299)	1:92:A:LEU:HD12	1:130:A:VAL:H	10	1.3
(1,1299)	1:92:A:LEU:HD13	1:130:A:VAL:H	10	1.3
(1,911)	1:53:A:ARG:HD2	1:57:A:GLY:H	4	1.3
(1,685)	1:102:A:TYR:HE2	1:108:A:GLU:HG2	15	1.3
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	8	1.3
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	8	1.3
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	8	1.3
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	17	1.3
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	17	1.3
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	17	1.3
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	18	1.3
(1,193)	1:53:A:ARG:HB3	1:59:A:GLN:HA	4	1.3
(1,134)	1:48:A:VAL:HG21	1:50:A:TYR:HD1	7	1.3
(1,134)	1:48:A:VAL:HG22	1:50:A:TYR:HD1	7	1.3
(1,134)	1:48:A:VAL:HG23	1:50:A:TYR:HD1	7	1.3
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	17	1.3
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	1	1.3
(1,1306)	1:81:A:LYS:HE2	1:85:A:GLN:HE21	16	1.29
(1,1185)	1:24:A:ALA:HB1	1:103:A:GLN:H	12	1.29
(1,1185)	1:24:A:ALA:HB2	1:103:A:GLN:H	12	1.29
(1,1185)	1:24:A:ALA:HB3	1:103:A:GLN:H	12	1.29
(1,758)	1:28:A:LYS:HG2	1:30:A:VAL:H	7	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	14	1.29
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	14	1.29
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	14	1.29
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	11	1.29
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	11	1.29
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	11	1.29
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	6	1.29
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	6	1.29
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	6	1.29
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	6	1.29
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	6	1.29
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	6	1.29
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD21	1	1.29
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD22	1	1.29
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD23	1	1.29
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	15	1.29
(1,167)	1:53:A:ARG:HG2	1:54:A:PHE:HD1	19	1.29
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG11	1	1.28
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG12	1	1.28
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG13	1	1.28
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG21	1	1.28
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG22	1	1.28
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG23	1	1.28
(1,1310)	1:81:A:LYS:HE2	1:85:A:GLN:HE22	17	1.28
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	6	1.28
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	6	1.28
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	6	1.28
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	18	1.28
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	18	1.28
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	18	1.28
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	16	1.28
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	16	1.28
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	16	1.28
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	14	1.28
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	3	1.28
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	3	1.28
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	3	1.28
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	16	1.28
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	16	1.28
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	16	1.28
(1,537)	1:108:A:GLU:HB2	1:118:A:LYS:HG2	3	1.28
(1,537)	1:108:A:GLU:HB2	1:118:A:LYS:HG2	13	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:74:A:LEU:HD11	1:84:A:ASP:HB3	4	1.28
(1,375)	1:74:A:LEU:HD12	1:84:A:ASP:HB3	4	1.28
(1,375)	1:74:A:LEU:HD13	1:84:A:ASP:HB3	4	1.28
(1,371)	1:81:A:LYS:HD3	1:84:A:ASP:HB2	14	1.28
(1,190)	1:54:A:PHE:HD1	1:58:A:LYS:HD2	12	1.28
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	2	1.28
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	18	1.28
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	18	1.28
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	18	1.28
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	13	1.28
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	13	1.28
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	13	1.28
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG21	9	1.28
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG22	9	1.28
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG23	9	1.28
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD2	13	1.27
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD3	13	1.27
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	2	1.27
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	2	1.27
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	2	1.27
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	2	1.27
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	2	1.27
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	2	1.27
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG11	12	1.27
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG12	12	1.27
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG13	12	1.27
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG21	12	1.27
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG22	12	1.27
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG23	12	1.27
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG11	12	1.27
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG12	12	1.27
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG13	12	1.27
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG21	12	1.27
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG22	12	1.27
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG23	12	1.27
(1,1300)	1:92:A:LEU:HD21	1:130:A:VAL:H	1	1.27
(1,1300)	1:92:A:LEU:HD22	1:130:A:VAL:H	1	1.27
(1,1300)	1:92:A:LEU:HD23	1:130:A:VAL:H	1	1.27
(1,857)	1:49:A:HIS:HD2	1:51:A:ASP:H	7	1.27
(1,685)	1:102:A:TYR:HE2	1:108:A:GLU:HG2	3	1.27
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	1	1.27
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	17	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	11	1.27
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	11	1.27
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	11	1.27
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG21	7	1.27
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG22	7	1.27
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG23	7	1.27
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG21	13	1.27
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG22	13	1.27
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG23	13	1.27
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB1	17	1.27
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB2	17	1.27
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB3	17	1.27
(1,422)	1:38:A:THR:HG21	1:91:A:THR:HA	13	1.27
(1,422)	1:38:A:THR:HG22	1:91:A:THR:HA	13	1.27
(1,422)	1:38:A:THR:HG23	1:91:A:THR:HA	13	1.27
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	6	1.27
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	20	1.27
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	20	1.27
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	20	1.27
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	3	1.27
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	4	1.27
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	13	1.26
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	13	1.26
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	13	1.26
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	13	1.26
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	13	1.26
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	13	1.26
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD2	4	1.26
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD3	4	1.26
(1,1543)	1:85:A:GLN:HB2	1:98:A:PHE:HD2	16	1.26
(1,1543)	1:85:A:GLN:HB3	1:98:A:PHE:HD2	16	1.26
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG11	6	1.26
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG12	6	1.26
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG13	6	1.26
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG21	6	1.26
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG22	6	1.26
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG23	6	1.26
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	13	1.26
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	13	1.26
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	13	1.26
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	13	1.26
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	13	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	13	1.26
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	1	1.26
(1,758)	1:28:A:LYS:HG2	1:30:A:VAL:H	12	1.26
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	8	1.26
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	8	1.26
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	8	1.26
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	18	1.26
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	18	1.26
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	18	1.26
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	6	1.26
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	16	1.26
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	16	1.26
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	16	1.26
(1,594)	1:122:A:VAL:HA	1:123:A:PHE:HD1	3	1.26
(1,594)	1:122:A:VAL:HA	1:123:A:PHE:HD1	13	1.26
(1,594)	1:122:A:VAL:HA	1:123:A:PHE:HD1	17	1.26
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	10	1.26
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	10	1.26
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	10	1.26
(1,519)	1:80:A:ILE:HB	1:105:A:ALA:HA	16	1.26
(1,417)	1:90:A:MET:HE1	1:94:A:GLU:HG2	4	1.26
(1,417)	1:90:A:MET:HE2	1:94:A:GLU:HG2	4	1.26
(1,417)	1:90:A:MET:HE3	1:94:A:GLU:HG2	4	1.26
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD11	4	1.26
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD12	4	1.26
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD13	4	1.26
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	11	1.26
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	11	1.26
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	11	1.26
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD11	5	1.25
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD12	5	1.25
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD13	5	1.25
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD21	5	1.25
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD22	5	1.25
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD23	5	1.25
(1,1324)	1:19:A:PRO:HG2	1:55:A:PRO:HG2	11	1.25
(1,1324)	1:19:A:PRO:HG3	1:55:A:PRO:HG2	11	1.25
(1,1253)	1:123:A:PHE:HD2	1:124:A:GLU:H	13	1.25
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	14	1.25
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	14	1.25
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	14	1.25
(1,923)	1:71:A:GLN:HE21	1:72:A:PHE:H	14	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	16	1.25
(1,800)	1:41:A:GLN:H	1:44:A:LYS:HB2	6	1.25
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	2	1.25
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	2	1.25
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	2	1.25
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	10	1.25
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	10	1.25
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	10	1.25
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	11	1.25
(1,539)	1:102:A:TYR:HE2	1:108:A:GLU:HA	15	1.25
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	13	1.25
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	13	1.25
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	13	1.25
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	1	1.25
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	1	1.25
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	1	1.25
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD11	3	1.25
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD12	3	1.25
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD13	3	1.25
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	18	1.24
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	18	1.24
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	18	1.24
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	18	1.24
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	18	1.24
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	18	1.24
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	15	1.24
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	15	1.24
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	15	1.24
(1,758)	1:28:A:LYS:HG2	1:30:A:VAL:H	5	1.24
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG21	15	1.24
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG22	15	1.24
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG23	15	1.24
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	13	1.24
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	13	1.24
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	13	1.24
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	20	1.24
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	20	1.24
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	20	1.24
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	6	1.24
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	6	1.24
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	6	1.24
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	17	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	17	1.24
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	17	1.24
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD21	13	1.24
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD22	13	1.24
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD23	13	1.24
(1,177)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	19	1.24
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG21	18	1.24
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG22	18	1.24
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG23	18	1.24
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	14	1.24
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG21	3	1.24
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG22	3	1.24
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG23	3	1.24
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	12	1.23
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	12	1.23
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	12	1.23
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	12	1.23
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	12	1.23
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	12	1.23
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	15	1.23
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	15	1.23
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	15	1.23
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	15	1.23
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	15	1.23
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	15	1.23
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	20	1.23
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	20	1.23
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	20	1.23
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	20	1.23
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	20	1.23
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	20	1.23
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	9	1.23
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	9	1.23
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	9	1.23
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	9	1.23
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	9	1.23
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	9	1.23
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG11	7	1.23
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG12	7	1.23
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG13	7	1.23
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG21	7	1.23
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG22	7	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG23	7	1.23
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG11	16	1.23
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG12	16	1.23
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG13	16	1.23
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG21	16	1.23
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG22	16	1.23
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG23	16	1.23
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	20	1.23
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	20	1.23
(1,1253)	1:123:A:PHE:HD2	1:124:A:GLU:H	17	1.23
(1,903)	1:59:A:GLN:HE22	1:62:A:SER:HB2	16	1.23
(1,897)	1:59:A:GLN:HE21	1:62:A:SER:HB3	16	1.23
(1,857)	1:49:A:HIS:HD2	1:51:A:ASP:H	6	1.23
(1,674)	1:106:A:TYR:HE1	1:111:A:TYR:HB2	19	1.23
(1,673)	1:52:A:GLY:HA3	1:123:A:PHE:HD1	2	1.23
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	4	1.23
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	4	1.23
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	4	1.23
(1,560)	1:106:A:TYR:HD1	1:111:A:TYR:HB3	19	1.23
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	19	1.23
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	19	1.23
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	19	1.23
(1,547)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	2	1.23
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD21	9	1.23
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD22	9	1.23
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD23	9	1.23
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	3	1.22
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	3	1.22
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	3	1.22
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	3	1.22
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	3	1.22
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	3	1.22
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	18	1.22
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	18	1.22
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	18	1.22
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	18	1.22
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	18	1.22
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	18	1.22
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD2	16	1.22
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD3	16	1.22
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD2	16	1.22
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD3	16	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1310)	1:81:A:LYS:HE2	1:85:A:GLN:HE22	18	1.22
(1,1306)	1:81:A:LYS:HE2	1:85:A:GLN:HE21	12	1.22
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	8	1.22
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	16	1.22
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG21	1	1.22
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG22	1	1.22
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG23	1	1.22
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	13	1.22
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	19	1.22
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	19	1.22
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	19	1.22
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	14	1.22
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	14	1.22
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	14	1.22
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	2	1.22
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	2	1.22
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	2	1.22
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	17	1.22
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	17	1.22
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	17	1.22
(1,537)	1:108:A:GLU:HB2	1:118:A:LYS:HG2	14	1.22
(1,315)	1:80:A:ILE:HD11	1:100:A:ILE:HG21	9	1.22
(1,315)	1:80:A:ILE:HD11	1:100:A:ILE:HG22	9	1.22
(1,315)	1:80:A:ILE:HD11	1:100:A:ILE:HG23	9	1.22
(1,315)	1:80:A:ILE:HD12	1:100:A:ILE:HG21	9	1.22
(1,315)	1:80:A:ILE:HD12	1:100:A:ILE:HG22	9	1.22
(1,315)	1:80:A:ILE:HD12	1:100:A:ILE:HG23	9	1.22
(1,315)	1:80:A:ILE:HD13	1:100:A:ILE:HG21	9	1.22
(1,315)	1:80:A:ILE:HD13	1:100:A:ILE:HG22	9	1.22
(1,315)	1:80:A:ILE:HD13	1:100:A:ILE:HG23	9	1.22
(1,211)	1:49:A:HIS:HB3	1:64:A:ARG:HA	3	1.22
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	9	1.22
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	10	1.22
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	10	1.22
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	10	1.22
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	19	1.21
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	19	1.21
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	19	1.21
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	19	1.21
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	19	1.21
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	19	1.21
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	19	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	19	1.21
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	19	1.21
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	19	1.21
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	19	1.21
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	19	1.21
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	8	1.21
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	8	1.21
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	8	1.21
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	8	1.21
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	8	1.21
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	8	1.21
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	7	1.21
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	7	1.21
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	7	1.21
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	7	1.21
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	7	1.21
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	7	1.21
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	15	1.21
(1,1253)	1:123:A:PHE:HD2	1:124:A:GLU:H	9	1.21
(1,953)	1:49:A:HIS:HE1	1:68:A:LYS:H	17	1.21
(1,758)	1:28:A:LYS:HG2	1:30:A:VAL:H	8	1.21
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	6	1.21
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	6	1.21
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	6	1.21
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	11	1.21
(1,594)	1:122:A:VAL:HA	1:123:A:PHE:HD1	9	1.21
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	10	1.21
(1,198)	1:59:A:GLN:HG2	1:61:A:ASP:H	20	1.21
(1,176)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	19	1.21
(1,167)	1:53:A:ARG:HG2	1:54:A:PHE:HD1	11	1.21
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	13	1.21
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	13	1.21
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	13	1.21
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	5	1.2
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	5	1.2
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	5	1.2
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	5	1.2
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	5	1.2
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	5	1.2
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	12	1.2
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	12	1.2
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	12	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	12	1.2
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	12	1.2
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	12	1.2
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	19	1.2
(1,1219)	1:111:A:TYR:H	1:115:A:ILE:HB	17	1.2
(1,1069)	1:86:A:GLY:H	1:98:A:PHE:HD2	3	1.2
(1,772)	1:32:A:THR:H	1:95:A:LYS:HB3	1	1.2
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	2	1.2
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	2	1.2
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	2	1.2
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG21	4	1.2
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG22	4	1.2
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG23	4	1.2
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	2	1.2
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	2	1.2
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	2	1.2
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	12	1.2
(1,582)	1:55:A:PRO:HG2	1:120:A:THR:HB	16	1.2
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	8	1.2
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	8	1.2
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	8	1.2
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	4	1.2
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	4	1.2
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	4	1.2
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD11	4	1.2
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD12	4	1.2
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD13	4	1.2
(1,134)	1:48:A:VAL:HG21	1:50:A:TYR:HD1	18	1.2
(1,134)	1:48:A:VAL:HG22	1:50:A:TYR:HD1	18	1.2
(1,134)	1:48:A:VAL:HG23	1:50:A:TYR:HD1	18	1.2
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG11	16	1.2
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG12	16	1.2
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG13	16	1.2
(1,28)	1:27:A:GLU:HG2	1:99:A:THR:HB	19	1.2
(1,3)	1:28:A:LYS:HG3	1:30:A:VAL:H	4	1.2
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	1	1.19
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	1	1.19
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	1	1.19
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	1	1.19
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	1	1.19
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	1	1.19
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	13	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	13	1.19
(1,1325)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	11	1.19
(1,1325)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	11	1.19
(1,1307)	1:81:A:LYS:HE3	1:85:A:GLN:HE21	2	1.19
(1,1253)	1:123:A:PHE:HD2	1:124:A:GLU:H	14	1.19
(1,923)	1:71:A:GLN:HE21	1:72:A:PHE:H	11	1.19
(1,686)	1:102:A:TYR:HE2	1:118:A:LYS:HA	15	1.19
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	13	1.19
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	13	1.19
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	13	1.19
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	15	1.19
(1,632)	1:93:A:GLY:H	1:127:A:LEU:HG	17	1.19
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	18	1.19
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	18	1.19
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	18	1.19
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	20	1.19
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	13	1.19
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	15	1.19
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	15	1.19
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	15	1.19
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	5	1.19
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	5	1.19
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	5	1.19
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	6	1.19
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	5	1.19
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	5	1.19
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	5	1.19
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	5	1.19
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	5	1.19
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	5	1.19
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	5	1.19
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	5	1.19
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	5	1.19
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	18	1.19
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	16	1.19
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	16	1.19
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	16	1.19
(1,167)	1:53:A:ARG:HG2	1:54:A:PHE:HD1	15	1.19
(1,165)	1:53:A:ARG:HG2	1:60:A:PHE:H	3	1.19
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	5	1.19
(1,76)	1:38:A:THR:HB	1:40:A:PRO:HD3	10	1.19
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD2	1	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD3	1	1.18
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD2	1	1.18
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD3	1	1.18
(1,1325)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	10	1.18
(1,1325)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	10	1.18
(1,1325)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	19	1.18
(1,1325)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	19	1.18
(1,1300)	1:92:A:LEU:HD21	1:130:A:VAL:H	16	1.18
(1,1300)	1:92:A:LEU:HD22	1:130:A:VAL:H	16	1.18
(1,1300)	1:92:A:LEU:HD23	1:130:A:VAL:H	16	1.18
(1,751)	1:27:A:GLU:HG2	1:28:A:LYS:H	14	1.18
(1,696)	1:83:A:TRP:HZ2	1:123:A:PHE:HB3	16	1.18
(1,686)	1:102:A:TYR:HE2	1:118:A:LYS:HA	10	1.18
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	9	1.18
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	15	1.18
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	15	1.18
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	15	1.18
(1,415)	1:90:A:MET:HE1	1:94:A:GLU:HA	9	1.18
(1,415)	1:90:A:MET:HE2	1:94:A:GLU:HA	9	1.18
(1,415)	1:90:A:MET:HE3	1:94:A:GLU:HA	9	1.18
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG21	5	1.18
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG22	5	1.18
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG23	5	1.18
(1,134)	1:48:A:VAL:HG21	1:50:A:TYR:HD1	13	1.18
(1,134)	1:48:A:VAL:HG22	1:50:A:TYR:HD1	13	1.18
(1,134)	1:48:A:VAL:HG23	1:50:A:TYR:HD1	13	1.18
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	6	1.18
(1,1543)	1:85:A:GLN:HB2	1:98:A:PHE:HD2	19	1.17
(1,1543)	1:85:A:GLN:HB3	1:98:A:PHE:HD2	19	1.17
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE2	17	1.17
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE3	17	1.17
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE2	17	1.17
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE3	17	1.17
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD2	2	1.17
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD3	2	1.17
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD2	2	1.17
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD3	2	1.17
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG11	14	1.17
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG12	14	1.17
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG13	14	1.17
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG21	14	1.17
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG22	14	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG23	14	1.17
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG11	14	1.17
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG12	14	1.17
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG13	14	1.17
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG21	14	1.17
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG22	14	1.17
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG23	14	1.17
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	3	1.17
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	3	1.17
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	3	1.17
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	5	1.17
(1,1253)	1:123:A:PHE:HD2	1:124:A:GLU:H	1	1.17
(1,1253)	1:123:A:PHE:HD2	1:124:A:GLU:H	3	1.17
(1,1253)	1:123:A:PHE:HD2	1:124:A:GLU:H	4	1.17
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	17	1.17
(1,960)	1:50:A:TYR:HE2	1:70:A:PHE:H	2	1.17
(1,923)	1:71:A:GLN:HE21	1:72:A:PHE:H	4	1.17
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	6	1.17
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	6	1.17
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	6	1.17
(1,149)	1:50:A:TYR:HB2	1:123:A:PHE:HD2	10	1.17
(1,28)	1:27:A:GLU:HG2	1:99:A:THR:HB	5	1.17
(1,1440)	1:53:A:ARG:HD2	1:57:A:GLY:H	1	1.16
(1,1440)	1:53:A:ARG:HD3	1:57:A:GLY:H	1	1.16
(1,1440)	1:53:A:ARG:HD2	1:57:A:GLY:H	4	1.16
(1,1440)	1:53:A:ARG:HD3	1:57:A:GLY:H	4	1.16
(1,1311)	1:81:A:LYS:HE3	1:85:A:GLN:HE22	8	1.16
(1,1253)	1:123:A:PHE:HD2	1:124:A:GLU:H	7	1.16
(1,1253)	1:123:A:PHE:HD2	1:124:A:GLU:H	20	1.16
(1,1085)	1:89:A:THR:H	1:90:A:MET:HE1	2	1.16
(1,1085)	1:89:A:THR:H	1:90:A:MET:HE2	2	1.16
(1,1085)	1:89:A:THR:H	1:90:A:MET:HE3	2	1.16
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	19	1.16
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	19	1.16
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	19	1.16
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG11	3	1.16
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG12	3	1.16
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG13	3	1.16
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG21	4	1.16
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG22	4	1.16
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG23	4	1.16
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	17	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	5	1.16
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	5	1.16
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	5	1.16
(1,516)	1:81:A:LYS:H	1:105:A:ALA:HA	3	1.16
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD21	12	1.16
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD22	12	1.16
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD23	12	1.16
(1,176)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	11	1.16
(1,165)	1:53:A:ARG:HG2	1:60:A:PHE:H	19	1.16
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	1	1.16
(1,76)	1:38:A:THR:HB	1:40:A:PRO:HD3	2	1.16
(1,1253)	1:123:A:PHE:HD2	1:124:A:GLU:H	6	1.15
(1,1235)	1:55:A:PRO:HG3	1:120:A:THR:H	7	1.15
(1,1111)	1:38:A:THR:HG21	1:92:A:LEU:H	13	1.15
(1,1111)	1:38:A:THR:HG22	1:92:A:LEU:H	13	1.15
(1,1111)	1:38:A:THR:HG23	1:92:A:LEU:H	13	1.15
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	3	1.15
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	3	1.15
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	3	1.15
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	1	1.15
(1,681)	1:50:A:TYR:H	1:50:A:TYR:HD2	5	1.15
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	14	1.15
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	14	1.15
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	14	1.15
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	3	1.15
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	3	1.15
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	3	1.15
(1,609)	1:123:A:PHE:HA	1:124:A:GLU:HG3	19	1.15
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD21	19	1.15
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD22	19	1.15
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD23	19	1.15
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	13	1.15
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	13	1.15
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	13	1.15
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	13	1.15
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	13	1.15
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	13	1.15
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	13	1.15
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	13	1.15
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	13	1.15
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG21	16	1.15
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG22	16	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG23	16	1.15
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	17	1.15
(1,146)	1:49:A:HIS:HD2	1:50:A:TYR:HA	6	1.15
(1,134)	1:48:A:VAL:HG21	1:50:A:TYR:HD1	12	1.15
(1,134)	1:48:A:VAL:HG22	1:50:A:TYR:HD1	12	1.15
(1,134)	1:48:A:VAL:HG23	1:50:A:TYR:HD1	12	1.15
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	19	1.15
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	19	1.15
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	19	1.15
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	8	1.15
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	8	1.15
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	8	1.15
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG11	1	1.15
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG12	1	1.15
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG13	1	1.15
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG11	7	1.15
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG12	7	1.15
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG13	7	1.15
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	10	1.14
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	10	1.14
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	10	1.14
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	10	1.14
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	10	1.14
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	10	1.14
(1,1440)	1:53:A:ARG:HD2	1:57:A:GLY:H	2	1.14
(1,1440)	1:53:A:ARG:HD3	1:57:A:GLY:H	2	1.14
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	9	1.14
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	9	1.14
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	9	1.14
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	9	1.14
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	9	1.14
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	9	1.14
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	9	1.14
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	9	1.14
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	9	1.14
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	9	1.14
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	9	1.14
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	9	1.14
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	9	1.14
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	9	1.14
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	9	1.14
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	9	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	9	1.14
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	9	1.14
(1,1309)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	3	1.14
(1,1300)	1:92:A:LEU:HD21	1:130:A:VAL:H	19	1.14
(1,1300)	1:92:A:LEU:HD22	1:130:A:VAL:H	19	1.14
(1,1300)	1:92:A:LEU:HD23	1:130:A:VAL:H	19	1.14
(1,1253)	1:123:A:PHE:HD2	1:124:A:GLU:H	10	1.14
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	1	1.14
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	1	1.14
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	1	1.14
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	15	1.14
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	5	1.14
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	5	1.14
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	5	1.14
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	18	1.14
(1,582)	1:55:A:PRO:HG2	1:120:A:THR:HB	5	1.14
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	7	1.14
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	17	1.14
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	17	1.14
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	17	1.14
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	12	1.14
(1,165)	1:53:A:ARG:HG2	1:60:A:PHE:H	7	1.14
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	4	1.14
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	4	1.14
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	4	1.14
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	9	1.14
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	9	1.14
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	9	1.14
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	13	1.13
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	13	1.13
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	13	1.13
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	13	1.13
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	13	1.13
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	13	1.13
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG2	19	1.13
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG3	19	1.13
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	5	1.13
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	20	1.13
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	20	1.13
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	20	1.13
(1,897)	1:59:A:GLN:HE21	1:62:A:SER:HB3	2	1.13
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	18	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	18	1.13
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	18	1.13
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	2	1.13
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	2	1.13
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	2	1.13
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	4	1.13
(1,609)	1:123:A:PHE:HA	1:124:A:GLU:HG3	8	1.13
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	5	1.13
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	19	1.13
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	18	1.13
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB1	5	1.13
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB2	5	1.13
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB3	5	1.13
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB1	5	1.13
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB2	5	1.13
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB3	5	1.13
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB1	5	1.13
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB2	5	1.13
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB3	5	1.13
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	19	1.13
(1,225)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	16	1.13
(1,195)	1:53:A:ARG:HG3	1:59:A:GLN:HA	12	1.13
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	12	1.13
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	12	1.13
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	12	1.13
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	11	1.13
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	11	1.13
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	11	1.13
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	9	1.12
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	9	1.12
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	9	1.12
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	9	1.12
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	9	1.12
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	9	1.12
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	18	1.12
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	18	1.12
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	18	1.12
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	18	1.12
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	18	1.12
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	18	1.12
(1,1299)	1:92:A:LEU:HD11	1:130:A:VAL:H	14	1.12
(1,1299)	1:92:A:LEU:HD12	1:130:A:VAL:H	14	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1299)	1:92:A:LEU:HD13	1:130:A:VAL:H	14	1.12
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	1	1.12
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	12	1.12
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	12	1.12
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	12	1.12
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	15	1.12
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	15	1.12
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	15	1.12
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	2	1.12
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	2	1.12
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	2	1.12
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	12	1.12
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	16	1.12
(1,557)	1:110:A:GLY:HA3	1:115:A:ILE:HB	4	1.12
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	18	1.12
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	18	1.12
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	18	1.12
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB1	19	1.12
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB2	19	1.12
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB3	19	1.12
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB1	20	1.12
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB2	20	1.12
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB3	20	1.12
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD21	13	1.12
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD22	13	1.12
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD23	13	1.12
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD21	19	1.12
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD22	19	1.12
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD23	19	1.12
(1,316)	1:80:A:ILE:HB	1:104:A:LEU:HB3	9	1.12
(1,211)	1:49:A:HIS:HB3	1:64:A:ARG:HA	15	1.12
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	2	1.12
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	2	1.12
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	2	1.12
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	6	1.12
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	6	1.12
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	6	1.12
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	8	1.12
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	8	1.12
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	8	1.12
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	7	1.11
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	7	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	7	1.11
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	7	1.11
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	7	1.11
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	7	1.11
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	1	1.11
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	1	1.11
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	1	1.11
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	1	1.11
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	1	1.11
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	1	1.11
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	17	1.11
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	17	1.11
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	17	1.11
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	17	1.11
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	17	1.11
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	17	1.11
(1,1333)	1:24:A:ALA:HB1	1:103:A:GLN:HG2	5	1.11
(1,1333)	1:24:A:ALA:HB1	1:103:A:GLN:HG3	5	1.11
(1,1333)	1:24:A:ALA:HB2	1:103:A:GLN:HG2	5	1.11
(1,1333)	1:24:A:ALA:HB2	1:103:A:GLN:HG3	5	1.11
(1,1333)	1:24:A:ALA:HB3	1:103:A:GLN:HG2	5	1.11
(1,1333)	1:24:A:ALA:HB3	1:103:A:GLN:HG3	5	1.11
(1,1300)	1:92:A:LEU:HD21	1:130:A:VAL:H	8	1.11
(1,1300)	1:92:A:LEU:HD22	1:130:A:VAL:H	8	1.11
(1,1300)	1:92:A:LEU:HD23	1:130:A:VAL:H	8	1.11
(1,1235)	1:55:A:PRO:HG3	1:120:A:THR:H	19	1.11
(1,1069)	1:86:A:GLY:H	1:98:A:PHE:HD2	16	1.11
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	2	1.11
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	19	1.11
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG21	11	1.11
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG22	11	1.11
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG23	11	1.11
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	8	1.11
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	16	1.11
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	18	1.11
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	5	1.11
(1,530)	1:106:A:TYR:HB3	1:111:A:TYR:HD2	20	1.11
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	3	1.11
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	19	1.11
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	18	1.11
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	18	1.11
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	18	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,146)	1:49:A:HIS:HD2	1:50:A:TYR:HA	7	1.11
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG21	11	1.11
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG22	11	1.11
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG23	11	1.11
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG21	18	1.11
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG22	18	1.11
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG23	18	1.11
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	9	1.11
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	6	1.1
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	6	1.1
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	6	1.1
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	6	1.1
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	6	1.1
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	6	1.1
(1,1253)	1:123:A:PHE:HD2	1:124:A:GLU:H	12	1.1
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	19	1.1
(1,923)	1:71:A:GLN:HE21	1:72:A:PHE:H	19	1.1
(1,744)	1:26:A:LEU:H	1:27:A:GLU:HG3	11	1.1
(1,695)	1:83:A:TRP:HZ2	1:123:A:PHE:HD1	2	1.1
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	8	1.1
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	8	1.1
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	8	1.1
(1,539)	1:102:A:TYR:HE2	1:108:A:GLU:HA	10	1.1
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD21	18	1.1
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD22	18	1.1
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD23	18	1.1
(1,422)	1:38:A:THR:HG21	1:91:A:THR:HA	8	1.1
(1,422)	1:38:A:THR:HG22	1:91:A:THR:HA	8	1.1
(1,422)	1:38:A:THR:HG23	1:91:A:THR:HA	8	1.1
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG21	1	1.1
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG22	1	1.1
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG23	1	1.1
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD21	16	1.1
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD22	16	1.1
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD23	16	1.1
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	11	1.1
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	11	1.1
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	11	1.1
(1,190)	1:54:A:PHE:HD1	1:58:A:LYS:HD2	3	1.1
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	13	1.1
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG21	4	1.1
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG22	4	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG23	4	1.1
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	19	1.1
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	19	1.1
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	19	1.1
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	11	1.1
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	11	1.1
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	11	1.1
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD2	3	1.09
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD3	3	1.09
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	11	1.09
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	11	1.09
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	11	1.09
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	11	1.09
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	11	1.09
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	11	1.09
(1,1440)	1:53:A:ARG:HD2	1:57:A:GLY:H	16	1.09
(1,1440)	1:53:A:ARG:HD3	1:57:A:GLY:H	16	1.09
(1,1300)	1:92:A:LEU:HD21	1:130:A:VAL:H	12	1.09
(1,1300)	1:92:A:LEU:HD22	1:130:A:VAL:H	12	1.09
(1,1300)	1:92:A:LEU:HD23	1:130:A:VAL:H	12	1.09
(1,1130)	1:90:A:MET:HE1	1:95:A:LYS:H	4	1.09
(1,1130)	1:90:A:MET:HE2	1:95:A:LYS:H	4	1.09
(1,1130)	1:90:A:MET:HE3	1:95:A:LYS:H	4	1.09
(1,1111)	1:38:A:THR:HG21	1:92:A:LEU:H	12	1.09
(1,1111)	1:38:A:THR:HG22	1:92:A:LEU:H	12	1.09
(1,1111)	1:38:A:THR:HG23	1:92:A:LEU:H	12	1.09
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	1	1.09
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	1	1.09
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	1	1.09
(1,923)	1:71:A:GLN:HE21	1:72:A:PHE:H	2	1.09
(1,923)	1:71:A:GLN:HE21	1:72:A:PHE:H	7	1.09
(1,695)	1:83:A:TRP:HZ2	1:123:A:PHE:HD1	5	1.09
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	4	1.09
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	3	1.09
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	8	1.09
(1,545)	1:108:A:GLU:HG2	1:118:A:LYS:HG2	13	1.09
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	11	1.09
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	11	1.09
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	11	1.09
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	15	1.09
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	15	1.09
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	15	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	8	1.09
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	8	1.09
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	8	1.09
(1,422)	1:38:A:THR:HG21	1:91:A:THR:HA	12	1.09
(1,422)	1:38:A:THR:HG22	1:91:A:THR:HA	12	1.09
(1,422)	1:38:A:THR:HG23	1:91:A:THR:HA	12	1.09
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	18	1.09
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	18	1.09
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	18	1.09
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	19	1.09
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	10	1.09
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	15	1.09
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	1	1.09
(1,193)	1:53:A:ARG:HB3	1:59:A:GLN:HA	8	1.09
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	20	1.09
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	20	1.09
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	20	1.09
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	3	1.08
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	3	1.08
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	3	1.08
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	3	1.08
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	3	1.08
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	3	1.08
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	11	1.08
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	11	1.08
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	11	1.08
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	11	1.08
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	11	1.08
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	11	1.08
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG21	5	1.08
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG22	5	1.08
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG23	5	1.08
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	16	1.08
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	12	1.08
(1,953)	1:49:A:HIS:HE1	1:68:A:LYS:H	8	1.08
(1,903)	1:59:A:GLN:HE22	1:62:A:SER:HB2	2	1.08
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG11	11	1.08
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG12	11	1.08
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG13	11	1.08
(1,688)	1:83:A:TRP:HD1	1:98:A:PHE:HD2	20	1.08
(1,685)	1:102:A:TYR:HE2	1:108:A:GLU:HG2	9	1.08
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	6	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	6	1.08
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	6	1.08
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	15	1.08
(1,587)	1:115:A:ILE:HD11	1:121:A:LEU:HG	4	1.08
(1,587)	1:115:A:ILE:HD12	1:121:A:LEU:HG	4	1.08
(1,587)	1:115:A:ILE:HD13	1:121:A:LEU:HG	4	1.08
(1,400)	1:74:A:LEU:HD21	1:88:A:ALA:HB1	11	1.08
(1,400)	1:74:A:LEU:HD21	1:88:A:ALA:HB2	11	1.08
(1,400)	1:74:A:LEU:HD21	1:88:A:ALA:HB3	11	1.08
(1,400)	1:74:A:LEU:HD22	1:88:A:ALA:HB1	11	1.08
(1,400)	1:74:A:LEU:HD22	1:88:A:ALA:HB2	11	1.08
(1,400)	1:74:A:LEU:HD22	1:88:A:ALA:HB3	11	1.08
(1,400)	1:74:A:LEU:HD23	1:88:A:ALA:HB1	11	1.08
(1,400)	1:74:A:LEU:HD23	1:88:A:ALA:HB2	11	1.08
(1,400)	1:74:A:LEU:HD23	1:88:A:ALA:HB3	11	1.08
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	5	1.08
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	16	1.08
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	20	1.08
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD2	15	1.07
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD3	15	1.07
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	7	1.07
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	7	1.07
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	7	1.07
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	7	1.07
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	7	1.07
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	7	1.07
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE21	8	1.07
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	8	1.07
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	14	1.07
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	14	1.07
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	14	1.07
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	14	1.07
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	14	1.07
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	14	1.07
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	10	1.07
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	10	1.07
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	10	1.07
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	10	1.07
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	10	1.07
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	10	1.07
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	10	1.07
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	10	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	10	1.07
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	10	1.07
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	10	1.07
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	10	1.07
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	10	1.07
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	10	1.07
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	10	1.07
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	10	1.07
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	10	1.07
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	10	1.07
(1,1311)	1:81:A:LYS:HE3	1:85:A:GLN:HE22	4	1.07
(1,1306)	1:81:A:LYS:HE2	1:85:A:GLN:HE21	11	1.07
(1,911)	1:53:A:ARG:HD2	1:57:A:GLY:H	3	1.07
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	9	1.07
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	17	1.07
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	18	1.07
(1,677)	1:105:A:ALA:HB1	1:106:A:TYR:HE2	18	1.07
(1,677)	1:105:A:ALA:HB2	1:106:A:TYR:HE2	18	1.07
(1,677)	1:105:A:ALA:HB3	1:106:A:TYR:HE2	18	1.07
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	10	1.07
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	10	1.07
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	10	1.07
(1,450)	1:32:A:THR:HB	1:95:A:LYS:HE3	5	1.07
(1,393)	1:74:A:LEU:HD21	1:88:A:ALA:HA	4	1.07
(1,393)	1:74:A:LEU:HD22	1:88:A:ALA:HA	4	1.07
(1,393)	1:74:A:LEU:HD23	1:88:A:ALA:HA	4	1.07
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD11	17	1.07
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD12	17	1.07
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD13	17	1.07
(1,211)	1:49:A:HIS:HB3	1:64:A:ARG:HA	12	1.07
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	7	1.07
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	8	1.06
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	8	1.06
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	8	1.06
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	8	1.06
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	8	1.06
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	8	1.06
(1,1543)	1:85:A:GLN:HB2	1:98:A:PHE:HD2	14	1.06
(1,1543)	1:85:A:GLN:HB3	1:98:A:PHE:HD2	14	1.06
(1,1219)	1:111:A:TYR:H	1:115:A:ILE:HB	9	1.06
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	18	1.06
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	15	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	10	1.06
(1,316)	1:80:A:ILE:HB	1:104:A:LEU:HB3	19	1.06
(1,240)	1:47:A:THR:HG21	1:69:A:PRO:HG3	7	1.06
(1,240)	1:47:A:THR:HG22	1:69:A:PRO:HG3	7	1.06
(1,240)	1:47:A:THR:HG23	1:69:A:PRO:HG3	7	1.06
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG21	6	1.06
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG22	6	1.06
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG23	6	1.06
(1,165)	1:53:A:ARG:HG2	1:60:A:PHE:H	18	1.06
(1,39)	1:32:A:THR:HB	1:95:A:LYS:HB2	1	1.06
(1,1658)	1:126:A:GLU:HG3	1:128:A:LEU:HD11	9	1.05
(1,1658)	1:126:A:GLU:HG3	1:128:A:LEU:HD12	9	1.05
(1,1658)	1:126:A:GLU:HG3	1:128:A:LEU:HD13	9	1.05
(1,1658)	1:126:A:GLU:HG3	1:128:A:LEU:HD21	9	1.05
(1,1658)	1:126:A:GLU:HG3	1:128:A:LEU:HD22	9	1.05
(1,1658)	1:126:A:GLU:HG3	1:128:A:LEU:HD23	9	1.05
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	19	1.05
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	19	1.05
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	19	1.05
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	19	1.05
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	19	1.05
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	19	1.05
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	13	1.05
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	13	1.05
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	13	1.05
(1,923)	1:71:A:GLN:HE21	1:72:A:PHE:H	3	1.05
(1,758)	1:28:A:LYS:HG2	1:30:A:VAL:H	13	1.05
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	2	1.05
(1,685)	1:102:A:TYR:HE2	1:108:A:GLU:HG2	16	1.05
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	12	1.05
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	19	1.05
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	19	1.05
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	19	1.05
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	20	1.05
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	20	1.05
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	20	1.05
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG21	1	1.05
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG22	1	1.05
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG23	1	1.05
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG21	5	1.05
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG22	5	1.05
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG23	5	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG21	15	1.05
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG22	15	1.05
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG23	15	1.05
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	7	1.05
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	7	1.05
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	7	1.05
(1,602)	1:100:A:ILE:HD11	1:123:A:PHE:HB3	14	1.05
(1,602)	1:100:A:ILE:HD12	1:123:A:PHE:HB3	14	1.05
(1,602)	1:100:A:ILE:HD13	1:123:A:PHE:HB3	14	1.05
(1,539)	1:102:A:TYR:HE2	1:108:A:GLU:HA	11	1.05
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	20	1.05
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	20	1.05
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	20	1.05
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	14	1.05
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	14	1.05
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	14	1.05
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	14	1.05
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	14	1.05
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	14	1.05
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	14	1.05
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	14	1.05
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	14	1.05
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	17	1.05
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	17	1.05
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	17	1.05
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	17	1.05
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	17	1.05
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	17	1.05
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	17	1.05
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	17	1.05
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	17	1.05
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG21	2	1.05
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG22	2	1.05
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG23	2	1.05
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG21	16	1.05
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG22	16	1.05
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG23	16	1.05
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	5	1.05
(1,191)	1:54:A:PHE:HD1	1:58:A:LYS:HD3	15	1.05
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	18	1.05
(1,130)	1:48:A:VAL:HG11	1:50:A:TYR:HD1	4	1.05
(1,130)	1:48:A:VAL:HG12	1:50:A:TYR:HD1	4	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,130)	1:48:A:VAL:HG13	1:50:A:TYR:HD1	4	1.05
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	1	1.05
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	1	1.05
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	1	1.05
(1,68)	1:38:A:THR:HG21	1:92:A:LEU:HA	12	1.05
(1,68)	1:38:A:THR:HG22	1:92:A:LEU:HA	12	1.05
(1,68)	1:38:A:THR:HG23	1:92:A:LEU:HA	12	1.05
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE21	19	1.04
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	19	1.04
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD2	20	1.04
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD3	20	1.04
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD2	20	1.04
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD3	20	1.04
(1,1324)	1:19:A:PRO:HG2	1:55:A:PRO:HG2	14	1.04
(1,1324)	1:19:A:PRO:HG3	1:55:A:PRO:HG2	14	1.04
(1,923)	1:71:A:GLN:HE21	1:72:A:PHE:H	16	1.04
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	4	1.04
(1,789)	1:38:A:THR:H	1:91:A:THR:HG21	2	1.04
(1,789)	1:38:A:THR:H	1:91:A:THR:HG22	2	1.04
(1,789)	1:38:A:THR:H	1:91:A:THR:HG23	2	1.04
(1,688)	1:83:A:TRP:HD1	1:98:A:PHE:HD2	4	1.04
(1,678)	1:80:A:ILE:HD11	1:106:A:TYR:HE2	8	1.04
(1,678)	1:80:A:ILE:HD12	1:106:A:TYR:HE2	8	1.04
(1,678)	1:80:A:ILE:HD13	1:106:A:TYR:HE2	8	1.04
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	13	1.04
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	13	1.04
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	13	1.04
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	7	1.04
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	16	1.04
(1,193)	1:53:A:ARG:HB3	1:59:A:GLN:HA	10	1.04
(1,76)	1:38:A:THR:HB	1:40:A:PRO:HD3	18	1.04
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG21	4	1.04
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG22	4	1.04
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG23	4	1.04
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	11	1.03
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	11	1.03
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	11	1.03
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	11	1.03
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	11	1.03
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	11	1.03
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG11	3	1.03
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG12	3	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG13	3	1.03
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG21	3	1.03
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG22	3	1.03
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG23	3	1.03
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	16	1.03
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	16	1.03
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	16	1.03
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	16	1.03
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	16	1.03
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	16	1.03
(1,1262)	1:123:A:PHE:HD2	1:125:A:VAL:H	2	1.03
(1,923)	1:71:A:GLN:HE21	1:72:A:PHE:H	5	1.03
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	4	1.03
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG21	17	1.03
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG22	17	1.03
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG23	17	1.03
(1,602)	1:100:A:ILE:HD11	1:123:A:PHE:HB3	13	1.03
(1,602)	1:100:A:ILE:HD12	1:123:A:PHE:HB3	13	1.03
(1,602)	1:100:A:ILE:HD13	1:123:A:PHE:HB3	13	1.03
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	2	1.03
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD21	15	1.03
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD22	15	1.03
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD23	15	1.03
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	3	1.03
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	1	1.03
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	1	1.03
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	1	1.03
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	3	1.03
(1,68)	1:38:A:THR:HG21	1:92:A:LEU:HA	13	1.03
(1,68)	1:38:A:THR:HG22	1:92:A:LEU:HA	13	1.03
(1,68)	1:38:A:THR:HG23	1:92:A:LEU:HA	13	1.03
(1,27)	1:27:A:GLU:HG3	1:99:A:THR:HB	1	1.03
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	4	1.02
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	4	1.02
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	4	1.02
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	4	1.02
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	4	1.02
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	4	1.02
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	20	1.02
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	20	1.02
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	20	1.02
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	20	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	20	1.02
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	20	1.02
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE2	5	1.02
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE3	5	1.02
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE2	5	1.02
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE3	5	1.02
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	2	1.02
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	2	1.02
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	2	1.02
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	2	1.02
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	2	1.02
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	2	1.02
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	3	1.02
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	3	1.02
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	3	1.02
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	3	1.02
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	3	1.02
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	3	1.02
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG21	17	1.02
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG22	17	1.02
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG23	17	1.02
(1,1064)	1:81:A:LYS:HD3	1:85:A:GLN:H	8	1.02
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	1	1.02
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	1	1.02
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	1	1.02
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	5	1.02
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	5	1.02
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	5	1.02
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	16	1.02
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	16	1.02
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	16	1.02
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	6	1.02
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	6	1.02
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	6	1.02
(1,464)	1:27:A:GLU:HB2	1:99:A:THR:HB	18	1.02
(1,240)	1:47:A:THR:HG21	1:69:A:PRO:HG3	15	1.02
(1,240)	1:47:A:THR:HG22	1:69:A:PRO:HG3	15	1.02
(1,240)	1:47:A:THR:HG23	1:69:A:PRO:HG3	15	1.02
(1,176)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	16	1.02
(1,85)	1:42:A:ALA:HA	1:74:A:LEU:HD21	18	1.02
(1,85)	1:42:A:ALA:HA	1:74:A:LEU:HD22	18	1.02
(1,85)	1:42:A:ALA:HA	1:74:A:LEU:HD23	18	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	3	1.02
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	2	1.01
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	2	1.01
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	13	1.01
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	13	1.01
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE2	14	1.01
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE3	14	1.01
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE2	14	1.01
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE3	14	1.01
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	15	1.01
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	15	1.01
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	15	1.01
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	15	1.01
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	15	1.01
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	15	1.01
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	4	1.01
(1,1069)	1:86:A:GLY:H	1:98:A:PHE:HD2	5	1.01
(1,695)	1:83:A:TRP:HZ2	1:123:A:PHE:HD1	15	1.01
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	14	1.01
(1,632)	1:93:A:GLY:H	1:127:A:LEU:HG	19	1.01
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	18	1.01
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	20	1.01
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	20	1.01
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	20	1.01
(1,194)	1:53:A:ARG:HG2	1:59:A:GLN:HA	10	1.01
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	16	1.01
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	2	1.01
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	2	1.01
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	2	1.01
(1,1648)	1:121:A:LEU:HD11	1:123:A:PHE:HD1	12	1.0
(1,1648)	1:121:A:LEU:HD12	1:123:A:PHE:HD1	12	1.0
(1,1648)	1:121:A:LEU:HD13	1:123:A:PHE:HD1	12	1.0
(1,1648)	1:121:A:LEU:HD21	1:123:A:PHE:HD1	12	1.0
(1,1648)	1:121:A:LEU:HD22	1:123:A:PHE:HD1	12	1.0
(1,1648)	1:121:A:LEU:HD23	1:123:A:PHE:HD1	12	1.0
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	14	1.0
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	14	1.0
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	14	1.0
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	14	1.0
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	14	1.0
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	14	1.0
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	16	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	16	1.0
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	16	1.0
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	16	1.0
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	16	1.0
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	16	1.0
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD11	15	1.0
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD12	15	1.0
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD13	15	1.0
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD21	15	1.0
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD22	15	1.0
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD23	15	1.0
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG11	2	1.0
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG12	2	1.0
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG13	2	1.0
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG21	2	1.0
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG22	2	1.0
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG23	2	1.0
(1,1306)	1:81:A:LYS:HE2	1:85:A:GLN:HE21	15	1.0
(1,786)	1:38:A:THR:H	1:91:A:THR:HA	2	1.0
(1,758)	1:28:A:LYS:HG2	1:30:A:VAL:H	1	1.0
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	16	1.0
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	14	1.0
(1,544)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	11	1.0
(1,544)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	13	1.0
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	7	1.0
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	7	1.0
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	7	1.0
(1,518)	1:80:A:ILE:HA	1:105:A:ALA:HA	5	1.0
(1,516)	1:81:A:LYS:H	1:105:A:ALA:HA	5	1.0
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	17	1.0
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	17	1.0
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	17	1.0
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	13	1.0
(1,158)	1:52:A:GLY:HA2	1:123:A:PHE:HD1	5	1.0
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	7	1.0
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	7	1.0
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	7	1.0
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG21	18	1.0
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG22	18	1.0
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG23	18	1.0
(1,26)	1:27:A:GLU:HG3	1:99:A:THR:H	1	1.0
(1,26)	1:27:A:GLU:HG3	1:99:A:THR:H	14	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	6	0.99
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	6	0.99
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	6	0.99
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	6	0.99
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	6	0.99
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	6	0.99
(1,1307)	1:81:A:LYS:HE3	1:85:A:GLN:HE21	10	0.99
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	6	0.99
(1,1199)	1:80:A:ILE:HG21	1:105:A:ALA:H	9	0.99
(1,1199)	1:80:A:ILE:HG22	1:105:A:ALA:H	9	0.99
(1,1199)	1:80:A:ILE:HG23	1:105:A:ALA:H	9	0.99
(1,1185)	1:24:A:ALA:HB1	1:103:A:GLN:H	11	0.99
(1,1185)	1:24:A:ALA:HB2	1:103:A:GLN:H	11	0.99
(1,1185)	1:24:A:ALA:HB3	1:103:A:GLN:H	11	0.99
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	20	0.99
(1,1111)	1:38:A:THR:HG21	1:92:A:LEU:H	8	0.99
(1,1111)	1:38:A:THR:HG22	1:92:A:LEU:H	8	0.99
(1,1111)	1:38:A:THR:HG23	1:92:A:LEU:H	8	0.99
(1,1085)	1:89:A:THR:H	1:90:A:MET:HE1	1	0.99
(1,1085)	1:89:A:THR:H	1:90:A:MET:HE2	1	0.99
(1,1085)	1:89:A:THR:H	1:90:A:MET:HE3	1	0.99
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	3	0.99
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	8	0.99
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	8	0.99
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	8	0.99
(1,781)	1:37:A:VAL:H	1:91:A:THR:HB	7	0.99
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	17	0.99
(1,632)	1:93:A:GLY:H	1:127:A:LEU:HG	1	0.99
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	5	0.99
(1,383)	1:66:A:ARG:HG2	1:68:A:LYS:H	20	0.99
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD11	17	0.99
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD12	17	0.99
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD13	17	0.99
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG21	18	0.99
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG22	18	0.99
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG23	18	0.99
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	15	0.99
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE2	12	0.98
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE3	12	0.98
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE2	12	0.98
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE3	12	0.98
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	10	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	10	0.98
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	10	0.98
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	10	0.98
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	10	0.98
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	10	0.98
(1,1325)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	18	0.98
(1,1325)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	18	0.98
(1,1085)	1:89:A:THR:H	1:90:A:MET:HE1	11	0.98
(1,1085)	1:89:A:THR:H	1:90:A:MET:HE2	11	0.98
(1,1085)	1:89:A:THR:H	1:90:A:MET:HE3	11	0.98
(1,960)	1:50:A:TYR:HE2	1:70:A:PHE:H	13	0.98
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	6	0.98
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	8	0.98
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	6	0.98
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	6	0.98
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	6	0.98
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	12	0.98
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	12	0.98
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	12	0.98
(1,435)	1:94:A:GLU:HA	1:95:A:LYS:HB2	1	0.98
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	7	0.98
(1,240)	1:47:A:THR:HG21	1:69:A:PRO:HG3	16	0.98
(1,240)	1:47:A:THR:HG22	1:69:A:PRO:HG3	16	0.98
(1,240)	1:47:A:THR:HG23	1:69:A:PRO:HG3	16	0.98
(1,194)	1:53:A:ARG:HG2	1:59:A:GLN:HA	5	0.98
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	4	0.98
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	4	0.98
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	4	0.98
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	19	0.98
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	19	0.98
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	19	0.98
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	11	0.98
(1,76)	1:38:A:THR:HB	1:40:A:PRO:HD3	5	0.98
(1,75)	1:38:A:THR:HB	1:40:A:PRO:HG3	16	0.98
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG11	3	0.98
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG12	3	0.98
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG13	3	0.98
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	17	0.97
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	17	0.97
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	17	0.97
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	17	0.97
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	17	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	17	0.97
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	5	0.97
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	5	0.97
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	5	0.97
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	5	0.97
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	5	0.97
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	5	0.97
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	15	0.97
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	15	0.97
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	15	0.97
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	15	0.97
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	15	0.97
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	15	0.97
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD11	11	0.97
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD12	11	0.97
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD13	11	0.97
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD21	11	0.97
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD22	11	0.97
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD23	11	0.97
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG11	15	0.97
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG12	15	0.97
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG13	15	0.97
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG21	15	0.97
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG22	15	0.97
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG23	15	0.97
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG11	15	0.97
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG12	15	0.97
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG13	15	0.97
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG21	15	0.97
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG22	15	0.97
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG23	15	0.97
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	3	0.97
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	3	0.97
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	3	0.97
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	5	0.97
(1,686)	1:102:A:TYR:HE2	1:118:A:LYS:HA	18	0.97
(1,651)	1:92:A:LEU:HD11	1:129:A:ALA:HA	18	0.97
(1,651)	1:92:A:LEU:HD12	1:129:A:ALA:HA	18	0.97
(1,651)	1:92:A:LEU:HD13	1:129:A:ALA:HA	18	0.97
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	15	0.97
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	15	0.97
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	15	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	20	0.97
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	20	0.97
(1,240)	1:47:A:THR:HG21	1:69:A:PRO:HG3	13	0.97
(1,240)	1:47:A:THR:HG22	1:69:A:PRO:HG3	13	0.97
(1,240)	1:47:A:THR:HG23	1:69:A:PRO:HG3	13	0.97
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	6	0.97
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG21	4	0.97
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG22	4	0.97
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG23	4	0.97
(1,28)	1:27:A:GLU:HG2	1:99:A:THR:HB	6	0.97
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	1	0.96
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	1	0.96
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	1	0.96
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	1	0.96
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	1	0.96
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	1	0.96
(1,1252)	1:100:A:ILE:HD11	1:123:A:PHE:H	9	0.96
(1,1252)	1:100:A:ILE:HD12	1:123:A:PHE:H	9	0.96
(1,1252)	1:100:A:ILE:HD13	1:123:A:PHE:H	9	0.96
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	13	0.96
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	13	0.96
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	13	0.96
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	3	0.96
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	16	0.96
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG21	13	0.96
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG22	13	0.96
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG23	13	0.96
(1,580)	1:115:A:ILE:HD11	1:119:A:ALA:HB1	9	0.96
(1,580)	1:115:A:ILE:HD11	1:119:A:ALA:HB2	9	0.96
(1,580)	1:115:A:ILE:HD11	1:119:A:ALA:HB3	9	0.96
(1,580)	1:115:A:ILE:HD12	1:119:A:ALA:HB1	9	0.96
(1,580)	1:115:A:ILE:HD12	1:119:A:ALA:HB2	9	0.96
(1,580)	1:115:A:ILE:HD12	1:119:A:ALA:HB3	9	0.96
(1,580)	1:115:A:ILE:HD13	1:119:A:ALA:HB1	9	0.96
(1,580)	1:115:A:ILE:HD13	1:119:A:ALA:HB2	9	0.96
(1,580)	1:115:A:ILE:HD13	1:119:A:ALA:HB3	9	0.96
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	13	0.96
(1,554)	1:106:A:TYR:HB2	1:110:A:GLY:HA2	4	0.96
(1,546)	1:108:A:GLU:HG3	1:118:A:LYS:HG2	2	0.96
(1,545)	1:108:A:GLU:HG2	1:118:A:LYS:HG2	6	0.96
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	20	0.96
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	20	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	20	0.96
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	20	0.96
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB1	12	0.96
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB2	12	0.96
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB3	12	0.96
(1,369)	1:83:A:TRP:H	1:84:A:ASP:HB2	14	0.96
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG21	13	0.96
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG22	13	0.96
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG23	13	0.96
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	13	0.96
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	19	0.96
(1,198)	1:59:A:GLN:HG2	1:61:A:ASP:H	18	0.96
(1,194)	1:53:A:ARG:HG2	1:59:A:GLN:HA	8	0.96
(1,193)	1:53:A:ARG:HB3	1:59:A:GLN:HA	19	0.96
(1,166)	1:53:A:ARG:HG3	1:60:A:PHE:H	4	0.96
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	5	0.96
(1,78)	1:40:A:PRO:HD3	1:91:A:THR:HG21	11	0.96
(1,78)	1:40:A:PRO:HD3	1:91:A:THR:HG22	11	0.96
(1,78)	1:40:A:PRO:HD3	1:91:A:THR:HG23	11	0.96
(1,75)	1:38:A:THR:HB	1:40:A:PRO:HG3	19	0.96
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG21	5	0.96
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG22	5	0.96
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG23	5	0.96
(1,66)	1:37:A:VAL:H	1:38:A:THR:HG21	15	0.96
(1,66)	1:37:A:VAL:H	1:38:A:THR:HG22	15	0.96
(1,66)	1:37:A:VAL:H	1:38:A:THR:HG23	15	0.96
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	15	0.96
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	15	0.96
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	15	0.96
(1,1298)	1:92:A:LEU:HG	1:130:A:VAL:H	18	0.95
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	18	0.95
(1,983)	1:73:A:THR:H	1:78:A:GLU:HB2	4	0.95
(1,953)	1:49:A:HIS:HE1	1:68:A:LYS:H	13	0.95
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	13	0.95
(1,696)	1:83:A:TRP:HZ2	1:123:A:PHE:HB3	5	0.95
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG21	6	0.95
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG22	6	0.95
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG23	6	0.95
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	18	0.95
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	2	0.95
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	15	0.95
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	16	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	10	0.95
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	10	0.95
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	10	0.95
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	14	0.95
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	14	0.95
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	14	0.95
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	8	0.95
(1,185)	1:53:A:ARG:HB3	1:57:A:GLY:HA2	16	0.95
(1,154)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	3	0.95
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	15	0.95
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	15	0.95
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	15	0.95
(1,106)	1:45:A:LYS:H	1:45:A:LYS:HE3	16	0.95
(1,93)	1:41:A:GLN:HG3	1:44:A:LYS:HG2	19	0.95
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG21	11	0.95
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG22	11	0.95
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG23	11	0.95
(1,76)	1:38:A:THR:HB	1:40:A:PRO:HD3	13	0.95
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	3	0.95
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	3	0.95
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	3	0.95
(1,1543)	1:85:A:GLN:HB2	1:98:A:PHE:HD2	4	0.94
(1,1543)	1:85:A:GLN:HB3	1:98:A:PHE:HD2	4	0.94
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD2	20	0.94
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD3	20	0.94
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG2	1	0.94
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG3	1	0.94
(1,1386)	1:41:A:GLN:H	1:44:A:LYS:HG2	4	0.94
(1,1386)	1:41:A:GLN:H	1:44:A:LYS:HG3	4	0.94
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG11	8	0.94
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG12	8	0.94
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG13	8	0.94
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG21	8	0.94
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG22	8	0.94
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG23	8	0.94
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG11	8	0.94
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG12	8	0.94
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG13	8	0.94
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG21	8	0.94
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG22	8	0.94
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG23	8	0.94
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	13	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	6	0.94
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	10	0.94
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	10	0.94
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	10	0.94
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	13	0.94
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	13	0.94
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	13	0.94
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	17	0.94
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	17	0.94
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	17	0.94
(1,923)	1:71:A:GLN:HE21	1:72:A:PHE:H	8	0.94
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	6	0.94
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	6	0.94
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	6	0.94
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	5	0.94
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	5	0.94
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	5	0.94
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG21	2	0.94
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG22	2	0.94
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG23	2	0.94
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG21	13	0.94
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG22	13	0.94
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG23	13	0.94
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	1	0.94
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	11	0.94
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	11	0.94
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	11	0.94
(1,68)	1:38:A:THR:HG21	1:92:A:LEU:HA	8	0.94
(1,68)	1:38:A:THR:HG22	1:92:A:LEU:HA	8	0.94
(1,68)	1:38:A:THR:HG23	1:92:A:LEU:HA	8	0.94
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	12	0.94
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	12	0.94
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	12	0.94
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	14	0.94
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	14	0.94
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	14	0.94
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG21	10	0.94
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG22	10	0.94
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG23	10	0.94
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	4	0.93
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	4	0.93
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	4	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	4	0.93
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	4	0.93
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	4	0.93
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	15	0.93
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	15	0.93
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	15	0.93
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	15	0.93
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	15	0.93
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	15	0.93
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD2	12	0.93
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD3	12	0.93
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE2	8	0.93
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE3	8	0.93
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE2	8	0.93
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE3	8	0.93
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG11	7	0.93
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG12	7	0.93
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG13	7	0.93
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG21	7	0.93
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG22	7	0.93
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG23	7	0.93
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	5	0.93
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	5	0.93
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	5	0.93
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	5	0.93
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	5	0.93
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	5	0.93
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	4	0.93
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	17	0.93
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	11	0.93
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	11	0.93
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	11	0.93
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	6	0.93
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	15	0.93
(1,1064)	1:81:A:LYS:HD3	1:85:A:GLN:H	19	0.93
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	16	0.93
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	16	0.93
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	16	0.93
(1,1025)	1:82:A:GLY:H	1:104:A:LEU:HA	1	0.93
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	18	0.93
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	18	0.93
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	18	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	1	0.93
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	1	0.93
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	1	0.93
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	19	0.93
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	14	0.93
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	14	0.93
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	14	0.93
(1,631)	1:92:A:LEU:H	1:127:A:LEU:HG	7	0.93
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	2	0.93
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	1	0.93
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	1	0.93
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	1	0.93
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	12	0.93
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	12	0.93
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	12	0.93
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	20	0.93
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	20	0.93
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	20	0.93
(1,449)	1:32:A:THR:HB	1:95:A:LYS:HE2	11	0.93
(1,310)	1:80:A:ILE:HA	1:81:A:LYS:HG2	14	0.93
(1,193)	1:53:A:ARG:HB3	1:59:A:GLN:HA	7	0.93
(1,158)	1:52:A:GLY:HA2	1:123:A:PHE:HD1	11	0.93
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	13	0.93
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB2	11	0.92
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB3	11	0.92
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB2	11	0.92
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB3	11	0.92
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	18	0.92
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	18	0.92
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	18	0.92
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	18	0.92
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	18	0.92
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	18	0.92
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD11	8	0.92
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD12	8	0.92
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD13	8	0.92
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD21	8	0.92
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD22	8	0.92
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD23	8	0.92
(1,1310)	1:81:A:LYS:HE2	1:85:A:GLN:HE22	16	0.92
(1,1248)	1:123:A:PHE:H	1:123:A:PHE:HD1	6	0.92
(1,1235)	1:55:A:PRO:HG3	1:120:A:THR:H	13	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	5	0.92
(1,1104)	1:91:A:THR:H	1:127:A:LEU:HG	7	0.92
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	18	0.92
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	9	0.92
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	9	0.92
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	9	0.92
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	7	0.92
(1,582)	1:55:A:PRO:HG2	1:120:A:THR:HB	1	0.92
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	1	0.92
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	1	0.92
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	1	0.92
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	3	0.92
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	3	0.92
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	3	0.92
(1,415)	1:90:A:MET:HE1	1:94:A:GLU:HA	7	0.92
(1,415)	1:90:A:MET:HE2	1:94:A:GLU:HA	7	0.92
(1,415)	1:90:A:MET:HE3	1:94:A:GLU:HA	7	0.92
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG21	3	0.92
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG22	3	0.92
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG23	3	0.92
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD21	17	0.92
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD22	17	0.92
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD23	17	0.92
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	17	0.92
(1,183)	1:53:A:ARG:HD2	1:57:A:GLY:HA2	16	0.92
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	3	0.92
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	3	0.92
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	3	0.92
(1,1648)	1:121:A:LEU:HD11	1:123:A:PHE:HD1	20	0.91
(1,1648)	1:121:A:LEU:HD12	1:123:A:PHE:HD1	20	0.91
(1,1648)	1:121:A:LEU:HD13	1:123:A:PHE:HD1	20	0.91
(1,1648)	1:121:A:LEU:HD21	1:123:A:PHE:HD1	20	0.91
(1,1648)	1:121:A:LEU:HD22	1:123:A:PHE:HD1	20	0.91
(1,1648)	1:121:A:LEU:HD23	1:123:A:PHE:HD1	20	0.91
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	13	0.91
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	13	0.91
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	13	0.91
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	13	0.91
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	13	0.91
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	13	0.91
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	3	0.91
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	3	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	3	0.91
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	3	0.91
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	3	0.91
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	3	0.91
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD11	9	0.91
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD12	9	0.91
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD13	9	0.91
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD21	9	0.91
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD22	9	0.91
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD23	9	0.91
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD11	19	0.91
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD12	19	0.91
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD13	19	0.91
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD21	19	0.91
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD22	19	0.91
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD23	19	0.91
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD2	10	0.91
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD3	10	0.91
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD11	14	0.91
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD12	14	0.91
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD13	14	0.91
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD21	14	0.91
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD22	14	0.91
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD23	14	0.91
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD11	14	0.91
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD12	14	0.91
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD13	14	0.91
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD21	14	0.91
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD22	14	0.91
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD23	14	0.91
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD11	14	0.91
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD12	14	0.91
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD13	14	0.91
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD21	14	0.91
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD22	14	0.91
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD23	14	0.91
(1,1323)	1:19:A:PRO:HG2	1:55:A:PRO:HB2	17	0.91
(1,1323)	1:19:A:PRO:HG3	1:55:A:PRO:HB2	17	0.91
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	11	0.91
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	11	0.91
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	11	0.91
(1,1252)	1:100:A:ILE:HD11	1:123:A:PHE:H	13	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1252)	1:100:A:ILE:HD12	1:123:A:PHE:H	13	0.91
(1,1252)	1:100:A:ILE:HD13	1:123:A:PHE:H	13	0.91
(1,1248)	1:123:A:PHE:H	1:123:A:PHE:HD1	7	0.91
(1,1069)	1:86:A:GLY:H	1:98:A:PHE:HD2	4	0.91
(1,820)	1:44:A:LYS:H	1:44:A:LYS:HG3	17	0.91
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	19	0.91
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	19	0.91
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	19	0.91
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	16	0.91
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	16	0.91
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	16	0.91
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB1	10	0.91
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB2	10	0.91
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB3	10	0.91
(1,198)	1:59:A:GLN:HG2	1:61:A:ASP:H	14	0.91
(1,27)	1:27:A:GLU:HG3	1:99:A:THR:HB	18	0.91
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	14	0.9
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	14	0.9
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	14	0.9
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	14	0.9
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	14	0.9
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	14	0.9
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	20	0.9
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	20	0.9
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	20	0.9
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	20	0.9
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	20	0.9
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	20	0.9
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	13	0.9
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	13	0.9
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	13	0.9
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	13	0.9
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	13	0.9
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	13	0.9
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD11	10	0.9
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD12	10	0.9
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD13	10	0.9
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD21	10	0.9
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD22	10	0.9
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD23	10	0.9
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG2	15	0.9
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG3	15	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1323)	1:19:A:PRO:HG2	1:55:A:PRO:HB2	20	0.9
(1,1323)	1:19:A:PRO:HG3	1:55:A:PRO:HB2	20	0.9
(1,1311)	1:81:A:LYS:HE3	1:85:A:GLN:HE22	19	0.9
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	11	0.9
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	11	0.9
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	11	0.9
(1,1300)	1:92:A:LEU:HD21	1:130:A:VAL:H	17	0.9
(1,1300)	1:92:A:LEU:HD22	1:130:A:VAL:H	17	0.9
(1,1300)	1:92:A:LEU:HD23	1:130:A:VAL:H	17	0.9
(1,1248)	1:123:A:PHE:H	1:123:A:PHE:HD1	20	0.9
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	7	0.9
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	7	0.9
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	7	0.9
(1,1219)	1:111:A:TYR:H	1:115:A:ILE:HB	4	0.9
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	18	0.9
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	8	0.9
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	3	0.9
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	3	0.9
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	3	0.9
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG21	11	0.9
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG22	11	0.9
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG23	11	0.9
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD11	12	0.9
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD12	12	0.9
(1,559)	1:111:A:TYR:HB2	1:115:A:ILE:HD13	12	0.9
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	3	0.9
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	3	0.9
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	3	0.9
(1,225)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	4	0.9
(1,211)	1:49:A:HIS:HB3	1:64:A:ARG:HA	8	0.9
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	10	0.9
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	10	0.9
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	10	0.9
(1,167)	1:53:A:ARG:HG2	1:54:A:PHE:HD1	4	0.9
(1,28)	1:27:A:GLU:HG2	1:99:A:THR:HB	9	0.9
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD11	20	0.89
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD12	20	0.89
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD13	20	0.89
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD21	20	0.89
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD22	20	0.89
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD23	20	0.89
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD2	19	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD3	19	0.89
(1,1346)	1:28:A:LYS:HG2	1:30:A:VAL:H	3	0.89
(1,1346)	1:28:A:LYS:HG3	1:30:A:VAL:H	3	0.89
(1,1328)	1:19:A:PRO:HG2	1:56:A:ASP:HA	7	0.89
(1,1328)	1:19:A:PRO:HG3	1:56:A:ASP:HA	7	0.89
(1,1310)	1:81:A:LYS:HE2	1:85:A:GLN:HE22	11	0.89
(1,1309)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	12	0.89
(1,1306)	1:81:A:LYS:HE2	1:85:A:GLN:HE21	2	0.89
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	2	0.89
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	2	0.89
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	2	0.89
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	4	0.89
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	4	0.89
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	4	0.89
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	14	0.89
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	14	0.89
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	14	0.89
(1,960)	1:50:A:TYR:HE2	1:70:A:PHE:H	19	0.89
(1,953)	1:49:A:HIS:HE1	1:68:A:LYS:H	9	0.89
(1,686)	1:102:A:TYR:HE2	1:118:A:LYS:HA	11	0.89
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG21	7	0.89
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG22	7	0.89
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG23	7	0.89
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	7	0.89
(1,519)	1:80:A:ILE:HB	1:105:A:ALA:HA	1	0.89
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	18	0.89
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	18	0.89
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	18	0.89
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	1	0.89
(1,449)	1:32:A:THR:HB	1:95:A:LYS:HE2	5	0.89
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	11	0.89
(1,158)	1:52:A:GLY:HA2	1:123:A:PHE:HD1	15	0.89
(1,76)	1:38:A:THR:HB	1:40:A:PRO:HD3	14	0.89
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG21	6	0.89
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG22	6	0.89
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG23	6	0.89
(1,1601)	1:97:A:LEU:HD11	1:124:A:GLU:HG3	9	0.88
(1,1601)	1:97:A:LEU:HD12	1:124:A:GLU:HG3	9	0.88
(1,1601)	1:97:A:LEU:HD13	1:124:A:GLU:HG3	9	0.88
(1,1601)	1:97:A:LEU:HD21	1:124:A:GLU:HG3	9	0.88
(1,1601)	1:97:A:LEU:HD22	1:124:A:GLU:HG3	9	0.88
(1,1601)	1:97:A:LEU:HD23	1:124:A:GLU:HG3	9	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD2	11	0.88
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD3	11	0.88
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	5	0.88
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	5	0.88
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	5	0.88
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	5	0.88
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	5	0.88
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	5	0.88
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	5	0.88
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	5	0.88
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	5	0.88
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	5	0.88
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	5	0.88
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	5	0.88
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	5	0.88
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	5	0.88
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	5	0.88
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	5	0.88
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	5	0.88
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	5	0.88
(1,1085)	1:89:A:THR:H	1:90:A:MET:HE1	6	0.88
(1,1085)	1:89:A:THR:H	1:90:A:MET:HE2	6	0.88
(1,1085)	1:89:A:THR:H	1:90:A:MET:HE3	6	0.88
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	3	0.88
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	12	0.88
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG11	13	0.88
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG12	13	0.88
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG13	13	0.88
(1,758)	1:28:A:LYS:HG2	1:30:A:VAL:H	20	0.88
(1,686)	1:102:A:TYR:HE2	1:118:A:LYS:HA	19	0.88
(1,682)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	12	0.88
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	8	0.88
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	8	0.88
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	8	0.88
(1,602)	1:100:A:ILE:HD11	1:123:A:PHE:HB3	4	0.88
(1,602)	1:100:A:ILE:HD12	1:123:A:PHE:HB3	4	0.88
(1,602)	1:100:A:ILE:HD13	1:123:A:PHE:HB3	4	0.88
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	20	0.88
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	20	0.88
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	20	0.88
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	17	0.88
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	11	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	11	0.88
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	11	0.88
(1,403)	1:89:A:THR:HG21	1:98:A:PHE:HD2	1	0.88
(1,403)	1:89:A:THR:HG22	1:98:A:PHE:HD2	1	0.88
(1,403)	1:89:A:THR:HG23	1:98:A:PHE:HD2	1	0.88
(1,393)	1:74:A:LEU:HD21	1:88:A:ALA:HA	11	0.88
(1,393)	1:74:A:LEU:HD22	1:88:A:ALA:HA	11	0.88
(1,393)	1:74:A:LEU:HD23	1:88:A:ALA:HA	11	0.88
(1,240)	1:47:A:THR:HG21	1:69:A:PRO:HG3	6	0.88
(1,240)	1:47:A:THR:HG22	1:69:A:PRO:HG3	6	0.88
(1,240)	1:47:A:THR:HG23	1:69:A:PRO:HG3	6	0.88
(1,194)	1:53:A:ARG:HG2	1:59:A:GLN:HA	19	0.88
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	7	0.88
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	17	0.88
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG21	5	0.88
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG22	5	0.88
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG23	5	0.88
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	10	0.88
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	6	0.87
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	6	0.87
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	6	0.87
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	6	0.87
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	6	0.87
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	6	0.87
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD2	4	0.87
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD3	4	0.87
(1,1442)	1:53:A:ARG:HD2	1:59:A:GLN:HA	4	0.87
(1,1442)	1:53:A:ARG:HD3	1:59:A:GLN:HA	4	0.87
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	8	0.87
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	16	0.87
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	19	0.87
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG11	7	0.87
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG12	7	0.87
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG13	7	0.87
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	11	0.87
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	1	0.87
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	2	0.87
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	2	0.87
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	2	0.87
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	8	0.87
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	8	0.87
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	8	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:32:A:THR:HB	1:95:A:LYS:HE3	11	0.87
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD11	13	0.87
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD12	13	0.87
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD13	13	0.87
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD21	1	0.87
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD22	1	0.87
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD23	1	0.87
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	6	0.87
(1,225)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	6	0.87
(1,211)	1:49:A:HIS:HB3	1:64:A:ARG:HA	6	0.87
(1,192)	1:59:A:GLN:HA	1:61:A:ASP:H	5	0.87
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	9	0.87
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	9	0.87
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	9	0.87
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	18	0.87
(1,130)	1:48:A:VAL:HG11	1:50:A:TYR:HD1	1	0.87
(1,130)	1:48:A:VAL:HG12	1:50:A:TYR:HD1	1	0.87
(1,130)	1:48:A:VAL:HG13	1:50:A:TYR:HD1	1	0.87
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG21	6	0.87
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG22	6	0.87
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG23	6	0.87
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	16	0.87
(1,1475)	1:59:A:GLN:HG2	1:61:A:ASP:H	16	0.86
(1,1475)	1:59:A:GLN:HG3	1:61:A:ASP:H	16	0.86
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD2	1	0.86
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD3	1	0.86
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD2	9	0.86
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD3	9	0.86
(1,1440)	1:53:A:ARG:HD2	1:57:A:GLY:H	3	0.86
(1,1440)	1:53:A:ARG:HD3	1:57:A:GLY:H	3	0.86
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG2	19	0.86
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG3	19	0.86
(1,1298)	1:92:A:LEU:HG	1:130:A:VAL:H	4	0.86
(1,1248)	1:123:A:PHE:H	1:123:A:PHE:HD1	12	0.86
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	19	0.86
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	19	0.86
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	19	0.86
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	1	0.86
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	20	0.86
(1,1195)	1:80:A:ILE:HB	1:105:A:ALA:H	16	0.86
(1,1025)	1:82:A:GLY:H	1:104:A:LEU:HA	4	0.86
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	7	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	7	0.86
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	7	0.86
(1,1004)	1:73:A:THR:HG21	1:76:A:ALA:H	12	0.86
(1,1004)	1:73:A:THR:HG22	1:76:A:ALA:H	12	0.86
(1,1004)	1:73:A:THR:HG23	1:76:A:ALA:H	12	0.86
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	10	0.86
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG21	8	0.86
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG22	8	0.86
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG23	8	0.86
(1,604)	1:123:A:PHE:HD2	1:124:A:GLU:HA	2	0.86
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	1	0.86
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	1	0.86
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	1	0.86
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	11	0.86
(1,211)	1:49:A:HIS:HB3	1:64:A:ARG:HA	17	0.86
(1,199)	1:59:A:GLN:HG3	1:61:A:ASP:H	16	0.86
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	5	0.86
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB2	6	0.85
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB3	6	0.85
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB2	6	0.85
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB3	6	0.85
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG11	3	0.85
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG12	3	0.85
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG13	3	0.85
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG21	3	0.85
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG22	3	0.85
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG23	3	0.85
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE2	2	0.85
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE3	2	0.85
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE2	2	0.85
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE3	2	0.85
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	7	0.85
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	7	0.85
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	15	0.85
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	7	0.85
(1,1105)	1:38:A:THR:H	1:92:A:LEU:H	7	0.85
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	14	0.85
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	14	0.85
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	14	0.85
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	20	0.85
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	19	0.85
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	19	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	19	0.85
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	6	0.85
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	6	0.85
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	6	0.85
(1,602)	1:100:A:ILE:HD11	1:123:A:PHE:HB3	1	0.85
(1,602)	1:100:A:ILE:HD12	1:123:A:PHE:HB3	1	0.85
(1,602)	1:100:A:ILE:HD13	1:123:A:PHE:HB3	1	0.85
(1,546)	1:108:A:GLU:HG3	1:118:A:LYS:HG2	18	0.85
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	16	0.85
(1,276)	1:74:A:LEU:HD11	1:88:A:ALA:H	4	0.85
(1,276)	1:74:A:LEU:HD12	1:88:A:ALA:H	4	0.85
(1,276)	1:74:A:LEU:HD13	1:88:A:ALA:H	4	0.85
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD21	15	0.85
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD22	15	0.85
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD23	15	0.85
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	4	0.85
(1,226)	1:49:A:HIS:HE1	1:67:A:GLY:HA2	15	0.85
(1,225)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	5	0.85
(1,177)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	10	0.85
(1,92)	1:41:A:GLN:HG2	1:44:A:LYS:HG2	3	0.85
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	1	0.85
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	1	0.85
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	1	0.85
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	6	0.85
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	6	0.85
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	6	0.85
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB2	3	0.84
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB3	3	0.84
(1,1394)	1:41:A:GLN:HE21	1:44:A:LYS:HG2	3	0.84
(1,1394)	1:41:A:GLN:HE21	1:44:A:LYS:HG3	3	0.84
(1,1394)	1:41:A:GLN:HE22	1:44:A:LYS:HG2	3	0.84
(1,1394)	1:41:A:GLN:HE22	1:44:A:LYS:HG3	3	0.84
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG11	3	0.84
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG12	3	0.84
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG13	3	0.84
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG21	3	0.84
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG22	3	0.84
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG23	3	0.84
(1,1328)	1:19:A:PRO:HG2	1:56:A:ASP:HA	17	0.84
(1,1328)	1:19:A:PRO:HG3	1:56:A:ASP:HA	17	0.84
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	4	0.84
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	20	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	19	0.84
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	1	0.84
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	1	0.84
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	1	0.84
(1,800)	1:41:A:GLN:H	1:44:A:LYS:HB2	4	0.84
(1,758)	1:28:A:LYS:HG2	1:30:A:VAL:H	14	0.84
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	13	0.84
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	13	0.84
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	13	0.84
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	13	0.84
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG21	9	0.84
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG22	9	0.84
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG23	9	0.84
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG21	18	0.84
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG22	18	0.84
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG23	18	0.84
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	7	0.84
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	7	0.84
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	7	0.84
(1,547)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	5	0.84
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	15	0.84
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	15	0.84
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	15	0.84
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD21	8	0.84
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD22	8	0.84
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD23	8	0.84
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	18	0.84
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	19	0.84
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	19	0.84
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	19	0.84
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	19	0.84
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	19	0.84
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	19	0.84
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	19	0.84
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	19	0.84
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	19	0.84
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	13	0.84
(1,265)	1:42:A:ALA:H	1:74:A:LEU:HB3	18	0.84
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	18	0.84
(1,194)	1:53:A:ARG:HG2	1:59:A:GLN:HA	7	0.84
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	1	0.84
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	1	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	1	0.84
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	7	0.84
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	16	0.84
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	16	0.84
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	16	0.84
(1,1648)	1:121:A:LEU:HD11	1:123:A:PHE:HD1	7	0.83
(1,1648)	1:121:A:LEU:HD12	1:123:A:PHE:HD1	7	0.83
(1,1648)	1:121:A:LEU:HD13	1:123:A:PHE:HD1	7	0.83
(1,1648)	1:121:A:LEU:HD21	1:123:A:PHE:HD1	7	0.83
(1,1648)	1:121:A:LEU:HD22	1:123:A:PHE:HD1	7	0.83
(1,1648)	1:121:A:LEU:HD23	1:123:A:PHE:HD1	7	0.83
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD2	10	0.83
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD3	10	0.83
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	15	0.83
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	15	0.83
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	15	0.83
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	15	0.83
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	15	0.83
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	15	0.83
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	7	0.83
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	7	0.83
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	7	0.83
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	7	0.83
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	7	0.83
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	7	0.83
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG11	11	0.83
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG12	11	0.83
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG13	11	0.83
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG21	11	0.83
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG22	11	0.83
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG23	11	0.83
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB2	6	0.83
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB3	6	0.83
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	15	0.83
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	15	0.83
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	15	0.83
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	14	0.83
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	11	0.83
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	12	0.83
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	12	0.83
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	12	0.83
(1,546)	1:108:A:GLU:HG3	1:118:A:LYS:HG2	12	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	3	0.83
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	3	0.83
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	3	0.83
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	3	0.83
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	3	0.83
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	3	0.83
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	3	0.83
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	3	0.83
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	3	0.83
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG21	1	0.83
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG22	1	0.83
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG23	1	0.83
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	10	0.83
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG11	11	0.83
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG12	11	0.83
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG13	11	0.83
(1,130)	1:48:A:VAL:HG11	1:50:A:TYR:HD1	15	0.83
(1,130)	1:48:A:VAL:HG12	1:50:A:TYR:HD1	15	0.83
(1,130)	1:48:A:VAL:HG13	1:50:A:TYR:HD1	15	0.83
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	19	0.83
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB2	13	0.82
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB3	13	0.82
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB2	13	0.82
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB3	13	0.82
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	11	0.82
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	11	0.82
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	11	0.82
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	11	0.82
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	11	0.82
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	11	0.82
(1,1599)	1:97:A:LEU:HD11	1:124:A:GLU:HB3	2	0.82
(1,1599)	1:97:A:LEU:HD12	1:124:A:GLU:HB3	2	0.82
(1,1599)	1:97:A:LEU:HD13	1:124:A:GLU:HB3	2	0.82
(1,1599)	1:97:A:LEU:HD21	1:124:A:GLU:HB3	2	0.82
(1,1599)	1:97:A:LEU:HD22	1:124:A:GLU:HB3	2	0.82
(1,1599)	1:97:A:LEU:HD23	1:124:A:GLU:HB3	2	0.82
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	6	0.82
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	6	0.82
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	6	0.82
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	6	0.82
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	6	0.82
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	6	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	10	0.82
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	10	0.82
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	10	0.82
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	10	0.82
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	10	0.82
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	10	0.82
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD2	5	0.82
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD3	5	0.82
(1,1323)	1:19:A:PRO:HG2	1:55:A:PRO:HB2	7	0.82
(1,1323)	1:19:A:PRO:HG3	1:55:A:PRO:HB2	7	0.82
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	2	0.82
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	2	0.82
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	2	0.82
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	4	0.82
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG11	17	0.82
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG12	17	0.82
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG13	17	0.82
(1,694)	1:80:A:ILE:HD11	1:83:A:TRP:HD1	16	0.82
(1,694)	1:80:A:ILE:HD12	1:83:A:TRP:HD1	16	0.82
(1,694)	1:80:A:ILE:HD13	1:83:A:TRP:HD1	16	0.82
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB1	3	0.82
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB2	3	0.82
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB3	3	0.82
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	19	0.82
(1,602)	1:100:A:ILE:HD11	1:123:A:PHE:HB3	3	0.82
(1,602)	1:100:A:ILE:HD12	1:123:A:PHE:HB3	3	0.82
(1,602)	1:100:A:ILE:HD13	1:123:A:PHE:HB3	3	0.82
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	3	0.82
(1,557)	1:110:A:GLY:HA3	1:115:A:ILE:HB	14	0.82
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	17	0.82
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	13	0.82
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	13	0.82
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	13	0.82
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	2	0.82
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	2	0.82
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	2	0.82
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	7	0.82
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	7	0.82
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	7	0.82
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG21	4	0.82
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG22	4	0.82
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG23	4	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	17	0.82
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD21	16	0.82
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD22	16	0.82
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD23	16	0.82
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	19	0.82
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	16	0.82
(1,89)	1:42:A:ALA:HB1	1:74:A:LEU:HA	14	0.82
(1,89)	1:42:A:ALA:HB2	1:74:A:LEU:HA	14	0.82
(1,89)	1:42:A:ALA:HB3	1:74:A:LEU:HA	14	0.82
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	15	0.82
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	16	0.82
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	16	0.82
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	16	0.82
(1,28)	1:27:A:GLU:HG2	1:99:A:THR:HB	17	0.82
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	20	0.82
(1,1625)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	14	0.81
(1,1625)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	14	0.81
(1,1310)	1:81:A:LYS:HE2	1:85:A:GLN:HE22	6	0.81
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	8	0.81
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	8	0.81
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	8	0.81
(1,751)	1:27:A:GLU:HG2	1:28:A:LYS:H	1	0.81
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	11	0.81
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	11	0.81
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	11	0.81
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG21	9	0.81
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG22	9	0.81
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG23	9	0.81
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	15	0.81
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	15	0.81
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	15	0.81
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	15	0.81
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	15	0.81
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	15	0.81
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	15	0.81
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	15	0.81
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	15	0.81
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	18	0.81
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	18	0.81
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	18	0.81
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	18	0.81
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	18	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	18	0.81
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	18	0.81
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	18	0.81
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	18	0.81
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	8	0.81
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	10	0.81
(1,28)	1:27:A:GLU:HG2	1:99:A:THR:HB	20	0.81
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	16	0.81
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	16	0.8
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	16	0.8
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	16	0.8
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	16	0.8
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	16	0.8
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	16	0.8
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG11	9	0.8
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG12	9	0.8
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG13	9	0.8
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG21	9	0.8
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG22	9	0.8
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG23	9	0.8
(1,1324)	1:19:A:PRO:HG2	1:55:A:PRO:HG2	16	0.8
(1,1324)	1:19:A:PRO:HG3	1:55:A:PRO:HG2	16	0.8
(1,1248)	1:123:A:PHE:H	1:123:A:PHE:HD1	10	0.8
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	7	0.8
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	20	0.8
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	20	0.8
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	20	0.8
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	17	0.8
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	17	0.8
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	17	0.8
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG21	10	0.8
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG22	10	0.8
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG23	10	0.8
(1,751)	1:27:A:GLU:HG2	1:28:A:LYS:H	15	0.8
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	19	0.8
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	13	0.8
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	10	0.8
(1,539)	1:102:A:TYR:HE2	1:108:A:GLU:HA	19	0.8
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD11	20	0.8
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD12	20	0.8
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD13	20	0.8
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD11	20	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD12	20	0.8
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD13	20	0.8
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD11	20	0.8
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD12	20	0.8
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD13	20	0.8
(1,375)	1:74:A:LEU:HD11	1:84:A:ASP:HB3	7	0.8
(1,375)	1:74:A:LEU:HD12	1:84:A:ASP:HB3	7	0.8
(1,375)	1:74:A:LEU:HD13	1:84:A:ASP:HB3	7	0.8
(1,329)	1:72:A:PHE:HD2	1:79:A:VAL:HG21	20	0.8
(1,329)	1:72:A:PHE:HD2	1:79:A:VAL:HG22	20	0.8
(1,329)	1:72:A:PHE:HD2	1:79:A:VAL:HG23	20	0.8
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG21	5	0.8
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG22	5	0.8
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG23	5	0.8
(1,310)	1:80:A:ILE:HA	1:81:A:LYS:HG2	19	0.8
(1,240)	1:47:A:THR:HG21	1:69:A:PRO:HG3	19	0.8
(1,240)	1:47:A:THR:HG22	1:69:A:PRO:HG3	19	0.8
(1,240)	1:47:A:THR:HG23	1:69:A:PRO:HG3	19	0.8
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	12	0.8
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	5	0.8
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	5	0.8
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	5	0.8
(1,155)	1:51:A:ASP:HB3	1:124:A:GLU:H	20	0.8
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	20	0.8
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG21	8	0.8
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG22	8	0.8
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG23	8	0.8
(1,27)	1:27:A:GLU:HG3	1:99:A:THR:HB	14	0.8
(1,1625)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	3	0.79
(1,1625)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	3	0.79
(1,1594)	1:97:A:LEU:HD11	1:123:A:PHE:H	18	0.79
(1,1594)	1:97:A:LEU:HD12	1:123:A:PHE:H	18	0.79
(1,1594)	1:97:A:LEU:HD13	1:123:A:PHE:H	18	0.79
(1,1594)	1:97:A:LEU:HD21	1:123:A:PHE:H	18	0.79
(1,1594)	1:97:A:LEU:HD22	1:123:A:PHE:H	18	0.79
(1,1594)	1:97:A:LEU:HD23	1:123:A:PHE:H	18	0.79
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	9	0.79
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	9	0.79
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	9	0.79
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	9	0.79
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	9	0.79
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	9	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	6	0.79
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	6	0.79
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	6	0.79
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	6	0.79
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	6	0.79
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	6	0.79
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	6	0.79
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	6	0.79
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	6	0.79
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	6	0.79
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	6	0.79
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	6	0.79
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	6	0.79
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	6	0.79
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	6	0.79
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	6	0.79
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	6	0.79
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	6	0.79
(1,1346)	1:28:A:LYS:HG2	1:30:A:VAL:H	10	0.79
(1,1346)	1:28:A:LYS:HG3	1:30:A:VAL:H	10	0.79
(1,1306)	1:81:A:LYS:HE2	1:85:A:GLN:HE21	8	0.79
(1,1248)	1:123:A:PHE:H	1:123:A:PHE:HD1	1	0.79
(1,1130)	1:90:A:MET:HE1	1:95:A:LYS:H	9	0.79
(1,1130)	1:90:A:MET:HE2	1:95:A:LYS:H	9	0.79
(1,1130)	1:90:A:MET:HE3	1:95:A:LYS:H	9	0.79
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	3	0.79
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	14	0.79
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	10	0.79
(1,682)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	19	0.79
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	5	0.79
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	14	0.79
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	14	0.79
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	14	0.79
(1,632)	1:93:A:GLY:H	1:127:A:LEU:HG	6	0.79
(1,557)	1:110:A:GLY:HA3	1:115:A:ILE:HB	18	0.79
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	18	0.79
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	18	0.79
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	18	0.79
(1,494)	1:102:A:TYR:HB2	1:102:A:TYR:HE2	4	0.79
(1,494)	1:102:A:TYR:HB2	1:102:A:TYR:HE2	17	0.79
(1,421)	1:91:A:THR:HA	1:127:A:LEU:HG	7	0.79
(1,385)	1:82:A:GLY:HA2	1:85:A:GLN:HB3	16	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	15	0.79
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	15	0.79
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	15	0.79
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD21	1	0.79
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD22	1	0.79
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD23	1	0.79
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG21	19	0.79
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG22	19	0.79
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG23	19	0.79
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	15	0.79
(1,198)	1:59:A:GLN:HG2	1:61:A:ASP:H	15	0.79
(1,152)	1:51:A:ASP:HB2	1:124:A:GLU:H	17	0.79
(1,89)	1:42:A:ALA:HB1	1:74:A:LEU:HA	17	0.79
(1,89)	1:42:A:ALA:HB2	1:74:A:LEU:HA	17	0.79
(1,89)	1:42:A:ALA:HB3	1:74:A:LEU:HA	17	0.79
(1,89)	1:42:A:ALA:HB1	1:74:A:LEU:HA	18	0.79
(1,89)	1:42:A:ALA:HB2	1:74:A:LEU:HA	18	0.79
(1,89)	1:42:A:ALA:HB3	1:74:A:LEU:HA	18	0.79
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	5	0.79
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	5	0.79
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	5	0.79
(1,27)	1:27:A:GLU:HG3	1:99:A:THR:HB	15	0.79
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	16	0.78
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	16	0.78
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	16	0.78
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	16	0.78
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	16	0.78
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	16	0.78
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD2	15	0.78
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD3	15	0.78
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD2	7	0.78
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD3	7	0.78
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD2	7	0.78
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD3	7	0.78
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG11	1	0.78
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG12	1	0.78
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG13	1	0.78
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG21	1	0.78
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG22	1	0.78
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG23	1	0.78
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	13	0.78
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	13	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	13	0.78
(1,1248)	1:123:A:PHE:H	1:123:A:PHE:HD1	9	0.78
(1,1248)	1:123:A:PHE:H	1:123:A:PHE:HD1	17	0.78
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	17	0.78
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	17	0.78
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	17	0.78
(1,1235)	1:55:A:PRO:HG3	1:120:A:THR:H	2	0.78
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	16	0.78
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	18	0.78
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	18	0.78
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	18	0.78
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	19	0.78
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	19	0.78
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	19	0.78
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	8	0.78
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	8	0.78
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	8	0.78
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	13	0.78
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	20	0.78
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	20	0.78
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	20	0.78
(1,953)	1:49:A:HIS:HE1	1:68:A:LYS:H	19	0.78
(1,696)	1:83:A:TRP:HZ2	1:123:A:PHE:HB3	2	0.78
(1,696)	1:83:A:TRP:HZ2	1:123:A:PHE:HB3	8	0.78
(1,689)	1:83:A:TRP:HD1	1:123:A:PHE:HD1	4	0.78
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	8	0.78
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	12	0.78
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	12	0.78
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	12	0.78
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	15	0.78
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	15	0.78
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	15	0.78
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	15	0.78
(1,547)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	8	0.78
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	5	0.78
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	5	0.78
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	5	0.78
(1,494)	1:102:A:TYR:HB2	1:102:A:TYR:HE2	18	0.78
(1,394)	1:74:A:LEU:HD11	1:88:A:ALA:HA	4	0.78
(1,394)	1:74:A:LEU:HD12	1:88:A:ALA:HA	4	0.78
(1,394)	1:74:A:LEU:HD13	1:88:A:ALA:HA	4	0.78
(1,383)	1:66:A:ARG:HG2	1:68:A:LYS:H	11	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG21	19	0.78
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG22	19	0.78
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG23	19	0.78
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD21	5	0.78
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD22	5	0.78
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD23	5	0.78
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD21	18	0.78
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD22	18	0.78
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD23	18	0.78
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	14	0.78
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	5	0.78
(1,165)	1:53:A:ARG:HG2	1:60:A:PHE:H	6	0.78
(1,165)	1:53:A:ARG:HG2	1:60:A:PHE:H	16	0.78
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	2	0.78
(1,130)	1:48:A:VAL:HG11	1:50:A:TYR:HD1	14	0.78
(1,130)	1:48:A:VAL:HG12	1:50:A:TYR:HD1	14	0.78
(1,130)	1:48:A:VAL:HG13	1:50:A:TYR:HD1	14	0.78
(1,121)	1:46:A:VAL:HG11	1:130:A:VAL:H	9	0.78
(1,121)	1:46:A:VAL:HG12	1:130:A:VAL:H	9	0.78
(1,121)	1:46:A:VAL:HG13	1:130:A:VAL:H	9	0.78
(1,92)	1:41:A:GLN:HG2	1:44:A:LYS:HG2	12	0.78
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG11	11	0.78
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG12	11	0.78
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG13	11	0.78
(1,26)	1:27:A:GLU:HG3	1:99:A:THR:H	18	0.78
(1,1625)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	13	0.77
(1,1625)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	13	0.77
(1,1599)	1:97:A:LEU:HD11	1:124:A:GLU:HB3	13	0.77
(1,1599)	1:97:A:LEU:HD12	1:124:A:GLU:HB3	13	0.77
(1,1599)	1:97:A:LEU:HD13	1:124:A:GLU:HB3	13	0.77
(1,1599)	1:97:A:LEU:HD21	1:124:A:GLU:HB3	13	0.77
(1,1599)	1:97:A:LEU:HD22	1:124:A:GLU:HB3	13	0.77
(1,1599)	1:97:A:LEU:HD23	1:124:A:GLU:HB3	13	0.77
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	2	0.77
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	2	0.77
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	2	0.77
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	2	0.77
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	2	0.77
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	2	0.77
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD11	1	0.77
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD12	1	0.77
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD13	1	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD21	1	0.77
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD22	1	0.77
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD23	1	0.77
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	6	0.77
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	6	0.77
(1,1248)	1:123:A:PHE:H	1:123:A:PHE:HD1	3	0.77
(1,1185)	1:24:A:ALA:HB1	1:103:A:GLN:H	2	0.77
(1,1185)	1:24:A:ALA:HB2	1:103:A:GLN:H	2	0.77
(1,1185)	1:24:A:ALA:HB3	1:103:A:GLN:H	2	0.77
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	6	0.77
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	6	0.77
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	6	0.77
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	4	0.77
(1,802)	1:41:A:GLN:H	1:74:A:LEU:HB3	6	0.77
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	20	0.77
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	11	0.77
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	11	0.77
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	11	0.77
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG21	14	0.77
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG22	14	0.77
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG23	14	0.77
(1,605)	1:100:A:ILE:HD11	1:124:A:GLU:HA	10	0.77
(1,605)	1:100:A:ILE:HD12	1:124:A:GLU:HA	10	0.77
(1,605)	1:100:A:ILE:HD13	1:124:A:GLU:HA	10	0.77
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	15	0.77
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	1	0.77
(1,543)	1:108:A:GLU:HA	1:118:A:LYS:HG2	13	0.77
(1,516)	1:81:A:LYS:H	1:105:A:ALA:HA	4	0.77
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	9	0.77
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	9	0.77
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	9	0.77
(1,419)	1:34:A:GLY:HA3	1:91:A:THR:HA	11	0.77
(1,417)	1:90:A:MET:HE1	1:94:A:GLU:HG2	9	0.77
(1,417)	1:90:A:MET:HE2	1:94:A:GLU:HG2	9	0.77
(1,417)	1:90:A:MET:HE3	1:94:A:GLU:HG2	9	0.77
(1,403)	1:89:A:THR:HG21	1:98:A:PHE:HD2	13	0.77
(1,403)	1:89:A:THR:HG22	1:98:A:PHE:HD2	13	0.77
(1,403)	1:89:A:THR:HG23	1:98:A:PHE:HD2	13	0.77
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	8	0.77
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	20	0.77
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	20	0.77
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	20	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	20	0.77
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	20	0.77
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	20	0.77
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	20	0.77
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	20	0.77
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	20	0.77
(1,278)	1:74:A:LEU:HD11	1:87:A:VAL:HB	3	0.77
(1,278)	1:74:A:LEU:HD12	1:87:A:VAL:HB	3	0.77
(1,278)	1:74:A:LEU:HD13	1:87:A:VAL:HB	3	0.77
(1,278)	1:74:A:LEU:HD11	1:87:A:VAL:HB	16	0.77
(1,278)	1:74:A:LEU:HD12	1:87:A:VAL:HB	16	0.77
(1,278)	1:74:A:LEU:HD13	1:87:A:VAL:HB	16	0.77
(1,130)	1:48:A:VAL:HG11	1:50:A:TYR:HD1	8	0.77
(1,130)	1:48:A:VAL:HG12	1:50:A:TYR:HD1	8	0.77
(1,130)	1:48:A:VAL:HG13	1:50:A:TYR:HD1	8	0.77
(1,75)	1:38:A:THR:HB	1:40:A:PRO:HG3	13	0.77
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG21	8	0.77
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG22	8	0.77
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG23	8	0.77
(1,1625)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	12	0.76
(1,1625)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	12	0.76
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	3	0.76
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	3	0.76
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	3	0.76
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	3	0.76
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	3	0.76
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	3	0.76
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	4	0.76
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	4	0.76
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	4	0.76
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	4	0.76
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	4	0.76
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	4	0.76
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	18	0.76
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	18	0.76
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	18	0.76
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	18	0.76
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	18	0.76
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	18	0.76
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	19	0.76
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	19	0.76
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	19	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	19	0.76
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	19	0.76
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	19	0.76
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	13	0.76
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	13	0.76
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG11	6	0.76
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG12	6	0.76
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG13	6	0.76
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG21	6	0.76
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG22	6	0.76
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG23	6	0.76
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG11	6	0.76
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG12	6	0.76
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG13	6	0.76
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG21	6	0.76
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG22	6	0.76
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG23	6	0.76
(1,1306)	1:81:A:LYS:HE2	1:85:A:GLN:HE21	19	0.76
(1,1298)	1:92:A:LEU:HG	1:130:A:VAL:H	7	0.76
(1,1248)	1:123:A:PHE:H	1:123:A:PHE:HD1	13	0.76
(1,1235)	1:55:A:PRO:HG3	1:120:A:THR:H	18	0.76
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	2	0.76
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	2	0.76
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	2	0.76
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	3	0.76
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	3	0.76
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	3	0.76
(1,1096)	1:91:A:THR:H	1:94:A:GLU:H	2	0.76
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	13	0.76
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	13	0.76
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	13	0.76
(1,960)	1:50:A:TYR:HE2	1:70:A:PHE:H	12	0.76
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG21	13	0.76
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG22	13	0.76
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG23	13	0.76
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	12	0.76
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	12	0.76
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	12	0.76
(1,632)	1:93:A:GLY:H	1:127:A:LEU:HG	4	0.76
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	14	0.76
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	20	0.76
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	5	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	12	0.76
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG21	20	0.76
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG22	20	0.76
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG23	20	0.76
(1,282)	1:75:A:GLY:HA2	1:84:A:ASP:HB3	11	0.76
(1,193)	1:53:A:ARG:HB3	1:59:A:GLN:HA	18	0.76
(1,176)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	18	0.76
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG21	20	0.76
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG22	20	0.76
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG23	20	0.76
(1,1648)	1:121:A:LEU:HD11	1:123:A:PHE:HD1	6	0.75
(1,1648)	1:121:A:LEU:HD12	1:123:A:PHE:HD1	6	0.75
(1,1648)	1:121:A:LEU:HD13	1:123:A:PHE:HD1	6	0.75
(1,1648)	1:121:A:LEU:HD21	1:123:A:PHE:HD1	6	0.75
(1,1648)	1:121:A:LEU:HD22	1:123:A:PHE:HD1	6	0.75
(1,1648)	1:121:A:LEU:HD23	1:123:A:PHE:HD1	6	0.75
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	12	0.75
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	12	0.75
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	12	0.75
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	12	0.75
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	12	0.75
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	12	0.75
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	19	0.75
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	19	0.75
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	19	0.75
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	19	0.75
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	19	0.75
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	19	0.75
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	11	0.75
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	11	0.75
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	11	0.75
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	11	0.75
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	11	0.75
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	11	0.75
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG11	3	0.75
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG12	3	0.75
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG13	3	0.75
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG21	3	0.75
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG22	3	0.75
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG23	3	0.75
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG11	3	0.75
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG12	3	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG13	3	0.75
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG21	3	0.75
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG22	3	0.75
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG23	3	0.75
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	2	0.75
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	2	0.75
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	2	0.75
(1,1300)	1:92:A:LEU:HD21	1:130:A:VAL:H	6	0.75
(1,1300)	1:92:A:LEU:HD22	1:130:A:VAL:H	6	0.75
(1,1300)	1:92:A:LEU:HD23	1:130:A:VAL:H	6	0.75
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	20	0.75
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	20	0.75
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	20	0.75
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	2	0.75
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	3	0.75
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	11	0.75
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	2	0.75
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	5	0.75
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	5	0.75
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	5	0.75
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	9	0.75
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	9	0.75
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	9	0.75
(1,1001)	1:73:A:THR:HB	1:76:A:ALA:H	12	0.75
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	7	0.75
(1,685)	1:102:A:TYR:HE2	1:108:A:GLU:HG2	13	0.75
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	14	0.75
(1,554)	1:106:A:TYR:HB2	1:110:A:GLY:HA2	1	0.75
(1,543)	1:108:A:GLU:HA	1:118:A:LYS:HG2	6	0.75
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	9	0.75
(1,494)	1:102:A:TYR:HB2	1:102:A:TYR:HE2	7	0.75
(1,444)	1:31:A:LEU:HG	1:95:A:LYS:HB3	3	0.75
(1,415)	1:90:A:MET:HE1	1:94:A:GLU:HA	14	0.75
(1,415)	1:90:A:MET:HE2	1:94:A:GLU:HA	14	0.75
(1,415)	1:90:A:MET:HE3	1:94:A:GLU:HA	14	0.75
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG21	9	0.75
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG22	9	0.75
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG23	9	0.75
(1,292)	1:76:A:ALA:HB1	1:78:A:GLU:HG2	15	0.75
(1,292)	1:76:A:ALA:HB2	1:78:A:GLU:HG2	15	0.75
(1,292)	1:76:A:ALA:HB3	1:78:A:GLU:HG2	15	0.75
(1,198)	1:59:A:GLN:HG2	1:61:A:ASP:H	4	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,130)	1:48:A:VAL:HG11	1:50:A:TYR:HD1	2	0.75
(1,130)	1:48:A:VAL:HG12	1:50:A:TYR:HD1	2	0.75
(1,130)	1:48:A:VAL:HG13	1:50:A:TYR:HD1	2	0.75
(1,28)	1:27:A:GLU:HG2	1:99:A:THR:HB	16	0.75
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD2	6	0.74
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD3	6	0.74
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD2	8	0.74
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD3	8	0.74
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD2	13	0.74
(1,1455)	1:54:A:PHE:HD2	1:55:A:PRO:HD3	13	0.74
(1,1393)	1:41:A:GLN:HG2	1:44:A:LYS:HG2	19	0.74
(1,1393)	1:41:A:GLN:HG2	1:44:A:LYS:HG3	19	0.74
(1,1393)	1:41:A:GLN:HG3	1:44:A:LYS:HG2	19	0.74
(1,1393)	1:41:A:GLN:HG3	1:44:A:LYS:HG3	19	0.74
(1,1300)	1:92:A:LEU:HD21	1:130:A:VAL:H	20	0.74
(1,1300)	1:92:A:LEU:HD22	1:130:A:VAL:H	20	0.74
(1,1300)	1:92:A:LEU:HD23	1:130:A:VAL:H	20	0.74
(1,1252)	1:100:A:ILE:HD11	1:123:A:PHE:H	17	0.74
(1,1252)	1:100:A:ILE:HD12	1:123:A:PHE:H	17	0.74
(1,1252)	1:100:A:ILE:HD13	1:123:A:PHE:H	17	0.74
(1,1248)	1:123:A:PHE:H	1:123:A:PHE:HD1	4	0.74
(1,1195)	1:80:A:ILE:HB	1:105:A:ALA:H	13	0.74
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	8	0.74
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG11	13	0.74
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG12	13	0.74
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG13	13	0.74
(1,896)	1:59:A:GLN:HE21	1:62:A:SER:HB2	17	0.74
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	20	0.74
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	20	0.74
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	20	0.74
(1,632)	1:93:A:GLY:H	1:127:A:LEU:HG	20	0.74
(1,631)	1:92:A:LEU:H	1:127:A:LEU:HG	15	0.74
(1,581)	1:55:A:PRO:HG3	1:120:A:THR:HB	13	0.74
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	11	0.74
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	11	0.74
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	11	0.74
(1,544)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	3	0.74
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	18	0.74
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	18	0.74
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	18	0.74
(1,464)	1:27:A:GLU:HB2	1:99:A:THR:HB	4	0.74
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	7	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	7	0.74
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	7	0.74
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	13	0.74
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	13	0.74
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	13	0.74
(1,403)	1:89:A:THR:HG21	1:98:A:PHE:HD2	2	0.74
(1,403)	1:89:A:THR:HG22	1:98:A:PHE:HD2	2	0.74
(1,403)	1:89:A:THR:HG23	1:98:A:PHE:HD2	2	0.74
(1,403)	1:89:A:THR:HG21	1:98:A:PHE:HD2	19	0.74
(1,403)	1:89:A:THR:HG22	1:98:A:PHE:HD2	19	0.74
(1,403)	1:89:A:THR:HG23	1:98:A:PHE:HD2	19	0.74
(1,385)	1:82:A:GLY:HA2	1:85:A:GLN:HB3	19	0.74
(1,283)	1:73:A:THR:HG21	1:76:A:ALA:HA	14	0.74
(1,283)	1:73:A:THR:HG22	1:76:A:ALA:HA	14	0.74
(1,283)	1:73:A:THR:HG23	1:76:A:ALA:HA	14	0.74
(1,226)	1:49:A:HIS:HE1	1:67:A:GLY:HA2	3	0.74
(1,194)	1:53:A:ARG:HG2	1:59:A:GLN:HA	3	0.74
(1,185)	1:53:A:ARG:HB3	1:57:A:GLY:HA2	1	0.74
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	2	0.74
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	2	0.74
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	2	0.74
(1,146)	1:49:A:HIS:HD2	1:50:A:TYR:HA	2	0.74
(1,1648)	1:121:A:LEU:HD11	1:123:A:PHE:HD1	10	0.73
(1,1648)	1:121:A:LEU:HD12	1:123:A:PHE:HD1	10	0.73
(1,1648)	1:121:A:LEU:HD13	1:123:A:PHE:HD1	10	0.73
(1,1648)	1:121:A:LEU:HD21	1:123:A:PHE:HD1	10	0.73
(1,1648)	1:121:A:LEU:HD22	1:123:A:PHE:HD1	10	0.73
(1,1648)	1:121:A:LEU:HD23	1:123:A:PHE:HD1	10	0.73
(1,1625)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	18	0.73
(1,1625)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	18	0.73
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	17	0.73
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	17	0.73
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	17	0.73
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	17	0.73
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	17	0.73
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	17	0.73
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	8	0.73
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	8	0.73
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	8	0.73
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	8	0.73
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	8	0.73
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	8	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1543)	1:85:A:GLN:HB2	1:98:A:PHE:HD2	7	0.73
(1,1543)	1:85:A:GLN:HB3	1:98:A:PHE:HD2	7	0.73
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG11	14	0.73
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG12	14	0.73
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG13	14	0.73
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG21	14	0.73
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG22	14	0.73
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG23	14	0.73
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	20	0.73
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	20	0.73
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	20	0.73
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	20	0.73
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	20	0.73
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	20	0.73
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG11	11	0.73
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG12	11	0.73
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG13	11	0.73
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG21	11	0.73
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG22	11	0.73
(1,1374)	1:38:A:THR:HB	1:130:A:VAL:HG23	11	0.73
(1,1346)	1:28:A:LYS:HG2	1:30:A:VAL:H	11	0.73
(1,1346)	1:28:A:LYS:HG3	1:30:A:VAL:H	11	0.73
(1,1300)	1:92:A:LEU:HD21	1:130:A:VAL:H	5	0.73
(1,1300)	1:92:A:LEU:HD22	1:130:A:VAL:H	5	0.73
(1,1300)	1:92:A:LEU:HD23	1:130:A:VAL:H	5	0.73
(1,1235)	1:55:A:PRO:HG3	1:120:A:THR:H	14	0.73
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	8	0.73
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	8	0.73
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	8	0.73
(1,1004)	1:73:A:THR:HG21	1:76:A:ALA:H	7	0.73
(1,1004)	1:73:A:THR:HG22	1:76:A:ALA:H	7	0.73
(1,1004)	1:73:A:THR:HG23	1:76:A:ALA:H	7	0.73
(1,912)	1:53:A:ARG:HD3	1:57:A:GLY:H	20	0.73
(1,910)	1:55:A:PRO:HA	1:57:A:GLY:H	14	0.73
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	19	0.73
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	18	0.73
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	18	0.73
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	18	0.73
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG11	16	0.73
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG12	16	0.73
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG13	16	0.73
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	18	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,632)	1:93:A:GLY:H	1:127:A:LEU:HG	3	0.73
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG21	4	0.73
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG22	4	0.73
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG23	4	0.73
(1,581)	1:55:A:PRO:HG3	1:120:A:THR:HB	7	0.73
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	5	0.73
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	6	0.73
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	6	0.73
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	6	0.73
(1,240)	1:47:A:THR:HG21	1:69:A:PRO:HG3	8	0.73
(1,240)	1:47:A:THR:HG22	1:69:A:PRO:HG3	8	0.73
(1,240)	1:47:A:THR:HG23	1:69:A:PRO:HG3	8	0.73
(1,191)	1:54:A:PHE:HD1	1:58:A:LYS:HD3	16	0.73
(1,185)	1:53:A:ARG:HB3	1:57:A:GLY:HA2	6	0.73
(1,152)	1:51:A:ASP:HB2	1:124:A:GLU:H	2	0.73
(1,152)	1:51:A:ASP:HB2	1:124:A:GLU:H	12	0.73
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG21	2	0.73
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG22	2	0.73
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG23	2	0.73
(1,81)	1:42:A:ALA:HA	1:74:A:LEU:H	14	0.73
(1,3)	1:28:A:LYS:HG3	1:30:A:VAL:H	2	0.73
(1,1543)	1:85:A:GLN:HB2	1:98:A:PHE:HD2	8	0.72
(1,1543)	1:85:A:GLN:HB3	1:98:A:PHE:HD2	8	0.72
(1,1323)	1:19:A:PRO:HG2	1:55:A:PRO:HB2	5	0.72
(1,1323)	1:19:A:PRO:HG3	1:55:A:PRO:HB2	5	0.72
(1,1323)	1:19:A:PRO:HG2	1:55:A:PRO:HB2	10	0.72
(1,1323)	1:19:A:PRO:HG3	1:55:A:PRO:HB2	10	0.72
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	2	0.72
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	7	0.72
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	18	0.72
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	18	0.72
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	18	0.72
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	14	0.72
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	14	0.72
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	14	0.72
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	17	0.72
(1,857)	1:49:A:HIS:HD2	1:51:A:ASP:H	18	0.72
(1,820)	1:44:A:LYS:H	1:44:A:LYS:HG3	19	0.72
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	11	0.72
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	11	0.72
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	11	0.72
(1,781)	1:37:A:VAL:H	1:91:A:THR:HB	2	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,781)	1:37:A:VAL:H	1:91:A:THR:HB	8	0.72
(1,702)	1:80:A:ILE:HG21	1:83:A:TRP:HE3	6	0.72
(1,702)	1:80:A:ILE:HG22	1:83:A:TRP:HE3	6	0.72
(1,702)	1:80:A:ILE:HG23	1:83:A:TRP:HE3	6	0.72
(1,694)	1:80:A:ILE:HD11	1:83:A:TRP:HD1	4	0.72
(1,694)	1:80:A:ILE:HD12	1:83:A:TRP:HD1	4	0.72
(1,694)	1:80:A:ILE:HD13	1:83:A:TRP:HD1	4	0.72
(1,689)	1:83:A:TRP:HD1	1:123:A:PHE:HD1	6	0.72
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB1	11	0.72
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB2	11	0.72
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB3	11	0.72
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	11	0.72
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	16	0.72
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	10	0.72
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	10	0.72
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	10	0.72
(1,383)	1:66:A:ARG:HG2	1:68:A:LYS:H	2	0.72
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG21	14	0.72
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG22	14	0.72
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG23	14	0.72
(1,183)	1:53:A:ARG:HD2	1:57:A:GLY:HA2	3	0.72
(1,168)	1:53:A:ARG:HG2	1:122:A:VAL:HB	12	0.72
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	14	0.72
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	14	0.72
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	14	0.72
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG21	3	0.72
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG22	3	0.72
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG23	3	0.72
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG21	19	0.72
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG22	19	0.72
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG23	19	0.72
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	14	0.72
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	7	0.71
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	7	0.71
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	7	0.71
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	7	0.71
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	7	0.71
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	7	0.71
(1,1575)	1:92:A:LEU:HD11	1:130:A:VAL:H	7	0.71
(1,1575)	1:92:A:LEU:HD12	1:130:A:VAL:H	7	0.71
(1,1575)	1:92:A:LEU:HD13	1:130:A:VAL:H	7	0.71
(1,1575)	1:92:A:LEU:HD21	1:130:A:VAL:H	7	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1575)	1:92:A:LEU:HD22	1:130:A:VAL:H	7	0.71
(1,1575)	1:92:A:LEU:HD23	1:130:A:VAL:H	7	0.71
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	12	0.71
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	12	0.71
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	12	0.71
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	12	0.71
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	12	0.71
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	12	0.71
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	12	0.71
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	12	0.71
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	12	0.71
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	12	0.71
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	12	0.71
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	12	0.71
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	12	0.71
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	12	0.71
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	12	0.71
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	12	0.71
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	12	0.71
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	12	0.71
(1,1324)	1:19:A:PRO:HG2	1:55:A:PRO:HG2	17	0.71
(1,1324)	1:19:A:PRO:HG3	1:55:A:PRO:HG2	17	0.71
(1,1306)	1:81:A:LYS:HE2	1:85:A:GLN:HE21	10	0.71
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	9	0.71
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	9	0.71
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	9	0.71
(1,1235)	1:55:A:PRO:HG3	1:120:A:THR:H	6	0.71
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	3	0.71
(1,953)	1:49:A:HIS:HE1	1:68:A:LYS:H	5	0.71
(1,912)	1:53:A:ARG:HD3	1:57:A:GLY:H	4	0.71
(1,762)	1:31:A:LEU:H	1:95:A:LYS:HB3	1	0.71
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	3	0.71
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	3	0.71
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	3	0.71
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG21	13	0.71
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG22	13	0.71
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG23	13	0.71
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	11	0.71
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	9	0.71
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	9	0.71
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	9	0.71
(1,519)	1:80:A:ILE:HB	1:105:A:ALA:HA	5	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	8	0.71
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	8	0.71
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	8	0.71
(1,419)	1:34:A:GLY:HA3	1:91:A:THR:HA	15	0.71
(1,415)	1:90:A:MET:HE1	1:94:A:GLU:HA	10	0.71
(1,415)	1:90:A:MET:HE2	1:94:A:GLU:HA	10	0.71
(1,415)	1:90:A:MET:HE3	1:94:A:GLU:HA	10	0.71
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD21	4	0.71
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD22	4	0.71
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD23	4	0.71
(1,193)	1:53:A:ARG:HB3	1:59:A:GLN:HA	3	0.71
(1,185)	1:53:A:ARG:HB3	1:57:A:GLY:HA2	2	0.71
(1,183)	1:53:A:ARG:HD2	1:57:A:GLY:HA2	2	0.71
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	6	0.71
(1,152)	1:51:A:ASP:HB2	1:124:A:GLU:H	8	0.71
(1,130)	1:48:A:VAL:HG11	1:50:A:TYR:HD1	11	0.71
(1,130)	1:48:A:VAL:HG12	1:50:A:TYR:HD1	11	0.71
(1,130)	1:48:A:VAL:HG13	1:50:A:TYR:HD1	11	0.71
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	9	0.71
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	16	0.71
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	10	0.71
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	10	0.71
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	10	0.71
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB2	16	0.7
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB3	16	0.7
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB2	16	0.7
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB3	16	0.7
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	15	0.7
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	15	0.7
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	15	0.7
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	15	0.7
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	15	0.7
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	15	0.7
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	16	0.7
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	16	0.7
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	16	0.7
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	16	0.7
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	16	0.7
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	16	0.7
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	8	0.7
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	8	0.7
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	8	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	8	0.7
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	8	0.7
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	8	0.7
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG2	14	0.7
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG3	14	0.7
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD2	14	0.7
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD3	14	0.7
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD2	14	0.7
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD3	14	0.7
(1,1252)	1:100:A:ILE:HD11	1:123:A:PHE:H	4	0.7
(1,1252)	1:100:A:ILE:HD12	1:123:A:PHE:H	4	0.7
(1,1252)	1:100:A:ILE:HD13	1:123:A:PHE:H	4	0.7
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	6	0.7
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	6	0.7
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	6	0.7
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	10	0.7
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	10	0.7
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	10	0.7
(1,929)	1:63:A:SER:H	1:64:A:ARG:HG3	18	0.7
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD21	17	0.7
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD22	17	0.7
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD23	17	0.7
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG21	1	0.7
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG22	1	0.7
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG23	1	0.7
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	8	0.7
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	2	0.7
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	12	0.7
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	10	0.7
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	10	0.7
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	10	0.7
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD11	16	0.7
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD12	16	0.7
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD13	16	0.7
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	14	0.7
(1,154)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	15	0.7
(1,1599)	1:97:A:LEU:HD11	1:124:A:GLU:HB3	9	0.69
(1,1599)	1:97:A:LEU:HD12	1:124:A:GLU:HB3	9	0.69
(1,1599)	1:97:A:LEU:HD13	1:124:A:GLU:HB3	9	0.69
(1,1599)	1:97:A:LEU:HD21	1:124:A:GLU:HB3	9	0.69
(1,1599)	1:97:A:LEU:HD22	1:124:A:GLU:HB3	9	0.69
(1,1599)	1:97:A:LEU:HD23	1:124:A:GLU:HB3	9	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	1	0.69
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	1	0.69
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	1	0.69
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	1	0.69
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	1	0.69
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	1	0.69
(1,1442)	1:53:A:ARG:HD2	1:59:A:GLN:HA	19	0.69
(1,1442)	1:53:A:ARG:HD3	1:59:A:GLN:HA	19	0.69
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE2	16	0.69
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE3	16	0.69
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE2	16	0.69
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE3	16	0.69
(1,1299)	1:92:A:LEU:HD11	1:130:A:VAL:H	15	0.69
(1,1299)	1:92:A:LEU:HD12	1:130:A:VAL:H	15	0.69
(1,1299)	1:92:A:LEU:HD13	1:130:A:VAL:H	15	0.69
(1,1248)	1:123:A:PHE:H	1:123:A:PHE:HD1	14	0.69
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	6	0.69
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	6	0.69
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	6	0.69
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	10	0.69
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	10	0.69
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	10	0.69
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	1	0.69
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	19	0.69
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	17	0.69
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	17	0.69
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	17	0.69
(1,959)	1:49:A:HIS:HD2	1:70:A:PHE:H	14	0.69
(1,896)	1:59:A:GLN:HE21	1:62:A:SER:HB2	20	0.69
(1,806)	1:42:A:ALA:H	1:74:A:LEU:HG	18	0.69
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	7	0.69
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	15	0.69
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	15	0.69
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	15	0.69
(1,631)	1:92:A:LEU:H	1:127:A:LEU:HG	1	0.69
(1,581)	1:55:A:PRO:HG3	1:120:A:THR:HB	12	0.69
(1,536)	1:102:A:TYR:HE2	1:108:A:GLU:HB2	3	0.69
(1,516)	1:81:A:LYS:H	1:105:A:ALA:HA	11	0.69
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	19	0.69
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	19	0.69
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	19	0.69
(1,417)	1:90:A:MET:HE1	1:94:A:GLU:HG2	7	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:90:A:MET:HE2	1:94:A:GLU:HG2	7	0.69
(1,417)	1:90:A:MET:HE3	1:94:A:GLU:HG2	7	0.69
(1,346)	1:81:A:LYS:HB3	1:82:A:GLY:HA3	3	0.69
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD21	13	0.69
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD22	13	0.69
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD23	13	0.69
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD11	9	0.69
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD12	9	0.69
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD13	9	0.69
(1,310)	1:80:A:ILE:HA	1:81:A:LYS:HG2	1	0.69
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD21	14	0.69
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD22	14	0.69
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD23	14	0.69
(1,198)	1:59:A:GLN:HG2	1:61:A:ASP:H	1	0.69
(1,185)	1:53:A:ARG:HB3	1:57:A:GLY:HA2	4	0.69
(1,75)	1:38:A:THR:HB	1:40:A:PRO:HG3	14	0.69
(1,1585)	1:95:A:LYS:HG2	1:125:A:VAL:H	1	0.68
(1,1585)	1:95:A:LYS:HG3	1:125:A:VAL:H	1	0.68
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD11	13	0.68
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD12	13	0.68
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD13	13	0.68
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD21	13	0.68
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD22	13	0.68
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD23	13	0.68
(1,1440)	1:53:A:ARG:HD2	1:57:A:GLY:H	6	0.68
(1,1440)	1:53:A:ARG:HD3	1:57:A:GLY:H	6	0.68
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG11	20	0.68
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG12	20	0.68
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG13	20	0.68
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG21	20	0.68
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG22	20	0.68
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG23	20	0.68
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG11	20	0.68
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG12	20	0.68
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG13	20	0.68
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG21	20	0.68
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG22	20	0.68
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG23	20	0.68
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG21	4	0.68
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG22	4	0.68
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG23	4	0.68
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	13	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB1	13	0.68
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB2	13	0.68
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB3	13	0.68
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	20	0.68
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	20	0.68
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	20	0.68
(1,1003)	1:74:A:LEU:HB3	1:76:A:ALA:H	7	0.68
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG11	1	0.68
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG12	1	0.68
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG13	1	0.68
(1,929)	1:63:A:SER:H	1:64:A:ARG:HG3	14	0.68
(1,781)	1:37:A:VAL:H	1:91:A:THR:HB	1	0.68
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	12	0.68
(1,689)	1:83:A:TRP:HD1	1:123:A:PHE:HD1	14	0.68
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG21	7	0.68
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG22	7	0.68
(1,669)	1:111:A:TYR:HB3	1:115:A:ILE:HG23	7	0.68
(1,651)	1:92:A:LEU:HD11	1:129:A:ALA:HA	14	0.68
(1,651)	1:92:A:LEU:HD12	1:129:A:ALA:HA	14	0.68
(1,651)	1:92:A:LEU:HD13	1:129:A:ALA:HA	14	0.68
(1,547)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	3	0.68
(1,545)	1:108:A:GLU:HG2	1:118:A:LYS:HG2	3	0.68
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	5	0.68
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	5	0.68
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	5	0.68
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	14	0.68
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	14	0.68
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	14	0.68
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	18	0.68
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD11	8	0.68
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD12	8	0.68
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD13	8	0.68
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD11	8	0.68
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD12	8	0.68
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD13	8	0.68
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD11	8	0.68
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD12	8	0.68
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD13	8	0.68
(1,385)	1:82:A:GLY:HA2	1:85:A:GLN:HB3	3	0.68
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD11	20	0.68
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD12	20	0.68
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD13	20	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG21	20	0.68
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG22	20	0.68
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG23	20	0.68
(1,310)	1:80:A:ILE:HA	1:81:A:LYS:HG2	8	0.68
(1,211)	1:49:A:HIS:HB3	1:64:A:ARG:HA	2	0.68
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG21	12	0.68
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG22	12	0.68
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG23	12	0.68
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	3	0.68
(1,130)	1:48:A:VAL:HG11	1:50:A:TYR:HD1	6	0.68
(1,130)	1:48:A:VAL:HG12	1:50:A:TYR:HD1	6	0.68
(1,130)	1:48:A:VAL:HG13	1:50:A:TYR:HD1	6	0.68
(1,105)	1:45:A:LYS:H	1:45:A:LYS:HE2	4	0.68
(1,3)	1:28:A:LYS:HG3	1:30:A:VAL:H	9	0.68
(1,1601)	1:97:A:LEU:HD11	1:124:A:GLU:HG3	8	0.67
(1,1601)	1:97:A:LEU:HD12	1:124:A:GLU:HG3	8	0.67
(1,1601)	1:97:A:LEU:HD13	1:124:A:GLU:HG3	8	0.67
(1,1601)	1:97:A:LEU:HD21	1:124:A:GLU:HG3	8	0.67
(1,1601)	1:97:A:LEU:HD22	1:124:A:GLU:HG3	8	0.67
(1,1601)	1:97:A:LEU:HD23	1:124:A:GLU:HG3	8	0.67
(1,1601)	1:97:A:LEU:HD11	1:124:A:GLU:HG3	19	0.67
(1,1601)	1:97:A:LEU:HD12	1:124:A:GLU:HG3	19	0.67
(1,1601)	1:97:A:LEU:HD13	1:124:A:GLU:HG3	19	0.67
(1,1601)	1:97:A:LEU:HD21	1:124:A:GLU:HG3	19	0.67
(1,1601)	1:97:A:LEU:HD22	1:124:A:GLU:HG3	19	0.67
(1,1601)	1:97:A:LEU:HD23	1:124:A:GLU:HG3	19	0.67
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	14	0.67
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	14	0.67
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	14	0.67
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	14	0.67
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	14	0.67
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	14	0.67
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	11	0.67
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	11	0.67
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	11	0.67
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	11	0.67
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	11	0.67
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	11	0.67
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	16	0.67
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	16	0.67
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	16	0.67
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	16	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	16	0.67
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	16	0.67
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD11	12	0.67
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD12	12	0.67
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD13	12	0.67
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD21	12	0.67
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD22	12	0.67
(1,1456)	1:54:A:PHE:HD2	1:121:A:LEU:HD23	12	0.67
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	8	0.67
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	8	0.67
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD2	12	0.67
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD3	12	0.67
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD2	12	0.67
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD3	12	0.67
(1,1386)	1:41:A:GLN:H	1:44:A:LYS:HG2	6	0.67
(1,1386)	1:41:A:GLN:H	1:44:A:LYS:HG3	6	0.67
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG11	9	0.67
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG12	9	0.67
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG13	9	0.67
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG21	9	0.67
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG22	9	0.67
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG23	9	0.67
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	4	0.67
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	4	0.67
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	4	0.67
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	4	0.67
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	4	0.67
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	4	0.67
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	9	0.67
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	9	0.67
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	9	0.67
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	9	0.67
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	9	0.67
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	9	0.67
(1,1324)	1:19:A:PRO:HG2	1:55:A:PRO:HG2	18	0.67
(1,1324)	1:19:A:PRO:HG3	1:55:A:PRO:HG2	18	0.67
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG21	9	0.67
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG22	9	0.67
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG23	9	0.67
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	11	0.67
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	16	0.67
(1,1041)	1:80:A:ILE:HG21	1:83:A:TRP:H	9	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1041)	1:80:A:ILE:HG22	1:83:A:TRP:H	9	0.67
(1,1041)	1:80:A:ILE:HG23	1:83:A:TRP:H	9	0.67
(1,747)	1:27:A:GLU:H	1:98:A:PHE:HA	14	0.67
(1,686)	1:102:A:TYR:HE2	1:118:A:LYS:HA	9	0.67
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	7	0.67
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	7	0.67
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	7	0.67
(1,587)	1:115:A:ILE:HD11	1:121:A:LEU:HG	8	0.67
(1,587)	1:115:A:ILE:HD12	1:121:A:LEU:HG	8	0.67
(1,587)	1:115:A:ILE:HD13	1:121:A:LEU:HG	8	0.67
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG21	5	0.67
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG22	5	0.67
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG23	5	0.67
(1,582)	1:55:A:PRO:HG2	1:120:A:THR:HB	3	0.67
(1,537)	1:108:A:GLU:HB2	1:118:A:LYS:HG2	2	0.67
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	16	0.67
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	16	0.67
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	16	0.67
(1,504)	1:82:A:GLY:H	1:104:A:LEU:HD11	19	0.67
(1,504)	1:82:A:GLY:H	1:104:A:LEU:HD12	19	0.67
(1,504)	1:82:A:GLY:H	1:104:A:LEU:HD13	19	0.67
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	10	0.67
(1,278)	1:74:A:LEU:HD11	1:87:A:VAL:HB	19	0.67
(1,278)	1:74:A:LEU:HD12	1:87:A:VAL:HB	19	0.67
(1,278)	1:74:A:LEU:HD13	1:87:A:VAL:HB	19	0.67
(1,211)	1:49:A:HIS:HB3	1:64:A:ARG:HA	14	0.67
(1,194)	1:53:A:ARG:HG2	1:59:A:GLN:HA	18	0.67
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	8	0.67
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	8	0.67
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	8	0.67
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG21	4	0.67
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG22	4	0.67
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG23	4	0.67
(1,1648)	1:121:A:LEU:HD11	1:123:A:PHE:HD1	19	0.66
(1,1648)	1:121:A:LEU:HD12	1:123:A:PHE:HD1	19	0.66
(1,1648)	1:121:A:LEU:HD13	1:123:A:PHE:HD1	19	0.66
(1,1648)	1:121:A:LEU:HD21	1:123:A:PHE:HD1	19	0.66
(1,1648)	1:121:A:LEU:HD22	1:123:A:PHE:HD1	19	0.66
(1,1648)	1:121:A:LEU:HD23	1:123:A:PHE:HD1	19	0.66
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB2	3	0.66
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB3	3	0.66
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB2	3	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB3	3	0.66
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB2	14	0.66
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB3	14	0.66
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB2	14	0.66
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB3	14	0.66
(1,1599)	1:97:A:LEU:HD11	1:124:A:GLU:HB3	3	0.66
(1,1599)	1:97:A:LEU:HD12	1:124:A:GLU:HB3	3	0.66
(1,1599)	1:97:A:LEU:HD13	1:124:A:GLU:HB3	3	0.66
(1,1599)	1:97:A:LEU:HD21	1:124:A:GLU:HB3	3	0.66
(1,1599)	1:97:A:LEU:HD22	1:124:A:GLU:HB3	3	0.66
(1,1599)	1:97:A:LEU:HD23	1:124:A:GLU:HB3	3	0.66
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	11	0.66
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	11	0.66
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE21	2	0.66
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE22	2	0.66
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	17	0.66
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	17	0.66
(1,1307)	1:81:A:LYS:HE3	1:85:A:GLN:HE21	15	0.66
(1,1300)	1:92:A:LEU:HD21	1:130:A:VAL:H	13	0.66
(1,1300)	1:92:A:LEU:HD22	1:130:A:VAL:H	13	0.66
(1,1300)	1:92:A:LEU:HD23	1:130:A:VAL:H	13	0.66
(1,1195)	1:80:A:ILE:HB	1:105:A:ALA:H	4	0.66
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	3	0.66
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	17	0.66
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	17	0.66
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	17	0.66
(1,1039)	1:80:A:ILE:HD11	1:83:A:TRP:H	9	0.66
(1,1039)	1:80:A:ILE:HD12	1:83:A:TRP:H	9	0.66
(1,1039)	1:80:A:ILE:HD13	1:83:A:TRP:H	9	0.66
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	19	0.66
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	19	0.66
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	19	0.66
(1,966)	1:69:A:PRO:HB3	1:70:A:PHE:H	19	0.66
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG21	19	0.66
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG22	19	0.66
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG23	19	0.66
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	9	0.66
(1,547)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	1	0.66
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	11	0.66
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	11	0.66
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	11	0.66
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	2	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	2	0.66
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	2	0.66
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD11	6	0.66
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD12	6	0.66
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD13	6	0.66
(1,310)	1:80:A:ILE:HA	1:81:A:LYS:HG2	11	0.66
(1,284)	1:73:A:THR:HG21	1:76:A:ALA:HB1	14	0.66
(1,284)	1:73:A:THR:HG21	1:76:A:ALA:HB2	14	0.66
(1,284)	1:73:A:THR:HG21	1:76:A:ALA:HB3	14	0.66
(1,284)	1:73:A:THR:HG22	1:76:A:ALA:HB1	14	0.66
(1,284)	1:73:A:THR:HG22	1:76:A:ALA:HB2	14	0.66
(1,284)	1:73:A:THR:HG22	1:76:A:ALA:HB3	14	0.66
(1,284)	1:73:A:THR:HG23	1:76:A:ALA:HB1	14	0.66
(1,284)	1:73:A:THR:HG23	1:76:A:ALA:HB2	14	0.66
(1,284)	1:73:A:THR:HG23	1:76:A:ALA:HB3	14	0.66
(1,229)	1:69:A:PRO:HA	1:128:A:LEU:HG	7	0.66
(1,198)	1:59:A:GLN:HG2	1:61:A:ASP:H	6	0.66
(1,197)	1:59:A:GLN:HG2	1:60:A:PHE:H	18	0.66
(1,190)	1:54:A:PHE:HD1	1:58:A:LYS:HD2	13	0.66
(1,152)	1:51:A:ASP:HB2	1:124:A:GLU:H	18	0.66
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG11	1	0.66
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG12	1	0.66
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG13	1	0.66
(1,106)	1:45:A:LYS:H	1:45:A:LYS:HE3	20	0.66
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG21	9	0.66
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG22	9	0.66
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG23	9	0.66
(1,1599)	1:97:A:LEU:HD11	1:124:A:GLU:HB3	1	0.65
(1,1599)	1:97:A:LEU:HD12	1:124:A:GLU:HB3	1	0.65
(1,1599)	1:97:A:LEU:HD13	1:124:A:GLU:HB3	1	0.65
(1,1599)	1:97:A:LEU:HD21	1:124:A:GLU:HB3	1	0.65
(1,1599)	1:97:A:LEU:HD22	1:124:A:GLU:HB3	1	0.65
(1,1599)	1:97:A:LEU:HD23	1:124:A:GLU:HB3	1	0.65
(1,1599)	1:97:A:LEU:HD11	1:124:A:GLU:HB3	8	0.65
(1,1599)	1:97:A:LEU:HD12	1:124:A:GLU:HB3	8	0.65
(1,1599)	1:97:A:LEU:HD13	1:124:A:GLU:HB3	8	0.65
(1,1599)	1:97:A:LEU:HD21	1:124:A:GLU:HB3	8	0.65
(1,1599)	1:97:A:LEU:HD22	1:124:A:GLU:HB3	8	0.65
(1,1599)	1:97:A:LEU:HD23	1:124:A:GLU:HB3	8	0.65
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB2	16	0.65
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB3	16	0.65
(1,1476)	1:59:A:GLN:HE21	1:62:A:SER:HB2	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1476)	1:59:A:GLN:HE21	1:62:A:SER:HB3	16	0.65
(1,1476)	1:59:A:GLN:HE22	1:62:A:SER:HB2	16	0.65
(1,1476)	1:59:A:GLN:HE22	1:62:A:SER:HB3	16	0.65
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG2	19	0.65
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG3	19	0.65
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	4	0.65
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	4	0.65
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	4	0.65
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	4	0.65
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	4	0.65
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	4	0.65
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG11	4	0.65
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG12	4	0.65
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG13	4	0.65
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG11	4	0.65
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG12	4	0.65
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG13	4	0.65
(1,1332)	1:24:A:ALA:HA	1:103:A:GLN:HG2	18	0.65
(1,1332)	1:24:A:ALA:HA	1:103:A:GLN:HG3	18	0.65
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	9	0.65
(1,1104)	1:91:A:THR:H	1:127:A:LEU:HG	15	0.65
(1,912)	1:53:A:ARG:HD3	1:57:A:GLY:H	1	0.65
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	12	0.65
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	12	0.65
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	12	0.65
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG11	1	0.65
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG12	1	0.65
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG13	1	0.65
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG21	18	0.65
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG22	18	0.65
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG23	18	0.65
(1,554)	1:106:A:TYR:HB2	1:110:A:GLY:HA2	20	0.65
(1,518)	1:80:A:ILE:HA	1:105:A:ALA:HA	1	0.65
(1,385)	1:82:A:GLY:HA2	1:85:A:GLN:HB3	6	0.65
(1,385)	1:82:A:GLY:HA2	1:85:A:GLN:HB3	10	0.65
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG21	9	0.65
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG22	9	0.65
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG23	9	0.65
(1,283)	1:73:A:THR:HG21	1:76:A:ALA:HA	2	0.65
(1,283)	1:73:A:THR:HG22	1:76:A:ALA:HA	2	0.65
(1,283)	1:73:A:THR:HG23	1:76:A:ALA:HA	2	0.65
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD21	17	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD22	17	0.65
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD23	17	0.65
(1,211)	1:49:A:HIS:HB3	1:64:A:ARG:HA	19	0.65
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	13	0.65
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	14	0.65
(1,75)	1:38:A:THR:HB	1:40:A:PRO:HG3	7	0.65
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	19	0.65
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	19	0.65
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	19	0.65
(1,26)	1:27:A:GLU:HG3	1:99:A:THR:H	4	0.65
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	17	0.65
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB2	19	0.64
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB3	19	0.64
(1,1475)	1:59:A:GLN:HG2	1:61:A:ASP:H	3	0.64
(1,1475)	1:59:A:GLN:HG3	1:61:A:ASP:H	3	0.64
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	16	0.64
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	16	0.64
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	16	0.64
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	5	0.64
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	17	0.64
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	9	0.64
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	10	0.64
(1,903)	1:59:A:GLN:HE22	1:62:A:SER:HB2	9	0.64
(1,902)	1:59:A:GLN:HE22	1:62:A:SER:HB3	7	0.64
(1,897)	1:59:A:GLN:HE21	1:62:A:SER:HB3	7	0.64
(1,881)	1:54:A:PHE:H	1:54:A:PHE:HD1	8	0.64
(1,800)	1:41:A:GLN:H	1:44:A:LYS:HB2	20	0.64
(1,581)	1:55:A:PRO:HG3	1:120:A:THR:HB	15	0.64
(1,557)	1:110:A:GLY:HA3	1:115:A:ILE:HB	2	0.64
(1,537)	1:108:A:GLU:HB2	1:118:A:LYS:HG2	12	0.64
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	1	0.64
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	1	0.64
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	1	0.64
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG21	14	0.64
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG22	14	0.64
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG23	14	0.64
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	6	0.64
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	6	0.64
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	6	0.64
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	6	0.64
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	6	0.64
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	6	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	6	0.64
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	6	0.64
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	6	0.64
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	7	0.64
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	7	0.64
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	7	0.64
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	7	0.64
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	7	0.64
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	7	0.64
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	7	0.64
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	7	0.64
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	7	0.64
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	8	0.64
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	8	0.64
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	8	0.64
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	8	0.64
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	8	0.64
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	8	0.64
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	8	0.64
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	8	0.64
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	8	0.64
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD21	2	0.64
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD22	2	0.64
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD23	2	0.64
(1,185)	1:53:A:ARG:HB3	1:57:A:GLY:HA2	9	0.64
(1,28)	1:27:A:GLU:HG2	1:99:A:THR:HB	12	0.64
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	19	0.64
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	13	0.63
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	13	0.63
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	13	0.63
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	13	0.63
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	13	0.63
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	13	0.63
(1,1405)	1:44:A:LYS:HE2	1:45:A:LYS:H	15	0.63
(1,1405)	1:44:A:LYS:HE3	1:45:A:LYS:H	15	0.63
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE2	5	0.63
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE3	5	0.63
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE2	5	0.63
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE3	5	0.63
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG11	20	0.63
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG12	20	0.63
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG13	20	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG11	20	0.63
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG12	20	0.63
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG13	20	0.63
(1,1308)	1:81:A:LYS:HD2	1:85:A:GLN:HE21	8	0.63
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	2	0.63
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	2	0.63
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	2	0.63
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	16	0.63
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	16	0.63
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	16	0.63
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	11	0.63
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	12	0.63
(1,1185)	1:24:A:ALA:HB1	1:103:A:GLN:H	19	0.63
(1,1185)	1:24:A:ALA:HB2	1:103:A:GLN:H	19	0.63
(1,1185)	1:24:A:ALA:HB3	1:103:A:GLN:H	19	0.63
(1,1118)	1:34:A:GLY:H	1:94:A:GLU:H	2	0.63
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	10	0.63
(1,1006)	1:77:A:GLY:H	1:78:A:GLU:HB2	18	0.63
(1,689)	1:83:A:TRP:HD1	1:123:A:PHE:HD1	3	0.63
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	11	0.63
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	11	0.63
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	11	0.63
(1,644)	1:49:A:HIS:HB2	1:128:A:LEU:HG	5	0.63
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG21	12	0.63
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG22	12	0.63
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG23	12	0.63
(1,542)	1:108:A:GLU:HA	1:118:A:LYS:HG3	13	0.63
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD21	10	0.63
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD22	10	0.63
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD23	10	0.63
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	5	0.63
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	5	0.63
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	5	0.63
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	14	0.63
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	14	0.63
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	14	0.63
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD11	10	0.63
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD12	10	0.63
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD13	10	0.63
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD11	10	0.63
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD12	10	0.63
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD13	10	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD11	10	0.63
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD12	10	0.63
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD13	10	0.63
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD11	19	0.63
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD12	19	0.63
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD13	19	0.63
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD11	19	0.63
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD12	19	0.63
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD13	19	0.63
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD11	19	0.63
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD12	19	0.63
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD13	19	0.63
(1,349)	1:82:A:GLY:HA3	1:100:A:ILE:HG21	4	0.63
(1,349)	1:82:A:GLY:HA3	1:100:A:ILE:HG22	4	0.63
(1,349)	1:82:A:GLY:HA3	1:100:A:ILE:HG23	4	0.63
(1,316)	1:80:A:ILE:HB	1:104:A:LEU:HB3	13	0.63
(1,176)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	9	0.63
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	14	0.63
(1,154)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	14	0.63
(1,146)	1:49:A:HIS:HD2	1:50:A:TYR:HA	18	0.63
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	17	0.63
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	17	0.63
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	17	0.63
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG11	8	0.63
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG12	8	0.63
(1,59)	1:38:A:THR:HA	1:130:A:VAL:HG13	8	0.63
(1,26)	1:27:A:GLU:HG3	1:99:A:THR:H	15	0.63
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	17	0.62
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	17	0.62
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	17	0.62
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	17	0.62
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	17	0.62
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	17	0.62
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD11	7	0.62
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD12	7	0.62
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD13	7	0.62
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD21	7	0.62
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD22	7	0.62
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD23	7	0.62
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	4	0.62
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	4	0.62
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG11	11	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG12	11	0.62
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG13	11	0.62
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG21	11	0.62
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG22	11	0.62
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG23	11	0.62
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG11	11	0.62
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG12	11	0.62
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG13	11	0.62
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG21	11	0.62
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG22	11	0.62
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG23	11	0.62
(1,1195)	1:80:A:ILE:HB	1:105:A:ALA:H	1	0.62
(1,1106)	1:37:A:VAL:H	1:92:A:LEU:H	8	0.62
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	5	0.62
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	5	0.62
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	5	0.62
(1,911)	1:53:A:ARG:HD2	1:57:A:GLY:H	6	0.62
(1,630)	1:127:A:LEU:HG	1:129:A:ALA:HA	14	0.62
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD11	19	0.62
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD12	19	0.62
(1,568)	1:111:A:TYR:H	1:115:A:ILE:HD13	19	0.62
(1,539)	1:102:A:TYR:HE2	1:108:A:GLU:HA	1	0.62
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	19	0.62
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	19	0.62
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	19	0.62
(1,346)	1:81:A:LYS:HB3	1:82:A:GLY:HA3	6	0.62
(1,346)	1:81:A:LYS:HB3	1:82:A:GLY:HA3	17	0.62
(1,197)	1:59:A:GLN:HG2	1:60:A:PHE:H	3	0.62
(1,197)	1:59:A:GLN:HG2	1:60:A:PHE:H	15	0.62
(1,165)	1:53:A:ARG:HG2	1:60:A:PHE:H	17	0.62
(1,121)	1:46:A:VAL:HG11	1:130:A:VAL:H	3	0.62
(1,121)	1:46:A:VAL:HG12	1:130:A:VAL:H	3	0.62
(1,121)	1:46:A:VAL:HG13	1:130:A:VAL:H	3	0.62
(1,106)	1:45:A:LYS:H	1:45:A:LYS:HE3	10	0.62
(1,89)	1:42:A:ALA:HB1	1:74:A:LEU:HA	10	0.62
(1,89)	1:42:A:ALA:HB2	1:74:A:LEU:HA	10	0.62
(1,89)	1:42:A:ALA:HB3	1:74:A:LEU:HA	10	0.62
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	8	0.62
(1,76)	1:38:A:THR:HB	1:40:A:PRO:HD3	6	0.62
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	14	0.62
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	14	0.62
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	14	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:27:A:GLU:HG3	1:99:A:THR:HB	4	0.62
(1,26)	1:27:A:GLU:HG3	1:99:A:THR:H	19	0.62
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	12	0.62
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	15	0.62
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	17	0.61
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	17	0.61
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	17	0.61
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	17	0.61
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	17	0.61
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	17	0.61
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	2	0.61
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	2	0.61
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	2	0.61
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	2	0.61
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	2	0.61
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	2	0.61
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE21	13	0.61
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE22	13	0.61
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG11	4	0.61
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG12	4	0.61
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG13	4	0.61
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG21	4	0.61
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG22	4	0.61
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG23	4	0.61
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	14	0.61
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	14	0.61
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	14	0.61
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	14	0.61
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	14	0.61
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	14	0.61
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	14	0.61
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	14	0.61
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	14	0.61
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	14	0.61
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	14	0.61
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	14	0.61
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	14	0.61
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	14	0.61
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	14	0.61
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	14	0.61
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	14	0.61
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	14	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1346)	1:28:A:LYS:HG2	1:30:A:VAL:H	19	0.61
(1,1346)	1:28:A:LYS:HG3	1:30:A:VAL:H	19	0.61
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD2	18	0.61
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD3	18	0.61
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD2	18	0.61
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD3	18	0.61
(1,1325)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	2	0.61
(1,1325)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	2	0.61
(1,1310)	1:81:A:LYS:HE2	1:85:A:GLN:HE22	7	0.61
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	3	0.61
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	3	0.61
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	3	0.61
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	14	0.61
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	16	0.61
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	16	0.61
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	16	0.61
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	12	0.61
(1,1049)	1:81:A:LYS:HD3	1:84:A:ASP:H	19	0.61
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	15	0.61
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	15	0.61
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	15	0.61
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG11	4	0.61
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG12	4	0.61
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG13	4	0.61
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG11	8	0.61
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG12	8	0.61
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG13	8	0.61
(1,806)	1:42:A:ALA:H	1:74:A:LEU:HG	17	0.61
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	3	0.61
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	3	0.61
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	3	0.61
(1,747)	1:27:A:GLU:H	1:98:A:PHE:HA	3	0.61
(1,632)	1:93:A:GLY:H	1:127:A:LEU:HG	16	0.61
(1,631)	1:92:A:LEU:H	1:127:A:LEU:HG	20	0.61
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	6	0.61
(1,543)	1:108:A:GLU:HA	1:118:A:LYS:HG2	3	0.61
(1,518)	1:80:A:ILE:HA	1:105:A:ALA:HA	3	0.61
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	10	0.61
(1,500)	1:81:A:LYS:HB2	1:104:A:LEU:HA	8	0.61
(1,375)	1:74:A:LEU:HD11	1:84:A:ASP:HB3	11	0.61
(1,375)	1:74:A:LEU:HD12	1:84:A:ASP:HB3	11	0.61
(1,375)	1:74:A:LEU:HD13	1:84:A:ASP:HB3	11	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	3	0.61
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	20	0.61
(1,234)	1:69:A:PRO:HB3	1:128:A:LEU:HG	7	0.61
(1,200)	1:59:A:GLN:HG3	1:60:A:PHE:H	16	0.61
(1,190)	1:54:A:PHE:HD1	1:58:A:LYS:HD2	11	0.61
(1,158)	1:52:A:GLY:HA2	1:123:A:PHE:HD1	18	0.61
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG11	6	0.61
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG12	6	0.61
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG13	6	0.61
(1,105)	1:45:A:LYS:H	1:45:A:LYS:HE2	14	0.61
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG21	6	0.61
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG22	6	0.61
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG23	6	0.61
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	2	0.61
(1,1624)	1:108:A:GLU:HG2	1:118:A:LYS:HG2	6	0.6
(1,1624)	1:108:A:GLU:HG3	1:118:A:LYS:HG2	6	0.6
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	15	0.6
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	15	0.6
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	15	0.6
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	15	0.6
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	15	0.6
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	15	0.6
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	20	0.6
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	20	0.6
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	6	0.6
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	6	0.6
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	6	0.6
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	6	0.6
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	6	0.6
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	6	0.6
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	7	0.6
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	7	0.6
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	7	0.6
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	7	0.6
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	7	0.6
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	7	0.6
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE2	1	0.6
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE3	1	0.6
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE2	1	0.6
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE3	1	0.6
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD11	10	0.6
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD12	10	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD13	10	0.6
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD21	10	0.6
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD22	10	0.6
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD23	10	0.6
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD11	10	0.6
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD12	10	0.6
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD13	10	0.6
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD21	10	0.6
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD22	10	0.6
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD23	10	0.6
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD11	10	0.6
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD12	10	0.6
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD13	10	0.6
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD21	10	0.6
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD22	10	0.6
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD23	10	0.6
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	15	0.6
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	15	0.6
(1,1324)	1:19:A:PRO:HG2	1:55:A:PRO:HG2	2	0.6
(1,1324)	1:19:A:PRO:HG3	1:55:A:PRO:HG2	2	0.6
(1,1118)	1:34:A:GLY:H	1:94:A:GLU:H	15	0.6
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	5	0.6
(1,1069)	1:86:A:GLY:H	1:98:A:PHE:HD2	14	0.6
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	11	0.6
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	11	0.6
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	11	0.6
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	1	0.6
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	1	0.6
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	1	0.6
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	13	0.6
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	13	0.6
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	13	0.6
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	1	0.6
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	10	0.6
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG21	15	0.6
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG22	15	0.6
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG23	15	0.6
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	18	0.6
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	18	0.6
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	18	0.6
(1,630)	1:127:A:LEU:HG	1:129:A:ALA:HA	17	0.6
(1,539)	1:102:A:TYR:HE2	1:108:A:GLU:HA	9	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	6	0.6
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	8	0.6
(1,310)	1:80:A:ILE:HA	1:81:A:LYS:HG2	13	0.6
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	2	0.6
(1,292)	1:76:A:ALA:HB1	1:78:A:GLU:HG2	11	0.6
(1,292)	1:76:A:ALA:HB2	1:78:A:GLU:HG2	11	0.6
(1,292)	1:76:A:ALA:HB3	1:78:A:GLU:HG2	11	0.6
(1,271)	1:74:A:LEU:HD21	1:88:A:ALA:H	11	0.6
(1,271)	1:74:A:LEU:HD22	1:88:A:ALA:H	11	0.6
(1,271)	1:74:A:LEU:HD23	1:88:A:ALA:H	11	0.6
(1,209)	1:64:A:ARG:HA	1:68:A:LYS:H	8	0.6
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	14	0.6
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	14	0.6
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	14	0.6
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	20	0.6
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	15	0.6
(1,153)	1:51:A:ASP:HB2	1:124:A:GLU:HB3	17	0.6
(1,121)	1:46:A:VAL:HG11	1:130:A:VAL:H	12	0.6
(1,121)	1:46:A:VAL:HG12	1:130:A:VAL:H	12	0.6
(1,121)	1:46:A:VAL:HG13	1:130:A:VAL:H	12	0.6
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	1	0.6
(1,1625)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	11	0.59
(1,1625)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	11	0.59
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB2	18	0.59
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB3	18	0.59
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB2	18	0.59
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB3	18	0.59
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD2	16	0.59
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD3	16	0.59
(1,1613)	1:102:A:TYR:HE2	1:118:A:LYS:HB2	13	0.59
(1,1613)	1:102:A:TYR:HE2	1:118:A:LYS:HB3	13	0.59
(1,1594)	1:97:A:LEU:HD11	1:123:A:PHE:H	5	0.59
(1,1594)	1:97:A:LEU:HD12	1:123:A:PHE:H	5	0.59
(1,1594)	1:97:A:LEU:HD13	1:123:A:PHE:H	5	0.59
(1,1594)	1:97:A:LEU:HD21	1:123:A:PHE:H	5	0.59
(1,1594)	1:97:A:LEU:HD22	1:123:A:PHE:H	5	0.59
(1,1594)	1:97:A:LEU:HD23	1:123:A:PHE:H	5	0.59
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB2	6	0.59
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB3	6	0.59
(1,1476)	1:59:A:GLN:HE21	1:62:A:SER:HB2	20	0.59
(1,1476)	1:59:A:GLN:HE21	1:62:A:SER:HB3	20	0.59
(1,1476)	1:59:A:GLN:HE22	1:62:A:SER:HB2	20	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1476)	1:59:A:GLN:HE22	1:62:A:SER:HB3	20	0.59
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB2	9	0.59
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB3	9	0.59
(1,1069)	1:86:A:GLY:H	1:98:A:PHE:HD2	8	0.59
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	18	0.59
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	18	0.59
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	18	0.59
(1,806)	1:42:A:ALA:H	1:74:A:LEU:HG	10	0.59
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG21	2	0.59
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG22	2	0.59
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG23	2	0.59
(1,632)	1:93:A:GLY:H	1:127:A:LEU:HG	14	0.59
(1,537)	1:108:A:GLU:HB2	1:118:A:LYS:HG2	16	0.59
(1,516)	1:81:A:LYS:H	1:105:A:ALA:HA	14	0.59
(1,457)	1:29:A:LYS:H	1:97:A:LEU:HB2	7	0.59
(1,364)	1:80:A:ILE:HD11	1:83:A:TRP:HA	16	0.59
(1,364)	1:80:A:ILE:HD12	1:83:A:TRP:HA	16	0.59
(1,364)	1:80:A:ILE:HD13	1:83:A:TRP:HA	16	0.59
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD11	6	0.59
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD12	6	0.59
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD13	6	0.59
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD11	18	0.59
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD12	18	0.59
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD13	18	0.59
(1,305)	1:79:A:VAL:HB	1:80:A:ILE:HD11	9	0.59
(1,305)	1:79:A:VAL:HB	1:80:A:ILE:HD12	9	0.59
(1,305)	1:79:A:VAL:HB	1:80:A:ILE:HD13	9	0.59
(1,130)	1:48:A:VAL:HG11	1:50:A:TYR:HD1	18	0.59
(1,130)	1:48:A:VAL:HG12	1:50:A:TYR:HD1	18	0.59
(1,130)	1:48:A:VAL:HG13	1:50:A:TYR:HD1	18	0.59
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG21	14	0.59
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG22	14	0.59
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG23	14	0.59
(1,1594)	1:97:A:LEU:HD11	1:123:A:PHE:H	1	0.58
(1,1594)	1:97:A:LEU:HD12	1:123:A:PHE:H	1	0.58
(1,1594)	1:97:A:LEU:HD13	1:123:A:PHE:H	1	0.58
(1,1594)	1:97:A:LEU:HD21	1:123:A:PHE:H	1	0.58
(1,1594)	1:97:A:LEU:HD22	1:123:A:PHE:H	1	0.58
(1,1594)	1:97:A:LEU:HD23	1:123:A:PHE:H	1	0.58
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	8	0.58
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	8	0.58
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE21	3	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	3	0.58
(1,1505)	1:66:A:ARG:HG2	1:68:A:LYS:H	11	0.58
(1,1505)	1:66:A:ARG:HG3	1:68:A:LYS:H	11	0.58
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG11	10	0.58
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG12	10	0.58
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG13	10	0.58
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG21	10	0.58
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG22	10	0.58
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG23	10	0.58
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG11	10	0.58
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG12	10	0.58
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG13	10	0.58
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG21	10	0.58
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG22	10	0.58
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG23	10	0.58
(1,1442)	1:53:A:ARG:HD2	1:59:A:GLN:HA	13	0.58
(1,1442)	1:53:A:ARG:HD3	1:59:A:GLN:HA	13	0.58
(1,1440)	1:53:A:ARG:HD2	1:57:A:GLY:H	17	0.58
(1,1440)	1:53:A:ARG:HD3	1:57:A:GLY:H	17	0.58
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	18	0.58
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	18	0.58
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	6	0.58
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	6	0.58
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	6	0.58
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	4	0.58
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	4	0.58
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	4	0.58
(1,1195)	1:80:A:ILE:HB	1:105:A:ALA:H	19	0.58
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	18	0.58
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	10	0.58
(1,1004)	1:73:A:THR:HG21	1:76:A:ALA:H	2	0.58
(1,1004)	1:73:A:THR:HG22	1:76:A:ALA:H	2	0.58
(1,1004)	1:73:A:THR:HG23	1:76:A:ALA:H	2	0.58
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	16	0.58
(1,912)	1:53:A:ARG:HD3	1:57:A:GLY:H	2	0.58
(1,695)	1:83:A:TRP:HZ2	1:123:A:PHE:HD1	11	0.58
(1,695)	1:83:A:TRP:HZ2	1:123:A:PHE:HD1	19	0.58
(1,694)	1:80:A:ILE:HD11	1:83:A:TRP:HD1	2	0.58
(1,694)	1:80:A:ILE:HD12	1:83:A:TRP:HD1	2	0.58
(1,694)	1:80:A:ILE:HD13	1:83:A:TRP:HD1	2	0.58
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	19	0.58
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	19	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	19	0.58
(1,587)	1:115:A:ILE:HD11	1:121:A:LEU:HG	5	0.58
(1,587)	1:115:A:ILE:HD12	1:121:A:LEU:HG	5	0.58
(1,587)	1:115:A:ILE:HD13	1:121:A:LEU:HG	5	0.58
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	19	0.58
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	7	0.58
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	14	0.58
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	9	0.58
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	9	0.58
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	9	0.58
(1,385)	1:82:A:GLY:HA2	1:85:A:GLN:HB3	15	0.58
(1,343)	1:66:A:ARG:HG3	1:68:A:LYS:H	9	0.58
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD11	16	0.58
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD12	16	0.58
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD13	16	0.58
(1,193)	1:53:A:ARG:HB3	1:59:A:GLN:HA	5	0.58
(1,185)	1:53:A:ARG:HB3	1:57:A:GLY:HA2	8	0.58
(1,183)	1:53:A:ARG:HD2	1:57:A:GLY:HA2	1	0.58
(1,177)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	2	0.58
(1,176)	1:19:A:PRO:HG2	1:55:A:PRO:HG3	2	0.58
(1,166)	1:53:A:ARG:HG3	1:60:A:PHE:H	19	0.58
(1,105)	1:45:A:LYS:H	1:45:A:LYS:HE2	12	0.58
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	16	0.58
(1,76)	1:38:A:THR:HB	1:40:A:PRO:HD3	4	0.58
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	20	0.58
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	20	0.58
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	20	0.58
(1,42)	1:33:A:PRO:HA	1:94:A:GLU:HG2	17	0.58
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	17	0.58
(1,1619)	1:103:A:GLN:HG2	1:104:A:LEU:H	11	0.57
(1,1619)	1:103:A:GLN:HG3	1:104:A:LEU:H	11	0.57
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB2	3	0.57
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB3	3	0.57
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	20	0.57
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	20	0.57
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	20	0.57
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	20	0.57
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	20	0.57
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	20	0.57
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	13	0.57
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	13	0.57
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	13	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	13	0.57
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	13	0.57
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	13	0.57
(1,1333)	1:24:A:ALA:HB1	1:103:A:GLN:HG2	11	0.57
(1,1333)	1:24:A:ALA:HB1	1:103:A:GLN:HG3	11	0.57
(1,1333)	1:24:A:ALA:HB2	1:103:A:GLN:HG2	11	0.57
(1,1333)	1:24:A:ALA:HB2	1:103:A:GLN:HG3	11	0.57
(1,1333)	1:24:A:ALA:HB3	1:103:A:GLN:HG2	11	0.57
(1,1333)	1:24:A:ALA:HB3	1:103:A:GLN:HG3	11	0.57
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	3	0.57
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	3	0.57
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD2	17	0.57
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD3	17	0.57
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD2	17	0.57
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD3	17	0.57
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	6	0.57
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	6	0.57
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	6	0.57
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	12	0.57
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	12	0.57
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	12	0.57
(1,1006)	1:77:A:GLY:H	1:78:A:GLU:HB2	10	0.57
(1,1006)	1:77:A:GLY:H	1:78:A:GLU:HB2	14	0.57
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	1	0.57
(1,910)	1:55:A:PRO:HA	1:57:A:GLY:H	17	0.57
(1,859)	1:50:A:TYR:HD2	1:51:A:ASP:H	13	0.57
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	14	0.57
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	14	0.57
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	14	0.57
(1,692)	1:80:A:ILE:HG12	1:83:A:TRP:HD1	14	0.57
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG11	8	0.57
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG12	8	0.57
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG13	8	0.57
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	20	0.57
(1,611)	1:123:A:PHE:H	1:124:A:GLU:HG3	14	0.57
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	3	0.57
(1,346)	1:81:A:LYS:HB3	1:82:A:GLY:HA3	12	0.57
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	12	0.57
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	11	0.57
(1,283)	1:73:A:THR:HG21	1:76:A:ALA:HA	12	0.57
(1,283)	1:73:A:THR:HG22	1:76:A:ALA:HA	12	0.57
(1,283)	1:73:A:THR:HG23	1:76:A:ALA:HA	12	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG21	3	0.57
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG22	3	0.57
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG23	3	0.57
(1,165)	1:53:A:ARG:HG2	1:60:A:PHE:H	9	0.57
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	10	0.57
(1,154)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	1	0.57
(1,154)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	5	0.57
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG11	2	0.57
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG12	2	0.57
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG13	2	0.57
(1,121)	1:46:A:VAL:HG11	1:130:A:VAL:H	10	0.57
(1,121)	1:46:A:VAL:HG12	1:130:A:VAL:H	10	0.57
(1,121)	1:46:A:VAL:HG13	1:130:A:VAL:H	10	0.57
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG21	3	0.57
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG22	3	0.57
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG23	3	0.57
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG21	7	0.57
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG22	7	0.57
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG23	7	0.57
(1,78)	1:40:A:PRO:HD3	1:91:A:THR:HG21	7	0.57
(1,78)	1:40:A:PRO:HD3	1:91:A:THR:HG22	7	0.57
(1,78)	1:40:A:PRO:HD3	1:91:A:THR:HG23	7	0.57
(1,42)	1:33:A:PRO:HA	1:94:A:GLU:HG2	12	0.57
(1,27)	1:27:A:GLU:HG3	1:99:A:THR:HB	11	0.57
(1,1625)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	6	0.56
(1,1625)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	6	0.56
(1,1601)	1:97:A:LEU:HD11	1:124:A:GLU:HG3	16	0.56
(1,1601)	1:97:A:LEU:HD12	1:124:A:GLU:HG3	16	0.56
(1,1601)	1:97:A:LEU:HD13	1:124:A:GLU:HG3	16	0.56
(1,1601)	1:97:A:LEU:HD21	1:124:A:GLU:HG3	16	0.56
(1,1601)	1:97:A:LEU:HD22	1:124:A:GLU:HG3	16	0.56
(1,1601)	1:97:A:LEU:HD23	1:124:A:GLU:HG3	16	0.56
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	18	0.56
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	18	0.56
(1,1476)	1:59:A:GLN:HE21	1:62:A:SER:HB2	2	0.56
(1,1476)	1:59:A:GLN:HE21	1:62:A:SER:HB3	2	0.56
(1,1476)	1:59:A:GLN:HE22	1:62:A:SER:HB2	2	0.56
(1,1476)	1:59:A:GLN:HE22	1:62:A:SER:HB3	2	0.56
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG11	8	0.56
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG12	8	0.56
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG13	8	0.56
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG21	8	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG22	8	0.56
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG23	8	0.56
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	2	0.56
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	2	0.56
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	2	0.56
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	2	0.56
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	2	0.56
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	2	0.56
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	11	0.56
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	11	0.56
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	18	0.56
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	18	0.56
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	18	0.56
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	18	0.56
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	18	0.56
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	18	0.56
(1,1308)	1:81:A:LYS:HD2	1:85:A:GLN:HE21	19	0.56
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	7	0.56
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	7	0.56
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	7	0.56
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	9	0.56
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	9	0.56
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	9	0.56
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	12	0.56
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	12	0.56
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	12	0.56
(1,1219)	1:111:A:TYR:H	1:115:A:ILE:HB	8	0.56
(1,1118)	1:34:A:GLY:H	1:94:A:GLU:H	4	0.56
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	17	0.56
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	17	0.56
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	17	0.56
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	7	0.56
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	2	0.56
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	2	0.56
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	2	0.56
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	16	0.56
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	16	0.56
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	16	0.56
(1,857)	1:49:A:HIS:HD2	1:51:A:ASP:H	8	0.56
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	13	0.56
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	13	0.56
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	13	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	5	0.56
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	5	0.56
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	5	0.56
(1,632)	1:93:A:GLY:H	1:127:A:LEU:HG	18	0.56
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG21	16	0.56
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG22	16	0.56
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG23	16	0.56
(1,581)	1:55:A:PRO:HG3	1:120:A:THR:HB	18	0.56
(1,575)	1:102:A:TYR:HE2	1:118:A:LYS:HG2	17	0.56
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	12	0.56
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	12	0.56
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	12	0.56
(1,464)	1:27:A:GLU:HB2	1:99:A:THR:HB	5	0.56
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB1	14	0.56
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB2	14	0.56
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB3	14	0.56
(1,385)	1:82:A:GLY:HA2	1:85:A:GLN:HB3	2	0.56
(1,364)	1:80:A:ILE:HD11	1:83:A:TRP:HA	2	0.56
(1,364)	1:80:A:ILE:HD12	1:83:A:TRP:HA	2	0.56
(1,364)	1:80:A:ILE:HD13	1:83:A:TRP:HA	2	0.56
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD11	14	0.56
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD12	14	0.56
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD13	14	0.56
(1,265)	1:42:A:ALA:H	1:74:A:LEU:HB3	17	0.56
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	9	0.56
(1,211)	1:49:A:HIS:HB3	1:64:A:ARG:HA	18	0.56
(1,193)	1:53:A:ARG:HB3	1:59:A:GLN:HA	12	0.56
(1,152)	1:51:A:ASP:HB2	1:124:A:GLU:H	6	0.56
(1,152)	1:51:A:ASP:HB2	1:124:A:GLU:H	9	0.56
(1,105)	1:45:A:LYS:H	1:45:A:LYS:HE2	13	0.56
(1,81)	1:42:A:ALA:HA	1:74:A:LEU:H	17	0.56
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	17	0.56
(1,76)	1:38:A:THR:HB	1:40:A:PRO:HD3	9	0.56
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB2	10	0.55
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB3	10	0.55
(1,1505)	1:66:A:ARG:HG2	1:68:A:LYS:H	9	0.55
(1,1505)	1:66:A:ARG:HG3	1:68:A:LYS:H	9	0.55
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	4	0.55
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	4	0.55
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	13	0.55
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	18	0.55
(1,1050)	1:80:A:ILE:HG12	1:84:A:ASP:H	9	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	12	0.55
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	12	0.55
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	12	0.55
(1,1004)	1:73:A:THR:HG21	1:76:A:ALA:H	13	0.55
(1,1004)	1:73:A:THR:HG22	1:76:A:ALA:H	13	0.55
(1,1004)	1:73:A:THR:HG23	1:76:A:ALA:H	13	0.55
(1,952)	1:67:A:GLY:H	1:68:A:LYS:HB2	18	0.55
(1,881)	1:54:A:PHE:H	1:54:A:PHE:HD1	9	0.55
(1,800)	1:41:A:GLN:H	1:44:A:LYS:HB2	3	0.55
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG11	2	0.55
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG12	2	0.55
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG13	2	0.55
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG21	12	0.55
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG22	12	0.55
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG23	12	0.55
(1,695)	1:83:A:TRP:HZ2	1:123:A:PHE:HD1	8	0.55
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	7	0.55
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	7	0.55
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	7	0.55
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB1	9	0.55
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB2	9	0.55
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB3	9	0.55
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB1	13	0.55
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB2	13	0.55
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB3	13	0.55
(1,631)	1:92:A:LEU:H	1:127:A:LEU:HG	6	0.55
(1,630)	1:127:A:LEU:HG	1:129:A:ALA:HA	10	0.55
(1,629)	1:92:A:LEU:HA	1:127:A:LEU:HG	4	0.55
(1,623)	1:95:A:LYS:HB2	1:126:A:GLU:HA	9	0.55
(1,554)	1:106:A:TYR:HB2	1:110:A:GLY:HA2	8	0.55
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	13	0.55
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	13	0.55
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	13	0.55
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	4	0.55
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	4	0.55
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	4	0.55
(1,500)	1:81:A:LYS:HB2	1:104:A:LEU:HA	17	0.55
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD11	4	0.55
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD12	4	0.55
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD13	4	0.55
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD11	4	0.55
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD12	4	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD13	4	0.55
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD11	4	0.55
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD12	4	0.55
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD13	4	0.55
(1,464)	1:27:A:GLU:HB2	1:99:A:THR:HB	11	0.55
(1,385)	1:82:A:GLY:HA2	1:85:A:GLN:HB3	17	0.55
(1,354)	1:82:A:GLY:HA2	1:104:A:LEU:HB3	1	0.55
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	12	0.55
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	12	0.55
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	12	0.55
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG21	17	0.55
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG22	17	0.55
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG23	17	0.55
(1,278)	1:74:A:LEU:HD11	1:87:A:VAL:HB	6	0.55
(1,278)	1:74:A:LEU:HD12	1:87:A:VAL:HB	6	0.55
(1,278)	1:74:A:LEU:HD13	1:87:A:VAL:HB	6	0.55
(1,271)	1:74:A:LEU:HD21	1:88:A:ALA:H	4	0.55
(1,271)	1:74:A:LEU:HD22	1:88:A:ALA:H	4	0.55
(1,271)	1:74:A:LEU:HD23	1:88:A:ALA:H	4	0.55
(1,201)	1:59:A:GLN:H	1:59:A:GLN:HG3	17	0.55
(1,166)	1:53:A:ARG:HG3	1:60:A:PHE:H	13	0.55
(1,145)	1:49:A:HIS:HB2	1:126:A:GLU:HG2	16	0.55
(1,1599)	1:97:A:LEU:HD11	1:124:A:GLU:HB3	7	0.54
(1,1599)	1:97:A:LEU:HD12	1:124:A:GLU:HB3	7	0.54
(1,1599)	1:97:A:LEU:HD13	1:124:A:GLU:HB3	7	0.54
(1,1599)	1:97:A:LEU:HD21	1:124:A:GLU:HB3	7	0.54
(1,1599)	1:97:A:LEU:HD22	1:124:A:GLU:HB3	7	0.54
(1,1599)	1:97:A:LEU:HD23	1:124:A:GLU:HB3	7	0.54
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	2	0.54
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	2	0.54
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	2	0.54
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	2	0.54
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	2	0.54
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	2	0.54
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG11	16	0.54
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG12	16	0.54
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG13	16	0.54
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG21	16	0.54
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG22	16	0.54
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG23	16	0.54
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG11	16	0.54
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG12	16	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG13	16	0.54
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG21	16	0.54
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG22	16	0.54
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG23	16	0.54
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	18	0.54
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	18	0.54
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	18	0.54
(1,1298)	1:92:A:LEU:HG	1:130:A:VAL:H	3	0.54
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	6	0.54
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	15	0.54
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	5	0.54
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	5	0.54
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	5	0.54
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	10	0.54
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	10	0.54
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	10	0.54
(1,960)	1:50:A:TYR:HE2	1:70:A:PHE:H	4	0.54
(1,797)	1:41:A:GLN:H	1:41:A:GLN:HG2	8	0.54
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	5	0.54
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	5	0.54
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	5	0.54
(1,781)	1:37:A:VAL:H	1:91:A:THR:HB	6	0.54
(1,751)	1:27:A:GLU:HG2	1:28:A:LYS:H	3	0.54
(1,747)	1:27:A:GLU:H	1:98:A:PHE:HA	13	0.54
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	13	0.54
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	13	0.54
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	13	0.54
(1,730)	1:35:A:ASP:H	1:37:A:VAL:HG21	12	0.54
(1,730)	1:35:A:ASP:H	1:37:A:VAL:HG22	12	0.54
(1,730)	1:35:A:ASP:H	1:37:A:VAL:HG23	12	0.54
(1,730)	1:35:A:ASP:H	1:37:A:VAL:HG21	19	0.54
(1,730)	1:35:A:ASP:H	1:37:A:VAL:HG22	19	0.54
(1,730)	1:35:A:ASP:H	1:37:A:VAL:HG23	19	0.54
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG21	10	0.54
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG22	10	0.54
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG23	10	0.54
(1,631)	1:92:A:LEU:H	1:127:A:LEU:HG	4	0.54
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	6	0.54
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	15	0.54
(1,518)	1:80:A:ILE:HA	1:105:A:ALA:HA	14	0.54
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	5	0.54
(1,481)	1:100:A:ILE:HG21	1:104:A:LEU:HA	4	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,481)	1:100:A:ILE:HG22	1:104:A:LEU:HA	4	0.54
(1,481)	1:100:A:ILE:HG23	1:104:A:LEU:HA	4	0.54
(1,411)	1:90:A:MET:HE1	1:127:A:LEU:H	4	0.54
(1,411)	1:90:A:MET:HE2	1:127:A:LEU:H	4	0.54
(1,411)	1:90:A:MET:HE3	1:127:A:LEU:H	4	0.54
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	7	0.54
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD21	1	0.54
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD22	1	0.54
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD23	1	0.54
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD21	13	0.54
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD22	13	0.54
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD23	13	0.54
(1,211)	1:49:A:HIS:HB3	1:64:A:ARG:HA	4	0.54
(1,185)	1:53:A:ARG:HB3	1:57:A:GLY:HA2	12	0.54
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG21	9	0.54
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG22	9	0.54
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG23	9	0.54
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	8	0.54
(1,92)	1:41:A:GLN:HG2	1:44:A:LYS:HG2	4	0.54
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG21	20	0.54
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG22	20	0.54
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG23	20	0.54
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG21	7	0.54
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG22	7	0.54
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG23	7	0.54
(1,62)	1:38:A:THR:HB	1:92:A:LEU:H	7	0.54
(1,1594)	1:97:A:LEU:HD11	1:123:A:PHE:H	11	0.53
(1,1594)	1:97:A:LEU:HD12	1:123:A:PHE:H	11	0.53
(1,1594)	1:97:A:LEU:HD13	1:123:A:PHE:H	11	0.53
(1,1594)	1:97:A:LEU:HD21	1:123:A:PHE:H	11	0.53
(1,1594)	1:97:A:LEU:HD22	1:123:A:PHE:H	11	0.53
(1,1594)	1:97:A:LEU:HD23	1:123:A:PHE:H	11	0.53
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	20	0.53
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	20	0.53
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	20	0.53
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	20	0.53
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	20	0.53
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	20	0.53
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	9	0.53
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	9	0.53
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE2	13	0.53
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE3	13	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE2	13	0.53
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE3	13	0.53
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG11	6	0.53
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG12	6	0.53
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG13	6	0.53
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG11	6	0.53
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG12	6	0.53
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG13	6	0.53
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	14	0.53
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	14	0.53
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	16	0.53
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	16	0.53
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	16	0.53
(1,1300)	1:92:A:LEU:HD21	1:130:A:VAL:H	2	0.53
(1,1300)	1:92:A:LEU:HD22	1:130:A:VAL:H	2	0.53
(1,1300)	1:92:A:LEU:HD23	1:130:A:VAL:H	2	0.53
(1,1235)	1:55:A:PRO:HG3	1:120:A:THR:H	20	0.53
(1,960)	1:50:A:TYR:HE2	1:70:A:PHE:H	15	0.53
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	7	0.53
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	12	0.53
(1,881)	1:54:A:PHE:H	1:54:A:PHE:HD1	12	0.53
(1,747)	1:27:A:GLU:H	1:98:A:PHE:HA	18	0.53
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG21	19	0.53
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG22	19	0.53
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG23	19	0.53
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	20	0.53
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	20	0.53
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	20	0.53
(1,661)	1:72:A:PHE:HB3	1:79:A:VAL:HG11	4	0.53
(1,661)	1:72:A:PHE:HB3	1:79:A:VAL:HG12	4	0.53
(1,661)	1:72:A:PHE:HB3	1:79:A:VAL:HG13	4	0.53
(1,578)	1:119:A:ALA:HB1	1:120:A:THR:HB	6	0.53
(1,578)	1:119:A:ALA:HB2	1:120:A:THR:HB	6	0.53
(1,578)	1:119:A:ALA:HB3	1:120:A:THR:HB	6	0.53
(1,557)	1:110:A:GLY:HA3	1:115:A:ILE:HB	6	0.53
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	6	0.53
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	6	0.53
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	6	0.53
(1,459)	1:97:A:LEU:HG	1:99:A:THR:H	20	0.53
(1,443)	1:32:A:THR:HG21	1:95:A:LYS:HB3	1	0.53
(1,443)	1:32:A:THR:HG22	1:95:A:LYS:HB3	1	0.53
(1,443)	1:32:A:THR:HG23	1:95:A:LYS:HB3	1	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:90:A:MET:HE1	1:94:A:GLU:HG2	14	0.53
(1,417)	1:90:A:MET:HE2	1:94:A:GLU:HG2	14	0.53
(1,417)	1:90:A:MET:HE3	1:94:A:GLU:HG2	14	0.53
(1,394)	1:74:A:LEU:HD11	1:88:A:ALA:HA	9	0.53
(1,394)	1:74:A:LEU:HD12	1:88:A:ALA:HA	9	0.53
(1,394)	1:74:A:LEU:HD13	1:88:A:ALA:HA	9	0.53
(1,316)	1:80:A:ILE:HB	1:104:A:LEU:HB3	17	0.53
(1,310)	1:80:A:ILE:HA	1:81:A:LYS:HG2	20	0.53
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	15	0.53
(1,240)	1:47:A:THR:HG21	1:69:A:PRO:HG3	17	0.53
(1,240)	1:47:A:THR:HG22	1:69:A:PRO:HG3	17	0.53
(1,240)	1:47:A:THR:HG23	1:69:A:PRO:HG3	17	0.53
(1,240)	1:47:A:THR:HG21	1:69:A:PRO:HG3	20	0.53
(1,240)	1:47:A:THR:HG22	1:69:A:PRO:HG3	20	0.53
(1,240)	1:47:A:THR:HG23	1:69:A:PRO:HG3	20	0.53
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	5	0.53
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	20	0.53
(1,185)	1:53:A:ARG:HB3	1:57:A:GLY:HA2	17	0.53
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG21	8	0.53
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG22	8	0.53
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG23	8	0.53
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	1	0.53
(1,105)	1:45:A:LYS:H	1:45:A:LYS:HE2	8	0.53
(1,89)	1:42:A:ALA:HB1	1:74:A:LEU:HA	8	0.53
(1,89)	1:42:A:ALA:HB2	1:74:A:LEU:HA	8	0.53
(1,89)	1:42:A:ALA:HB3	1:74:A:LEU:HA	8	0.53
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	2	0.53
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG21	1	0.53
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG22	1	0.53
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG23	1	0.53
(1,1648)	1:121:A:LEU:HD11	1:123:A:PHE:HD1	1	0.52
(1,1648)	1:121:A:LEU:HD12	1:123:A:PHE:HD1	1	0.52
(1,1648)	1:121:A:LEU:HD13	1:123:A:PHE:HD1	1	0.52
(1,1648)	1:121:A:LEU:HD21	1:123:A:PHE:HD1	1	0.52
(1,1648)	1:121:A:LEU:HD22	1:123:A:PHE:HD1	1	0.52
(1,1648)	1:121:A:LEU:HD23	1:123:A:PHE:HD1	1	0.52
(1,1619)	1:103:A:GLN:HG2	1:104:A:LEU:H	19	0.52
(1,1619)	1:103:A:GLN:HG3	1:104:A:LEU:H	19	0.52
(1,1601)	1:97:A:LEU:HD11	1:124:A:GLU:HG3	2	0.52
(1,1601)	1:97:A:LEU:HD12	1:124:A:GLU:HG3	2	0.52
(1,1601)	1:97:A:LEU:HD13	1:124:A:GLU:HG3	2	0.52
(1,1601)	1:97:A:LEU:HD21	1:124:A:GLU:HG3	2	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1601)	1:97:A:LEU:HD22	1:124:A:GLU:HG3	2	0.52
(1,1601)	1:97:A:LEU:HD23	1:124:A:GLU:HG3	2	0.52
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	8	0.52
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	8	0.52
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	8	0.52
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	8	0.52
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	8	0.52
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	8	0.52
(1,1594)	1:97:A:LEU:HD11	1:123:A:PHE:H	4	0.52
(1,1594)	1:97:A:LEU:HD12	1:123:A:PHE:H	4	0.52
(1,1594)	1:97:A:LEU:HD13	1:123:A:PHE:H	4	0.52
(1,1594)	1:97:A:LEU:HD21	1:123:A:PHE:H	4	0.52
(1,1594)	1:97:A:LEU:HD22	1:123:A:PHE:H	4	0.52
(1,1594)	1:97:A:LEU:HD23	1:123:A:PHE:H	4	0.52
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	9	0.52
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	9	0.52
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	9	0.52
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	9	0.52
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	9	0.52
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	9	0.52
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	9	0.52
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	9	0.52
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA2	14	0.52
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	14	0.52
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD11	18	0.52
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD12	18	0.52
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD13	18	0.52
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD21	18	0.52
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD22	18	0.52
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD23	18	0.52
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD11	18	0.52
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD12	18	0.52
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD13	18	0.52
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD21	18	0.52
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD22	18	0.52
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD23	18	0.52
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD11	18	0.52
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD12	18	0.52
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD13	18	0.52
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD21	18	0.52
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD22	18	0.52
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD23	18	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	20	0.52
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	20	0.52
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	20	0.52
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	20	0.52
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	20	0.52
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	20	0.52
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	14	0.52
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	14	0.52
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	14	0.52
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	9	0.52
(1,1023)	1:81:A:LYS:H	1:81:A:LYS:HG3	14	0.52
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	2	0.52
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	2	0.52
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	2	0.52
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	4	0.52
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	4	0.52
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	4	0.52
(1,960)	1:50:A:TYR:HE2	1:70:A:PHE:H	6	0.52
(1,912)	1:53:A:ARG:HD3	1:57:A:GLY:H	16	0.52
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	2	0.52
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	6	0.52
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	8	0.52
(1,806)	1:42:A:ALA:H	1:74:A:LEU:HG	6	0.52
(1,730)	1:35:A:ASP:H	1:37:A:VAL:HG21	15	0.52
(1,730)	1:35:A:ASP:H	1:37:A:VAL:HG22	15	0.52
(1,730)	1:35:A:ASP:H	1:37:A:VAL:HG23	15	0.52
(1,694)	1:80:A:ILE:HD11	1:83:A:TRP:HD1	15	0.52
(1,694)	1:80:A:ILE:HD12	1:83:A:TRP:HD1	15	0.52
(1,694)	1:80:A:ILE:HD13	1:83:A:TRP:HD1	15	0.52
(1,651)	1:92:A:LEU:HD11	1:129:A:ALA:HA	10	0.52
(1,651)	1:92:A:LEU:HD12	1:129:A:ALA:HA	10	0.52
(1,651)	1:92:A:LEU:HD13	1:129:A:ALA:HA	10	0.52
(1,544)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	6	0.52
(1,544)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	16	0.52
(1,500)	1:81:A:LYS:HB2	1:104:A:LEU:HA	15	0.52
(1,457)	1:29:A:LYS:H	1:97:A:LEU:HB2	3	0.52
(1,450)	1:32:A:THR:HB	1:95:A:LYS:HE3	10	0.52
(1,358)	1:80:A:ILE:HD11	1:83:A:TRP:HB2	9	0.52
(1,358)	1:80:A:ILE:HD12	1:83:A:TRP:HB2	9	0.52
(1,358)	1:80:A:ILE:HD13	1:83:A:TRP:HB2	9	0.52
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	7	0.52
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	7	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	7	0.52
(1,310)	1:80:A:ILE:HA	1:81:A:LYS:HG2	5	0.52
(1,265)	1:42:A:ALA:H	1:74:A:LEU:HB3	5	0.52
(1,197)	1:59:A:GLN:HG2	1:60:A:PHE:H	14	0.52
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG21	17	0.52
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG22	17	0.52
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG23	17	0.52
(1,159)	1:53:A:ARG:HB2	1:59:A:GLN:H	20	0.52
(1,42)	1:33:A:PRO:HA	1:94:A:GLU:HG2	4	0.52
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	14	0.52
(1,1656)	1:126:A:GLU:HB2	1:128:A:LEU:HD11	9	0.51
(1,1656)	1:126:A:GLU:HB2	1:128:A:LEU:HD12	9	0.51
(1,1656)	1:126:A:GLU:HB2	1:128:A:LEU:HD13	9	0.51
(1,1656)	1:126:A:GLU:HB2	1:128:A:LEU:HD21	9	0.51
(1,1656)	1:126:A:GLU:HB2	1:128:A:LEU:HD22	9	0.51
(1,1656)	1:126:A:GLU:HB2	1:128:A:LEU:HD23	9	0.51
(1,1656)	1:126:A:GLU:HB3	1:128:A:LEU:HD11	9	0.51
(1,1656)	1:126:A:GLU:HB3	1:128:A:LEU:HD12	9	0.51
(1,1656)	1:126:A:GLU:HB3	1:128:A:LEU:HD13	9	0.51
(1,1656)	1:126:A:GLU:HB3	1:128:A:LEU:HD21	9	0.51
(1,1656)	1:126:A:GLU:HB3	1:128:A:LEU:HD22	9	0.51
(1,1656)	1:126:A:GLU:HB3	1:128:A:LEU:HD23	9	0.51
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	16	0.51
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	16	0.51
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	16	0.51
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	16	0.51
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	16	0.51
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	16	0.51
(1,1594)	1:97:A:LEU:HD11	1:123:A:PHE:H	10	0.51
(1,1594)	1:97:A:LEU:HD12	1:123:A:PHE:H	10	0.51
(1,1594)	1:97:A:LEU:HD13	1:123:A:PHE:H	10	0.51
(1,1594)	1:97:A:LEU:HD21	1:123:A:PHE:H	10	0.51
(1,1594)	1:97:A:LEU:HD22	1:123:A:PHE:H	10	0.51
(1,1594)	1:97:A:LEU:HD23	1:123:A:PHE:H	10	0.51
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	2	0.51
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	2	0.51
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	19	0.51
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	19	0.51
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE21	7	0.51
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE22	7	0.51
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB2	12	0.51
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB3	12	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD2	11	0.51
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD3	11	0.51
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD2	11	0.51
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD3	11	0.51
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	18	0.51
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	18	0.51
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	18	0.51
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	3	0.51
(1,1162)	1:27:A:GLU:HB2	1:99:A:THR:H	18	0.51
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	4	0.51
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	15	0.51
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	9	0.51
(1,1006)	1:77:A:GLY:H	1:78:A:GLU:HB2	2	0.51
(1,966)	1:69:A:PRO:HB3	1:70:A:PHE:H	1	0.51
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	18	0.51
(1,881)	1:54:A:PHE:H	1:54:A:PHE:HD1	1	0.51
(1,682)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	13	0.51
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	1	0.51
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	1	0.51
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	1	0.51
(1,630)	1:127:A:LEU:HG	1:129:A:ALA:HA	12	0.51
(1,608)	1:97:A:LEU:HG	1:124:A:GLU:HG3	9	0.51
(1,601)	1:100:A:ILE:HD11	1:123:A:PHE:HB2	9	0.51
(1,601)	1:100:A:ILE:HD12	1:123:A:PHE:HB2	9	0.51
(1,601)	1:100:A:ILE:HD13	1:123:A:PHE:HB2	9	0.51
(1,545)	1:108:A:GLU:HG2	1:118:A:LYS:HG2	16	0.51
(1,543)	1:108:A:GLU:HA	1:118:A:LYS:HG2	14	0.51
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB1	3	0.51
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB2	3	0.51
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB3	3	0.51
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB1	3	0.51
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB2	3	0.51
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB3	3	0.51
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB1	3	0.51
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB2	3	0.51
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB3	3	0.51
(1,524)	1:80:A:ILE:HD11	1:105:A:ALA:HB1	9	0.51
(1,524)	1:80:A:ILE:HD11	1:105:A:ALA:HB2	9	0.51
(1,524)	1:80:A:ILE:HD11	1:105:A:ALA:HB3	9	0.51
(1,524)	1:80:A:ILE:HD12	1:105:A:ALA:HB1	9	0.51
(1,524)	1:80:A:ILE:HD12	1:105:A:ALA:HB2	9	0.51
(1,524)	1:80:A:ILE:HD12	1:105:A:ALA:HB3	9	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,524)	1:80:A:ILE:HD13	1:105:A:ALA:HB1	9	0.51
(1,524)	1:80:A:ILE:HD13	1:105:A:ALA:HB2	9	0.51
(1,524)	1:80:A:ILE:HD13	1:105:A:ALA:HB3	9	0.51
(1,518)	1:80:A:ILE:HA	1:105:A:ALA:HA	2	0.51
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD21	13	0.51
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD22	13	0.51
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD23	13	0.51
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB1	19	0.51
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB2	19	0.51
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB3	19	0.51
(1,422)	1:38:A:THR:HG21	1:91:A:THR:HA	1	0.51
(1,422)	1:38:A:THR:HG22	1:91:A:THR:HA	1	0.51
(1,422)	1:38:A:THR:HG23	1:91:A:THR:HA	1	0.51
(1,265)	1:42:A:ALA:H	1:74:A:LEU:HB3	14	0.51
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	18	0.51
(1,200)	1:59:A:GLN:HG3	1:60:A:PHE:H	20	0.51
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG21	20	0.51
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG22	20	0.51
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG23	20	0.51
(1,105)	1:45:A:LYS:H	1:45:A:LYS:HE2	9	0.51
(1,81)	1:42:A:ALA:HA	1:74:A:LEU:H	9	0.51
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	9	0.51
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	9	0.51
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	9	0.51
(1,20)	1:25:A:GLN:H	1:26:A:LEU:HB2	6	0.51
(1,1625)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	16	0.5
(1,1625)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	16	0.5
(1,1613)	1:102:A:TYR:HE2	1:118:A:LYS:HB2	10	0.5
(1,1613)	1:102:A:TYR:HE2	1:118:A:LYS:HB3	10	0.5
(1,1543)	1:85:A:GLN:HB2	1:98:A:PHE:HD2	6	0.5
(1,1543)	1:85:A:GLN:HB3	1:98:A:PHE:HD2	6	0.5
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG11	10	0.5
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG12	10	0.5
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG13	10	0.5
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG21	10	0.5
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG22	10	0.5
(1,1383)	1:40:A:PRO:HB2	1:130:A:VAL:HG23	10	0.5
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG11	10	0.5
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG12	10	0.5
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG13	10	0.5
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG21	10	0.5
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG22	10	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1383)	1:40:A:PRO:HB3	1:130:A:VAL:HG23	10	0.5
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	17	0.5
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	17	0.5
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	17	0.5
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	17	0.5
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	17	0.5
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	17	0.5
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	17	0.5
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	17	0.5
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	17	0.5
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	17	0.5
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	17	0.5
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	17	0.5
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	17	0.5
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	17	0.5
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	17	0.5
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	17	0.5
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	17	0.5
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	17	0.5
(1,1204)	1:100:A:ILE:HG21	1:106:A:TYR:H	7	0.5
(1,1204)	1:100:A:ILE:HG22	1:106:A:TYR:H	7	0.5
(1,1204)	1:100:A:ILE:HG23	1:106:A:TYR:H	7	0.5
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	7	0.5
(1,1106)	1:37:A:VAL:H	1:92:A:LEU:H	7	0.5
(1,1104)	1:91:A:THR:H	1:127:A:LEU:HG	1	0.5
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	17	0.5
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	14	0.5
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	17	0.5
(1,929)	1:63:A:SER:H	1:64:A:ARG:HG3	17	0.5
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	5	0.5
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	11	0.5
(1,857)	1:49:A:HIS:HD2	1:51:A:ASP:H	2	0.5
(1,857)	1:49:A:HIS:HD2	1:51:A:ASP:H	17	0.5
(1,689)	1:83:A:TRP:HD1	1:123:A:PHE:HD1	1	0.5
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	3	0.5
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	3	0.5
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	3	0.5
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	17	0.5
(1,539)	1:102:A:TYR:HE2	1:108:A:GLU:HA	20	0.5
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	8	0.5
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	8	0.5
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	8	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	14	0.5
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	14	0.5
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	14	0.5
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	12	0.5
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	12	0.5
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	12	0.5
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD21	15	0.5
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD22	15	0.5
(1,508)	1:80:A:ILE:HA	1:104:A:LEU:HD23	15	0.5
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	9	0.5
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	9	0.5
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	9	0.5
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	3	0.5
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	3	0.5
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	3	0.5
(1,422)	1:38:A:THR:HG21	1:91:A:THR:HA	19	0.5
(1,422)	1:38:A:THR:HG22	1:91:A:THR:HA	19	0.5
(1,422)	1:38:A:THR:HG23	1:91:A:THR:HA	19	0.5
(1,415)	1:90:A:MET:HE1	1:94:A:GLU:HA	3	0.5
(1,415)	1:90:A:MET:HE2	1:94:A:GLU:HA	3	0.5
(1,415)	1:90:A:MET:HE3	1:94:A:GLU:HA	3	0.5
(1,346)	1:81:A:LYS:HB3	1:82:A:GLY:HA3	10	0.5
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD11	9	0.5
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD12	9	0.5
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD13	9	0.5
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG21	3	0.5
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG22	3	0.5
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG23	3	0.5
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG21	2	0.5
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG22	2	0.5
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG23	2	0.5
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG21	15	0.5
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG22	15	0.5
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG23	15	0.5
(1,211)	1:49:A:HIS:HB3	1:64:A:ARG:HA	9	0.5
(1,152)	1:51:A:ASP:HB2	1:124:A:GLU:H	7	0.5
(1,71)	1:38:A:THR:HG21	1:92:A:LEU:HD21	10	0.5
(1,71)	1:38:A:THR:HG21	1:92:A:LEU:HD22	10	0.5
(1,71)	1:38:A:THR:HG21	1:92:A:LEU:HD23	10	0.5
(1,71)	1:38:A:THR:HG22	1:92:A:LEU:HD21	10	0.5
(1,71)	1:38:A:THR:HG22	1:92:A:LEU:HD22	10	0.5
(1,71)	1:38:A:THR:HG22	1:92:A:LEU:HD23	10	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:38:A:THR:HG23	1:92:A:LEU:HD21	10	0.5
(1,71)	1:38:A:THR:HG23	1:92:A:LEU:HD22	10	0.5
(1,71)	1:38:A:THR:HG23	1:92:A:LEU:HD23	10	0.5
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	1	0.49
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	1	0.49
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	1	0.49
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	1	0.49
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	1	0.49
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	1	0.49
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	8	0.49
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	8	0.49
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	8	0.49
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	8	0.49
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	8	0.49
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	8	0.49
(1,1584)	1:95:A:LYS:HG2	1:124:A:GLU:HB3	9	0.49
(1,1584)	1:95:A:LYS:HG3	1:124:A:GLU:HB3	9	0.49
(1,1575)	1:92:A:LEU:HD11	1:130:A:VAL:H	3	0.49
(1,1575)	1:92:A:LEU:HD12	1:130:A:VAL:H	3	0.49
(1,1575)	1:92:A:LEU:HD13	1:130:A:VAL:H	3	0.49
(1,1575)	1:92:A:LEU:HD21	1:130:A:VAL:H	3	0.49
(1,1575)	1:92:A:LEU:HD22	1:130:A:VAL:H	3	0.49
(1,1575)	1:92:A:LEU:HD23	1:130:A:VAL:H	3	0.49
(1,1543)	1:85:A:GLN:HB2	1:98:A:PHE:HD2	9	0.49
(1,1543)	1:85:A:GLN:HB3	1:98:A:PHE:HD2	9	0.49
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	6	0.49
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	6	0.49
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	12	0.49
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	12	0.49
(1,1505)	1:66:A:ARG:HG2	1:68:A:LYS:H	20	0.49
(1,1505)	1:66:A:ARG:HG3	1:68:A:LYS:H	20	0.49
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB2	1	0.49
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB3	1	0.49
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB2	19	0.49
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB3	19	0.49
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB2	17	0.49
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB3	17	0.49
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG2	4	0.49
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG3	4	0.49
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG2	8	0.49
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG3	8	0.49
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	5	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	5	0.49
(1,1307)	1:81:A:LYS:HE3	1:85:A:GLN:HE21	8	0.49
(1,1306)	1:81:A:LYS:HE2	1:85:A:GLN:HE21	4	0.49
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	5	0.49
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	5	0.49
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	5	0.49
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	7	0.49
(1,1195)	1:80:A:ILE:HB	1:105:A:ALA:H	3	0.49
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	1	0.49
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	16	0.49
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	16	0.49
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	16	0.49
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	5	0.49
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	5	0.49
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	5	0.49
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	15	0.49
(1,1006)	1:77:A:GLY:H	1:78:A:GLU:HB2	13	0.49
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	17	0.49
(1,820)	1:44:A:LYS:H	1:44:A:LYS:HG3	2	0.49
(1,747)	1:27:A:GLU:H	1:98:A:PHE:HA	4	0.49
(1,696)	1:83:A:TRP:HZ2	1:123:A:PHE:HB3	19	0.49
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG21	9	0.49
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG22	9	0.49
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG23	9	0.49
(1,660)	1:72:A:PHE:HB2	1:79:A:VAL:HG11	4	0.49
(1,660)	1:72:A:PHE:HB2	1:79:A:VAL:HG12	4	0.49
(1,660)	1:72:A:PHE:HB2	1:79:A:VAL:HG13	4	0.49
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	9	0.49
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	3	0.49
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	9	0.49
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	10	0.49
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD11	6	0.49
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD12	6	0.49
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD13	6	0.49
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD11	6	0.49
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD12	6	0.49
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD13	6	0.49
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD11	6	0.49
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD12	6	0.49
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD13	6	0.49
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG21	18	0.49
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG22	18	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG23	18	0.49
(1,449)	1:32:A:THR:HB	1:95:A:LYS:HE2	10	0.49
(1,419)	1:34:A:GLY:HA3	1:91:A:THR:HA	16	0.49
(1,413)	1:90:A:MET:HE1	1:91:A:THR:H	9	0.49
(1,413)	1:90:A:MET:HE2	1:91:A:THR:H	9	0.49
(1,413)	1:90:A:MET:HE3	1:91:A:THR:H	9	0.49
(1,400)	1:74:A:LEU:HD21	1:88:A:ALA:HB1	7	0.49
(1,400)	1:74:A:LEU:HD21	1:88:A:ALA:HB2	7	0.49
(1,400)	1:74:A:LEU:HD21	1:88:A:ALA:HB3	7	0.49
(1,400)	1:74:A:LEU:HD22	1:88:A:ALA:HB1	7	0.49
(1,400)	1:74:A:LEU:HD22	1:88:A:ALA:HB2	7	0.49
(1,400)	1:74:A:LEU:HD22	1:88:A:ALA:HB3	7	0.49
(1,400)	1:74:A:LEU:HD23	1:88:A:ALA:HB1	7	0.49
(1,400)	1:74:A:LEU:HD23	1:88:A:ALA:HB2	7	0.49
(1,400)	1:74:A:LEU:HD23	1:88:A:ALA:HB3	7	0.49
(1,375)	1:74:A:LEU:HD11	1:84:A:ASP:HB3	2	0.49
(1,375)	1:74:A:LEU:HD12	1:84:A:ASP:HB3	2	0.49
(1,375)	1:74:A:LEU:HD13	1:84:A:ASP:HB3	2	0.49
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	16	0.49
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG21	11	0.49
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG22	11	0.49
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG23	11	0.49
(1,283)	1:73:A:THR:HG21	1:76:A:ALA:HA	7	0.49
(1,283)	1:73:A:THR:HG22	1:76:A:ALA:HA	7	0.49
(1,283)	1:73:A:THR:HG23	1:76:A:ALA:HA	7	0.49
(1,266)	1:74:A:LEU:HD21	1:75:A:GLY:H	4	0.49
(1,266)	1:74:A:LEU:HD22	1:75:A:GLY:H	4	0.49
(1,266)	1:74:A:LEU:HD23	1:75:A:GLY:H	4	0.49
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	20	0.49
(1,146)	1:49:A:HIS:HD2	1:50:A:TYR:HA	3	0.49
(1,146)	1:49:A:HIS:HD2	1:50:A:TYR:HA	8	0.49
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG21	9	0.49
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG22	9	0.49
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG23	9	0.49
(1,49)	1:35:A:ASP:HA	1:37:A:VAL:HG21	12	0.49
(1,49)	1:35:A:ASP:HA	1:37:A:VAL:HG22	12	0.49
(1,49)	1:35:A:ASP:HA	1:37:A:VAL:HG23	12	0.49
(1,1624)	1:108:A:GLU:HG2	1:118:A:LYS:HG2	13	0.48
(1,1624)	1:108:A:GLU:HG3	1:118:A:LYS:HG2	13	0.48
(1,1599)	1:97:A:LEU:HD11	1:124:A:GLU:HB3	19	0.48
(1,1599)	1:97:A:LEU:HD12	1:124:A:GLU:HB3	19	0.48
(1,1599)	1:97:A:LEU:HD13	1:124:A:GLU:HB3	19	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1599)	1:97:A:LEU:HD21	1:124:A:GLU:HB3	19	0.48
(1,1599)	1:97:A:LEU:HD22	1:124:A:GLU:HB3	19	0.48
(1,1599)	1:97:A:LEU:HD23	1:124:A:GLU:HB3	19	0.48
(1,1594)	1:97:A:LEU:HD11	1:123:A:PHE:H	15	0.48
(1,1594)	1:97:A:LEU:HD12	1:123:A:PHE:H	15	0.48
(1,1594)	1:97:A:LEU:HD13	1:123:A:PHE:H	15	0.48
(1,1594)	1:97:A:LEU:HD21	1:123:A:PHE:H	15	0.48
(1,1594)	1:97:A:LEU:HD22	1:123:A:PHE:H	15	0.48
(1,1594)	1:97:A:LEU:HD23	1:123:A:PHE:H	15	0.48
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB2	17	0.48
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB3	17	0.48
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG2	11	0.48
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG3	11	0.48
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	1	0.48
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	1	0.48
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	1	0.48
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	1	0.48
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	1	0.48
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	1	0.48
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB2	3	0.48
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB3	3	0.48
(1,1265)	1:124:A:GLU:HB3	1:125:A:VAL:H	9	0.48
(1,1199)	1:80:A:ILE:HG21	1:105:A:ALA:H	19	0.48
(1,1199)	1:80:A:ILE:HG22	1:105:A:ALA:H	19	0.48
(1,1199)	1:80:A:ILE:HG23	1:105:A:ALA:H	19	0.48
(1,1106)	1:37:A:VAL:H	1:92:A:LEU:H	1	0.48
(1,1049)	1:81:A:LYS:HD3	1:84:A:ASP:H	8	0.48
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	14	0.48
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	14	0.48
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	14	0.48
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	7	0.48
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	7	0.48
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	7	0.48
(1,1003)	1:74:A:LEU:HB3	1:76:A:ALA:H	12	0.48
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	9	0.48
(1,857)	1:49:A:HIS:HD2	1:51:A:ASP:H	12	0.48
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	6	0.48
(1,786)	1:38:A:THR:H	1:91:A:THR:HA	8	0.48
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	20	0.48
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	20	0.48
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	20	0.48
(1,747)	1:27:A:GLU:H	1:98:A:PHE:HA	19	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	11	0.48
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	11	0.48
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	11	0.48
(1,651)	1:92:A:LEU:HD11	1:129:A:ALA:HA	4	0.48
(1,651)	1:92:A:LEU:HD12	1:129:A:ALA:HA	4	0.48
(1,651)	1:92:A:LEU:HD13	1:129:A:ALA:HA	4	0.48
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	6	0.48
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	6	0.48
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	6	0.48
(1,578)	1:119:A:ALA:HB1	1:120:A:THR:HB	7	0.48
(1,578)	1:119:A:ALA:HB2	1:120:A:THR:HB	7	0.48
(1,578)	1:119:A:ALA:HB3	1:120:A:THR:HB	7	0.48
(1,578)	1:119:A:ALA:HB1	1:120:A:THR:HB	13	0.48
(1,578)	1:119:A:ALA:HB2	1:120:A:THR:HB	13	0.48
(1,578)	1:119:A:ALA:HB3	1:120:A:THR:HB	13	0.48
(1,556)	1:106:A:TYR:HB2	1:110:A:GLY:HA3	11	0.48
(1,554)	1:106:A:TYR:HB2	1:110:A:GLY:HA2	5	0.48
(1,547)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	13	0.48
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB1	14	0.48
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB2	14	0.48
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB3	14	0.48
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB1	14	0.48
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB2	14	0.48
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB3	14	0.48
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB1	14	0.48
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB2	14	0.48
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB3	14	0.48
(1,464)	1:27:A:GLU:HB2	1:99:A:THR:HB	10	0.48
(1,459)	1:97:A:LEU:HG	1:99:A:THR:H	17	0.48
(1,422)	1:38:A:THR:HG21	1:91:A:THR:HA	10	0.48
(1,422)	1:38:A:THR:HG22	1:91:A:THR:HA	10	0.48
(1,422)	1:38:A:THR:HG23	1:91:A:THR:HA	10	0.48
(1,415)	1:90:A:MET:HE1	1:94:A:GLU:HA	15	0.48
(1,415)	1:90:A:MET:HE2	1:94:A:GLU:HA	15	0.48
(1,415)	1:90:A:MET:HE3	1:94:A:GLU:HA	15	0.48
(1,415)	1:90:A:MET:HE1	1:94:A:GLU:HA	17	0.48
(1,415)	1:90:A:MET:HE2	1:94:A:GLU:HA	17	0.48
(1,415)	1:90:A:MET:HE3	1:94:A:GLU:HA	17	0.48
(1,346)	1:81:A:LYS:HB3	1:82:A:GLY:HA3	4	0.48
(1,346)	1:81:A:LYS:HB3	1:82:A:GLY:HA3	15	0.48
(1,346)	1:81:A:LYS:HB3	1:82:A:GLY:HA3	16	0.48
(1,283)	1:73:A:THR:HG21	1:76:A:ALA:HA	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,283)	1:73:A:THR:HG22	1:76:A:ALA:HA	10	0.48
(1,283)	1:73:A:THR:HG23	1:76:A:ALA:HA	10	0.48
(1,265)	1:42:A:ALA:H	1:74:A:LEU:HB3	9	0.48
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG21	10	0.48
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG22	10	0.48
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG23	10	0.48
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	12	0.48
(1,155)	1:51:A:ASP:HB3	1:124:A:GLU:H	15	0.48
(1,154)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	11	0.48
(1,146)	1:49:A:HIS:HD2	1:50:A:TYR:HA	12	0.48
(1,89)	1:42:A:ALA:HB1	1:74:A:LEU:HA	5	0.48
(1,89)	1:42:A:ALA:HB2	1:74:A:LEU:HA	5	0.48
(1,89)	1:42:A:ALA:HB3	1:74:A:LEU:HA	5	0.48
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG21	14	0.48
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG22	14	0.48
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG23	14	0.48
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG21	19	0.48
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG22	19	0.48
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG23	19	0.48
(1,49)	1:35:A:ASP:HA	1:37:A:VAL:HG21	18	0.48
(1,49)	1:35:A:ASP:HA	1:37:A:VAL:HG22	18	0.48
(1,49)	1:35:A:ASP:HA	1:37:A:VAL:HG23	18	0.48
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	4	0.48
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	11	0.48
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD2	2	0.47
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD3	2	0.47
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	9	0.47
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	9	0.47
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	9	0.47
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	9	0.47
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	9	0.47
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	9	0.47
(1,1580)	1:95:A:LYS:HB2	1:128:A:LEU:HD11	9	0.47
(1,1580)	1:95:A:LYS:HB2	1:128:A:LEU:HD12	9	0.47
(1,1580)	1:95:A:LYS:HB2	1:128:A:LEU:HD13	9	0.47
(1,1580)	1:95:A:LYS:HB2	1:128:A:LEU:HD21	9	0.47
(1,1580)	1:95:A:LYS:HB2	1:128:A:LEU:HD22	9	0.47
(1,1580)	1:95:A:LYS:HB2	1:128:A:LEU:HD23	9	0.47
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB2	2	0.47
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB3	2	0.47
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG11	6	0.47
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG12	6	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG13	6	0.47
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG21	6	0.47
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG22	6	0.47
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG23	6	0.47
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG11	6	0.47
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG12	6	0.47
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG13	6	0.47
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG21	6	0.47
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG22	6	0.47
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG23	6	0.47
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	5	0.47
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	5	0.47
(1,1346)	1:28:A:LYS:HG2	1:30:A:VAL:H	18	0.47
(1,1346)	1:28:A:LYS:HG3	1:30:A:VAL:H	18	0.47
(1,1333)	1:24:A:ALA:HB1	1:103:A:GLN:HG2	14	0.47
(1,1333)	1:24:A:ALA:HB1	1:103:A:GLN:HG3	14	0.47
(1,1333)	1:24:A:ALA:HB2	1:103:A:GLN:HG2	14	0.47
(1,1333)	1:24:A:ALA:HB2	1:103:A:GLN:HG3	14	0.47
(1,1333)	1:24:A:ALA:HB3	1:103:A:GLN:HG2	14	0.47
(1,1333)	1:24:A:ALA:HB3	1:103:A:GLN:HG3	14	0.47
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	7	0.47
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	7	0.47
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	7	0.47
(1,1300)	1:92:A:LEU:HD21	1:130:A:VAL:H	11	0.47
(1,1300)	1:92:A:LEU:HD22	1:130:A:VAL:H	11	0.47
(1,1300)	1:92:A:LEU:HD23	1:130:A:VAL:H	11	0.47
(1,1252)	1:100:A:ILE:HD11	1:123:A:PHE:H	3	0.47
(1,1252)	1:100:A:ILE:HD12	1:123:A:PHE:H	3	0.47
(1,1252)	1:100:A:ILE:HD13	1:123:A:PHE:H	3	0.47
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	2	0.47
(1,1199)	1:80:A:ILE:HG21	1:105:A:ALA:H	13	0.47
(1,1199)	1:80:A:ILE:HG22	1:105:A:ALA:H	13	0.47
(1,1199)	1:80:A:ILE:HG23	1:105:A:ALA:H	13	0.47
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	4	0.47
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	4	0.47
(1,1137)	1:95:A:LYS:HG2	1:96:A:ALA:H	1	0.47
(1,1023)	1:81:A:LYS:H	1:81:A:LYS:HG3	13	0.47
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	5	0.47
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG11	9	0.47
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG12	9	0.47
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG13	9	0.47
(1,859)	1:50:A:TYR:HD2	1:51:A:ASP:H	2	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,857)	1:49:A:HIS:HD2	1:51:A:ASP:H	19	0.47
(1,820)	1:44:A:LYS:H	1:44:A:LYS:HG3	13	0.47
(1,758)	1:28:A:LYS:HG2	1:30:A:VAL:H	3	0.47
(1,696)	1:83:A:TRP:HZ2	1:123:A:PHE:HB3	15	0.47
(1,686)	1:102:A:TYR:HE2	1:118:A:LYS:HA	7	0.47
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG21	5	0.47
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG22	5	0.47
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG23	5	0.47
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB1	1	0.47
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB2	1	0.47
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB3	1	0.47
(1,632)	1:93:A:GLY:H	1:127:A:LEU:HG	15	0.47
(1,539)	1:102:A:TYR:HE2	1:108:A:GLU:HA	3	0.47
(1,536)	1:102:A:TYR:HE2	1:108:A:GLU:HB2	12	0.47
(1,519)	1:80:A:ILE:HB	1:105:A:ALA:HA	3	0.47
(1,519)	1:80:A:ILE:HB	1:105:A:ALA:HA	4	0.47
(1,516)	1:81:A:LYS:H	1:105:A:ALA:HA	13	0.47
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	12	0.47
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	15	0.47
(1,266)	1:74:A:LEU:HD21	1:75:A:GLY:H	14	0.47
(1,266)	1:74:A:LEU:HD22	1:75:A:GLY:H	14	0.47
(1,266)	1:74:A:LEU:HD23	1:75:A:GLY:H	14	0.47
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	2	0.47
(1,228)	1:47:A:THR:HG21	1:69:A:PRO:HA	16	0.47
(1,228)	1:47:A:THR:HG22	1:69:A:PRO:HA	16	0.47
(1,228)	1:47:A:THR:HG23	1:69:A:PRO:HA	16	0.47
(1,154)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	4	0.47
(1,145)	1:49:A:HIS:HB2	1:126:A:GLU:HG2	10	0.47
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	6	0.47
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	6	0.47
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	6	0.47
(1,38)	1:31:A:LEU:HG	1:32:A:THR:H	3	0.47
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	1	0.46
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	1	0.46
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	1	0.46
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	1	0.46
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	1	0.46
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	1	0.46
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB2	15	0.46
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB3	15	0.46
(1,1505)	1:66:A:ARG:HG2	1:68:A:LYS:H	2	0.46
(1,1505)	1:66:A:ARG:HG3	1:68:A:LYS:H	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	9	0.46
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	9	0.46
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	9	0.46
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	9	0.46
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	9	0.46
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	9	0.46
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD11	4	0.46
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD12	4	0.46
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD13	4	0.46
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD21	4	0.46
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD22	4	0.46
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD23	4	0.46
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD11	4	0.46
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD12	4	0.46
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD13	4	0.46
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD21	4	0.46
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD22	4	0.46
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD23	4	0.46
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD11	4	0.46
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD12	4	0.46
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD13	4	0.46
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD21	4	0.46
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD22	4	0.46
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD23	4	0.46
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD11	19	0.46
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD12	19	0.46
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD13	19	0.46
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD21	19	0.46
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD22	19	0.46
(1,1343)	1:28:A:LYS:HB2	1:97:A:LEU:HD23	19	0.46
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG11	4	0.46
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG12	4	0.46
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG13	4	0.46
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG21	4	0.46
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG22	4	0.46
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG23	4	0.46
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG11	4	0.46
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG12	4	0.46
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG13	4	0.46
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG21	4	0.46
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG22	4	0.46
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG23	4	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1265)	1:124:A:GLU:HB3	1:125:A:VAL:H	19	0.46
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	9	0.46
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	9	0.46
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	9	0.46
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG21	13	0.46
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG22	13	0.46
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG23	13	0.46
(1,1023)	1:81:A:LYS:H	1:81:A:LYS:HG3	1	0.46
(1,1023)	1:81:A:LYS:H	1:81:A:LYS:HG3	5	0.46
(1,1023)	1:81:A:LYS:H	1:81:A:LYS:HG3	11	0.46
(1,1006)	1:77:A:GLY:H	1:78:A:GLU:HB2	3	0.46
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	6	0.46
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	20	0.46
(1,859)	1:50:A:TYR:HD2	1:51:A:ASP:H	15	0.46
(1,857)	1:49:A:HIS:HD2	1:51:A:ASP:H	3	0.46
(1,702)	1:80:A:ILE:HG21	1:83:A:TRP:HE3	17	0.46
(1,702)	1:80:A:ILE:HG22	1:83:A:TRP:HE3	17	0.46
(1,702)	1:80:A:ILE:HG23	1:83:A:TRP:HE3	17	0.46
(1,694)	1:80:A:ILE:HD11	1:83:A:TRP:HD1	1	0.46
(1,694)	1:80:A:ILE:HD12	1:83:A:TRP:HD1	1	0.46
(1,694)	1:80:A:ILE:HD13	1:83:A:TRP:HD1	1	0.46
(1,645)	1:69:A:PRO:HG3	1:128:A:LEU:HG	2	0.46
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	7	0.46
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	7	0.46
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	7	0.46
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	9	0.46
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	9	0.46
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	9	0.46
(1,602)	1:100:A:ILE:HD11	1:123:A:PHE:HB3	11	0.46
(1,602)	1:100:A:ILE:HD12	1:123:A:PHE:HB3	11	0.46
(1,602)	1:100:A:ILE:HD13	1:123:A:PHE:HB3	11	0.46
(1,554)	1:106:A:TYR:HB2	1:110:A:GLY:HA2	13	0.46
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	20	0.46
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	20	0.46
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	20	0.46
(1,422)	1:38:A:THR:HG21	1:91:A:THR:HA	16	0.46
(1,422)	1:38:A:THR:HG22	1:91:A:THR:HA	16	0.46
(1,422)	1:38:A:THR:HG23	1:91:A:THR:HA	16	0.46
(1,383)	1:66:A:ARG:HG2	1:68:A:LYS:H	9	0.46
(1,315)	1:80:A:ILE:HD11	1:100:A:ILE:HG21	16	0.46
(1,315)	1:80:A:ILE:HD11	1:100:A:ILE:HG22	16	0.46
(1,315)	1:80:A:ILE:HD11	1:100:A:ILE:HG23	16	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:80:A:ILE:HD12	1:100:A:ILE:HG21	16	0.46
(1,315)	1:80:A:ILE:HD12	1:100:A:ILE:HG22	16	0.46
(1,315)	1:80:A:ILE:HD12	1:100:A:ILE:HG23	16	0.46
(1,315)	1:80:A:ILE:HD13	1:100:A:ILE:HG21	16	0.46
(1,315)	1:80:A:ILE:HD13	1:100:A:ILE:HG22	16	0.46
(1,315)	1:80:A:ILE:HD13	1:100:A:ILE:HG23	16	0.46
(1,283)	1:73:A:THR:HG21	1:76:A:ALA:HA	13	0.46
(1,283)	1:73:A:THR:HG22	1:76:A:ALA:HA	13	0.46
(1,283)	1:73:A:THR:HG23	1:76:A:ALA:HA	13	0.46
(1,211)	1:49:A:HIS:HB3	1:64:A:ARG:HA	20	0.46
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG21	20	0.46
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG22	20	0.46
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG23	20	0.46
(1,158)	1:52:A:GLY:HA2	1:123:A:PHE:HD1	16	0.46
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG21	14	0.46
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG22	14	0.46
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG23	14	0.46
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	4	0.46
(1,80)	1:38:A:THR:HB	1:40:A:PRO:HD2	11	0.46
(1,64)	1:38:A:THR:HG21	1:39:A:LYS:H	17	0.46
(1,64)	1:38:A:THR:HG22	1:39:A:LYS:H	17	0.46
(1,64)	1:38:A:THR:HG23	1:39:A:LYS:H	17	0.46
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD2	14	0.45
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD3	14	0.45
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	4	0.45
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	4	0.45
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	4	0.45
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	4	0.45
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	4	0.45
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	4	0.45
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	12	0.45
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	12	0.45
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	12	0.45
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	12	0.45
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	12	0.45
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	12	0.45
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	4	0.45
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	4	0.45
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	15	0.45
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	15	0.45
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	16	0.45
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	16	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	20	0.45
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	20	0.45
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE21	19	0.45
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE22	19	0.45
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD2	8	0.45
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD3	8	0.45
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD2	8	0.45
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD3	8	0.45
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB2	7	0.45
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB3	7	0.45
(1,1333)	1:24:A:ALA:HB1	1:103:A:GLN:HG2	19	0.45
(1,1333)	1:24:A:ALA:HB1	1:103:A:GLN:HG3	19	0.45
(1,1333)	1:24:A:ALA:HB2	1:103:A:GLN:HG2	19	0.45
(1,1333)	1:24:A:ALA:HB2	1:103:A:GLN:HG3	19	0.45
(1,1333)	1:24:A:ALA:HB3	1:103:A:GLN:HG2	19	0.45
(1,1333)	1:24:A:ALA:HB3	1:103:A:GLN:HG3	19	0.45
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG2	13	0.45
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG3	13	0.45
(1,1324)	1:19:A:PRO:HG2	1:55:A:PRO:HG2	10	0.45
(1,1324)	1:19:A:PRO:HG3	1:55:A:PRO:HG2	10	0.45
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	18	0.45
(1,1276)	1:96:A:ALA:H	1:127:A:LEU:H	18	0.45
(1,1235)	1:55:A:PRO:HG3	1:120:A:THR:H	4	0.45
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	10	0.45
(1,1195)	1:80:A:ILE:HB	1:105:A:ALA:H	2	0.45
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB1	2	0.45
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB2	2	0.45
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB3	2	0.45
(1,1097)	1:34:A:GLY:HA3	1:91:A:THR:H	11	0.45
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	6	0.45
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	6	0.45
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	6	0.45
(1,1004)	1:73:A:THR:HG21	1:76:A:ALA:H	17	0.45
(1,1004)	1:73:A:THR:HG22	1:76:A:ALA:H	17	0.45
(1,1004)	1:73:A:THR:HG23	1:76:A:ALA:H	17	0.45
(1,950)	1:64:A:ARG:HA	1:67:A:GLY:H	5	0.45
(1,911)	1:53:A:ARG:HD2	1:57:A:GLY:H	19	0.45
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	4	0.45
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	19	0.45
(1,881)	1:54:A:PHE:H	1:54:A:PHE:HD1	13	0.45
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	17	0.45
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	17	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	17	0.45
(1,744)	1:26:A:LEU:H	1:27:A:GLU:HG3	10	0.45
(1,684)	1:48:A:VAL:HG21	1:50:A:TYR:HE1	1	0.45
(1,684)	1:48:A:VAL:HG22	1:50:A:TYR:HE1	1	0.45
(1,684)	1:48:A:VAL:HG23	1:50:A:TYR:HE1	1	0.45
(1,660)	1:72:A:PHE:HB2	1:79:A:VAL:HG11	17	0.45
(1,660)	1:72:A:PHE:HB2	1:79:A:VAL:HG12	17	0.45
(1,660)	1:72:A:PHE:HB2	1:79:A:VAL:HG13	17	0.45
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	20	0.45
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB1	2	0.45
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB2	2	0.45
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB3	2	0.45
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	11	0.45
(1,630)	1:127:A:LEU:HG	1:129:A:ALA:HA	19	0.45
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG21	6	0.45
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG22	6	0.45
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG23	6	0.45
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	13	0.45
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	13	0.45
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	13	0.45
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG21	9	0.45
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG22	9	0.45
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG23	9	0.45
(1,464)	1:27:A:GLU:HB2	1:99:A:THR:HB	19	0.45
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB1	15	0.45
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB2	15	0.45
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB3	15	0.45
(1,419)	1:34:A:GLY:HA3	1:91:A:THR:HA	7	0.45
(1,385)	1:82:A:GLY:HA2	1:85:A:GLN:HB3	8	0.45
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD11	1	0.45
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD12	1	0.45
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD13	1	0.45
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	16	0.45
(1,198)	1:59:A:GLN:HG2	1:61:A:ASP:H	16	0.45
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	1	0.45
(1,161)	1:53:A:ARG:HA	1:60:A:PHE:H	13	0.45
(1,152)	1:51:A:ASP:HB2	1:124:A:GLU:H	19	0.45
(1,146)	1:49:A:HIS:HD2	1:50:A:TYR:HA	17	0.45
(1,146)	1:49:A:HIS:HD2	1:50:A:TYR:HA	19	0.45
(1,103)	1:45:A:LYS:HG2	1:46:A:VAL:H	9	0.45
(1,68)	1:38:A:THR:HG21	1:92:A:LEU:HA	10	0.45
(1,68)	1:38:A:THR:HG22	1:92:A:LEU:HA	10	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:38:A:THR:HG23	1:92:A:LEU:HA	10	0.45
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	5	0.45
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	5	0.45
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	5	0.45
(1,64)	1:38:A:THR:HG21	1:39:A:LYS:H	8	0.45
(1,64)	1:38:A:THR:HG22	1:39:A:LYS:H	8	0.45
(1,64)	1:38:A:THR:HG23	1:39:A:LYS:H	8	0.45
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG21	4	0.45
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG22	4	0.45
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG23	4	0.45
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	2	0.45
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	18	0.44
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	18	0.44
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	18	0.44
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	18	0.44
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	18	0.44
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	18	0.44
(1,1543)	1:85:A:GLN:HB2	1:98:A:PHE:HD2	12	0.44
(1,1543)	1:85:A:GLN:HB3	1:98:A:PHE:HD2	12	0.44
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	17	0.44
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	17	0.44
(1,1474)	1:59:A:GLN:HG2	1:60:A:PHE:H	18	0.44
(1,1474)	1:59:A:GLN:HG3	1:60:A:PHE:H	18	0.44
(1,1440)	1:53:A:ARG:HD2	1:57:A:GLY:H	19	0.44
(1,1440)	1:53:A:ARG:HD3	1:57:A:GLY:H	19	0.44
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG2	2	0.44
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG3	2	0.44
(1,1433)	1:51:A:ASP:HB2	1:124:A:GLU:HB3	20	0.44
(1,1433)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	20	0.44
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG11	10	0.44
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG12	10	0.44
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG13	10	0.44
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG21	10	0.44
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG22	10	0.44
(1,1379)	1:39:A:LYS:H	1:130:A:VAL:HG23	10	0.44
(1,1314)	1:13:A:GLU:H	1:13:A:GLU:HB2	2	0.44
(1,1314)	1:13:A:GLU:H	1:13:A:GLU:HB3	2	0.44
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	1	0.44
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	1	0.44
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	1	0.44
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	14	0.44
(1,1199)	1:80:A:ILE:HG21	1:105:A:ALA:H	2	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1199)	1:80:A:ILE:HG22	1:105:A:ALA:H	2	0.44
(1,1199)	1:80:A:ILE:HG23	1:105:A:ALA:H	2	0.44
(1,1199)	1:80:A:ILE:HG21	1:105:A:ALA:H	16	0.44
(1,1199)	1:80:A:ILE:HG22	1:105:A:ALA:H	16	0.44
(1,1199)	1:80:A:ILE:HG23	1:105:A:ALA:H	16	0.44
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	14	0.44
(1,1023)	1:81:A:LYS:H	1:81:A:LYS:HG3	20	0.44
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	8	0.44
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG11	5	0.44
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG12	5	0.44
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG13	5	0.44
(1,972)	1:70:A:PHE:HD2	1:71:A:GLN:H	20	0.44
(1,952)	1:67:A:GLY:H	1:68:A:LYS:HB2	5	0.44
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	2	0.44
(1,881)	1:54:A:PHE:H	1:54:A:PHE:HD1	19	0.44
(1,859)	1:50:A:TYR:HD2	1:51:A:ASP:H	7	0.44
(1,811)	1:43:A:GLY:H	1:74:A:LEU:HB2	11	0.44
(1,786)	1:38:A:THR:H	1:91:A:THR:HA	19	0.44
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	1	0.44
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	1	0.44
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	1	0.44
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	5	0.44
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	5	0.44
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	5	0.44
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG21	10	0.44
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG22	10	0.44
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG23	10	0.44
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG11	3	0.44
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG12	3	0.44
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG13	3	0.44
(1,575)	1:102:A:TYR:HE2	1:118:A:LYS:HG2	18	0.44
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD21	2	0.44
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD22	2	0.44
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD23	2	0.44
(1,411)	1:90:A:MET:HE1	1:127:A:LEU:H	17	0.44
(1,411)	1:90:A:MET:HE2	1:127:A:LEU:H	17	0.44
(1,411)	1:90:A:MET:HE3	1:127:A:LEU:H	17	0.44
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	10	0.44
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	10	0.44
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	10	0.44
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD21	3	0.44
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD22	3	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD23	3	0.44
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD11	5	0.44
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD12	5	0.44
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD13	5	0.44
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD21	19	0.44
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD22	19	0.44
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD23	19	0.44
(1,198)	1:59:A:GLN:HG2	1:61:A:ASP:H	5	0.44
(1,153)	1:51:A:ASP:HB2	1:124:A:GLU:HB3	12	0.44
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG21	3	0.44
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG22	3	0.44
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG23	3	0.44
(1,27)	1:27:A:GLU:HG3	1:99:A:THR:HB	10	0.44
(1,1648)	1:121:A:LEU:HD11	1:123:A:PHE:HD1	4	0.43
(1,1648)	1:121:A:LEU:HD12	1:123:A:PHE:HD1	4	0.43
(1,1648)	1:121:A:LEU:HD13	1:123:A:PHE:HD1	4	0.43
(1,1648)	1:121:A:LEU:HD21	1:123:A:PHE:HD1	4	0.43
(1,1648)	1:121:A:LEU:HD22	1:123:A:PHE:HD1	4	0.43
(1,1648)	1:121:A:LEU:HD23	1:123:A:PHE:HD1	4	0.43
(1,1648)	1:121:A:LEU:HD11	1:123:A:PHE:HD1	13	0.43
(1,1648)	1:121:A:LEU:HD12	1:123:A:PHE:HD1	13	0.43
(1,1648)	1:121:A:LEU:HD13	1:123:A:PHE:HD1	13	0.43
(1,1648)	1:121:A:LEU:HD21	1:123:A:PHE:HD1	13	0.43
(1,1648)	1:121:A:LEU:HD22	1:123:A:PHE:HD1	13	0.43
(1,1648)	1:121:A:LEU:HD23	1:123:A:PHE:HD1	13	0.43
(1,1624)	1:108:A:GLU:HG2	1:118:A:LYS:HG2	3	0.43
(1,1624)	1:108:A:GLU:HG3	1:118:A:LYS:HG2	3	0.43
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB2	2	0.43
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB3	2	0.43
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB2	2	0.43
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB3	2	0.43
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB2	12	0.43
(1,1623)	1:108:A:GLU:HG2	1:118:A:LYS:HB3	12	0.43
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB2	12	0.43
(1,1623)	1:108:A:GLU:HG3	1:118:A:LYS:HB3	12	0.43
(1,1612)	1:102:A:TYR:HB2	1:108:A:GLU:HG2	11	0.43
(1,1612)	1:102:A:TYR:HB2	1:108:A:GLU:HG3	11	0.43
(1,1599)	1:97:A:LEU:HD11	1:124:A:GLU:HB3	20	0.43
(1,1599)	1:97:A:LEU:HD12	1:124:A:GLU:HB3	20	0.43
(1,1599)	1:97:A:LEU:HD13	1:124:A:GLU:HB3	20	0.43
(1,1599)	1:97:A:LEU:HD21	1:124:A:GLU:HB3	20	0.43
(1,1599)	1:97:A:LEU:HD22	1:124:A:GLU:HB3	20	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1599)	1:97:A:LEU:HD23	1:124:A:GLU:HB3	20	0.43
(1,1584)	1:95:A:LYS:HG2	1:124:A:GLU:HB3	19	0.43
(1,1584)	1:95:A:LYS:HG3	1:124:A:GLU:HB3	19	0.43
(1,1543)	1:85:A:GLN:HB2	1:98:A:PHE:HD2	10	0.43
(1,1543)	1:85:A:GLN:HB3	1:98:A:PHE:HD2	10	0.43
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	7	0.43
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	7	0.43
(1,1470)	1:59:A:GLN:H	1:59:A:GLN:HG2	17	0.43
(1,1470)	1:59:A:GLN:H	1:59:A:GLN:HG3	17	0.43
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG11	18	0.43
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG12	18	0.43
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG13	18	0.43
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG21	18	0.43
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG22	18	0.43
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG23	18	0.43
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	19	0.43
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	19	0.43
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	12	0.43
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	12	0.43
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD11	14	0.43
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD12	14	0.43
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD13	14	0.43
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD21	14	0.43
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD22	14	0.43
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD23	14	0.43
(1,1323)	1:19:A:PRO:HG2	1:55:A:PRO:HB2	1	0.43
(1,1323)	1:19:A:PRO:HG3	1:55:A:PRO:HB2	1	0.43
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	14	0.43
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	4	0.43
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	4	0.43
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	4	0.43
(1,1281)	1:95:A:LYS:HB2	1:127:A:LEU:H	9	0.43
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	3	0.43
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	6	0.43
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	5	0.43
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	5	0.43
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	5	0.43
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	4	0.43
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	4	0.43
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	4	0.43
(1,912)	1:53:A:ARG:HD3	1:57:A:GLY:H	11	0.43
(1,859)	1:50:A:TYR:HD2	1:51:A:ASP:H	18	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	12	0.43
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	12	0.43
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	12	0.43
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	10	0.43
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	10	0.43
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	10	0.43
(1,714)	1:13:A:GLU:HA	1:14:A:ALA:H	2	0.43
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB1	15	0.43
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB2	15	0.43
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB3	15	0.43
(1,602)	1:100:A:ILE:HD11	1:123:A:PHE:HB3	17	0.43
(1,602)	1:100:A:ILE:HD12	1:123:A:PHE:HB3	17	0.43
(1,602)	1:100:A:ILE:HD13	1:123:A:PHE:HB3	17	0.43
(1,554)	1:106:A:TYR:HB2	1:110:A:GLY:HA2	7	0.43
(1,536)	1:102:A:TYR:HE2	1:108:A:GLU:HB2	14	0.43
(1,419)	1:34:A:GLY:HA3	1:91:A:THR:HA	6	0.43
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	12	0.43
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	12	0.43
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	12	0.43
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	12	0.43
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	12	0.43
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	12	0.43
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	12	0.43
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	12	0.43
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	12	0.43
(1,289)	1:76:A:ALA:HB1	1:78:A:GLU:HB2	18	0.43
(1,289)	1:76:A:ALA:HB2	1:78:A:GLU:HB2	18	0.43
(1,289)	1:76:A:ALA:HB3	1:78:A:GLU:HB2	18	0.43
(1,232)	1:48:A:VAL:H	1:69:A:PRO:HB3	4	0.43
(1,201)	1:59:A:GLN:H	1:59:A:GLN:HG3	2	0.43
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	17	0.43
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	19	0.43
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	19	0.43
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	19	0.43
(1,121)	1:46:A:VAL:HG11	1:130:A:VAL:H	19	0.43
(1,121)	1:46:A:VAL:HG12	1:130:A:VAL:H	19	0.43
(1,121)	1:46:A:VAL:HG13	1:130:A:VAL:H	19	0.43
(1,103)	1:45:A:LYS:HG2	1:46:A:VAL:H	16	0.43
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	6	0.43
(1,75)	1:38:A:THR:HB	1:40:A:PRO:HG3	4	0.43
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	10	0.42
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	10	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	10	0.42
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	10	0.42
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	10	0.42
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	10	0.42
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	3	0.42
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	3	0.42
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	6	0.42
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	6	0.42
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE21	12	0.42
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE22	12	0.42
(1,1442)	1:53:A:ARG:HD2	1:59:A:GLN:HA	10	0.42
(1,1442)	1:53:A:ARG:HD3	1:59:A:GLN:HA	10	0.42
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD11	13	0.42
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD12	13	0.42
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD13	13	0.42
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD21	13	0.42
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD22	13	0.42
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD23	13	0.42
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	1	0.42
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	1	0.42
(1,1346)	1:28:A:LYS:HG2	1:30:A:VAL:H	15	0.42
(1,1346)	1:28:A:LYS:HG3	1:30:A:VAL:H	15	0.42
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG11	11	0.42
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG12	11	0.42
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG13	11	0.42
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG21	11	0.42
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG22	11	0.42
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG23	11	0.42
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG11	11	0.42
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG12	11	0.42
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG13	11	0.42
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG21	11	0.42
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG22	11	0.42
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG23	11	0.42
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB2	20	0.42
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB3	20	0.42
(1,1310)	1:81:A:LYS:HE2	1:85:A:GLN:HE22	9	0.42
(1,1309)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	18	0.42
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	3	0.42
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	12	0.42
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	12	0.42
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	12	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	3	0.42
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	11	0.42
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	1	0.42
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	2	0.42
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB1	14	0.42
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB2	14	0.42
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB3	14	0.42
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	15	0.42
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	15	0.42
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	15	0.42
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	20	0.42
(1,1006)	1:77:A:GLY:H	1:78:A:GLU:HB2	17	0.42
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	16	0.42
(1,866)	1:51:A:ASP:H	1:124:A:GLU:HB3	16	0.42
(1,863)	1:50:A:TYR:HB2	1:51:A:ASP:H	5	0.42
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD21	5	0.42
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD22	5	0.42
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD23	5	0.42
(1,751)	1:27:A:GLU:HG2	1:28:A:LYS:H	6	0.42
(1,686)	1:102:A:TYR:HE2	1:118:A:LYS:HA	3	0.42
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG21	12	0.42
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG22	12	0.42
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG23	12	0.42
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG21	17	0.42
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG22	17	0.42
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG23	17	0.42
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG21	20	0.42
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG22	20	0.42
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG23	20	0.42
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD21	2	0.42
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD22	2	0.42
(1,510)	1:81:A:LYS:HE3	1:104:A:LEU:HD23	2	0.42
(1,465)	1:99:A:THR:HB	1:122:A:VAL:HG11	17	0.42
(1,465)	1:99:A:THR:HB	1:122:A:VAL:HG12	17	0.42
(1,465)	1:99:A:THR:HB	1:122:A:VAL:HG13	17	0.42
(1,419)	1:34:A:GLY:HA3	1:91:A:THR:HA	10	0.42
(1,419)	1:34:A:GLY:HA3	1:91:A:THR:HA	19	0.42
(1,415)	1:90:A:MET:HE1	1:94:A:GLU:HA	19	0.42
(1,415)	1:90:A:MET:HE2	1:94:A:GLU:HA	19	0.42
(1,415)	1:90:A:MET:HE3	1:94:A:GLU:HA	19	0.42
(1,385)	1:82:A:GLY:HA2	1:85:A:GLN:HB3	9	0.42
(1,346)	1:81:A:LYS:HB3	1:82:A:GLY:HA3	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,197)	1:59:A:GLN:HG2	1:60:A:PHE:H	4	0.42
(1,193)	1:53:A:ARG:HB3	1:59:A:GLN:HA	17	0.42
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	15	0.42
(1,152)	1:51:A:ASP:HB2	1:124:A:GLU:H	13	0.42
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG11	7	0.42
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG12	7	0.42
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG13	7	0.42
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	1	0.42
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	1	0.42
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	1	0.42
(1,103)	1:45:A:LYS:HG2	1:46:A:VAL:H	5	0.42
(1,92)	1:41:A:GLN:HG2	1:44:A:LYS:HG2	13	0.42
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	19	0.42
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG21	12	0.42
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG22	12	0.42
(1,60)	1:38:A:THR:HA	1:130:A:VAL:HG23	12	0.42
(1,40)	1:32:A:THR:HB	1:95:A:LYS:HB3	1	0.42
(1,28)	1:27:A:GLU:HG2	1:99:A:THR:HB	14	0.42
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	5	0.42
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	3	0.41
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	3	0.41
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	3	0.41
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	3	0.41
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	3	0.41
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	3	0.41
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	14	0.41
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	14	0.41
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	14	0.41
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	14	0.41
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	14	0.41
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	14	0.41
(1,1539)	1:85:A:GLN:HA	1:85:A:GLN:HE21	16	0.41
(1,1539)	1:85:A:GLN:HA	1:85:A:GLN:HE22	16	0.41
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	10	0.41
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	10	0.41
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG11	19	0.41
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG12	19	0.41
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG13	19	0.41
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG21	19	0.41
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG22	19	0.41
(1,1480)	1:60:A:PHE:HD2	1:114:A:VAL:HG23	19	0.41
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB2	11	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB3	11	0.41
(1,1440)	1:53:A:ARG:HD2	1:57:A:GLY:H	8	0.41
(1,1440)	1:53:A:ARG:HD3	1:57:A:GLY:H	8	0.41
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG2	5	0.41
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG3	5	0.41
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG11	15	0.41
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG12	15	0.41
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG13	15	0.41
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG21	15	0.41
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG22	15	0.41
(1,1387)	1:41:A:GLN:H	1:130:A:VAL:HG23	15	0.41
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD11	4	0.41
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD12	4	0.41
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD13	4	0.41
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD21	4	0.41
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD22	4	0.41
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD23	4	0.41
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	16	0.41
(1,1162)	1:27:A:GLU:HB2	1:99:A:THR:H	4	0.41
(1,1120)	1:34:A:GLY:HA2	1:94:A:GLU:H	15	0.41
(1,1116)	1:92:A:LEU:HD11	1:93:A:GLY:H	13	0.41
(1,1116)	1:92:A:LEU:HD12	1:93:A:GLY:H	13	0.41
(1,1116)	1:92:A:LEU:HD13	1:93:A:GLY:H	13	0.41
(1,1097)	1:34:A:GLY:HA3	1:91:A:THR:H	6	0.41
(1,1003)	1:74:A:LEU:HB3	1:76:A:ALA:H	6	0.41
(1,896)	1:59:A:GLN:HE21	1:62:A:SER:HB2	9	0.41
(1,824)	1:44:A:LYS:HB3	1:45:A:LYS:H	17	0.41
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG21	6	0.41
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG22	6	0.41
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG23	6	0.41
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	15	0.41
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	15	0.41
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	15	0.41
(1,751)	1:27:A:GLU:HG2	1:28:A:LYS:H	7	0.41
(1,747)	1:27:A:GLU:H	1:98:A:PHE:HA	15	0.41
(1,696)	1:83:A:TRP:HZ2	1:123:A:PHE:HB3	18	0.41
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	8	0.41
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	14	0.41
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	14	0.41
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	14	0.41
(1,632)	1:93:A:GLY:H	1:127:A:LEU:HG	12	0.41
(1,611)	1:123:A:PHE:H	1:124:A:GLU:HG3	3	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,581)	1:55:A:PRO:HG3	1:120:A:THR:HB	17	0.41
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	1	0.41
(1,522)	1:80:A:ILE:HG21	1:105:A:ALA:HA	16	0.41
(1,522)	1:80:A:ILE:HG22	1:105:A:ALA:HA	16	0.41
(1,522)	1:80:A:ILE:HG23	1:105:A:ALA:HA	16	0.41
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	11	0.41
(1,482)	1:100:A:ILE:HG21	1:104:A:LEU:HB2	20	0.41
(1,482)	1:100:A:ILE:HG22	1:104:A:LEU:HB2	20	0.41
(1,482)	1:100:A:ILE:HG23	1:104:A:LEU:HB2	20	0.41
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB1	15	0.41
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB2	15	0.41
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB3	15	0.41
(1,413)	1:90:A:MET:HE1	1:91:A:THR:H	4	0.41
(1,413)	1:90:A:MET:HE2	1:91:A:THR:H	4	0.41
(1,413)	1:90:A:MET:HE3	1:91:A:THR:H	4	0.41
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG21	2	0.41
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG22	2	0.41
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG23	2	0.41
(1,350)	1:82:A:GLY:HA3	1:104:A:LEU:HD11	19	0.41
(1,350)	1:82:A:GLY:HA3	1:104:A:LEU:HD12	19	0.41
(1,350)	1:82:A:GLY:HA3	1:104:A:LEU:HD13	19	0.41
(1,346)	1:81:A:LYS:HB3	1:82:A:GLY:HA3	18	0.41
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	8	0.41
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	8	0.41
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	8	0.41
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	4	0.41
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG21	4	0.41
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG22	4	0.41
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG23	4	0.41
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG21	16	0.41
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG22	16	0.41
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG23	16	0.41
(1,225)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	12	0.41
(1,197)	1:59:A:GLN:HG2	1:60:A:PHE:H	1	0.41
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG21	17	0.41
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG22	17	0.41
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG23	17	0.41
(1,130)	1:48:A:VAL:HG11	1:50:A:TYR:HD1	19	0.41
(1,130)	1:48:A:VAL:HG12	1:50:A:TYR:HD1	19	0.41
(1,130)	1:48:A:VAL:HG13	1:50:A:TYR:HD1	19	0.41
(1,121)	1:46:A:VAL:HG11	1:130:A:VAL:H	8	0.41
(1,121)	1:46:A:VAL:HG12	1:130:A:VAL:H	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:46:A:VAL:HG13	1:130:A:VAL:H	8	0.41
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG21	12	0.41
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG22	12	0.41
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG23	12	0.41
(1,81)	1:42:A:ALA:HA	1:74:A:LEU:H	18	0.41
(1,64)	1:38:A:THR:HG21	1:39:A:LYS:H	9	0.41
(1,64)	1:38:A:THR:HG22	1:39:A:LYS:H	9	0.41
(1,64)	1:38:A:THR:HG23	1:39:A:LYS:H	9	0.41
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	3	0.41
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	3	0.41
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	3	0.41
(1,42)	1:33:A:PRO:HA	1:94:A:GLU:HG2	20	0.41
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	18	0.41
(1,1612)	1:102:A:TYR:HB2	1:108:A:GLU:HG2	7	0.4
(1,1612)	1:102:A:TYR:HB2	1:108:A:GLU:HG3	7	0.4
(1,1594)	1:97:A:LEU:HD11	1:123:A:PHE:H	16	0.4
(1,1594)	1:97:A:LEU:HD12	1:123:A:PHE:H	16	0.4
(1,1594)	1:97:A:LEU:HD13	1:123:A:PHE:H	16	0.4
(1,1594)	1:97:A:LEU:HD21	1:123:A:PHE:H	16	0.4
(1,1594)	1:97:A:LEU:HD22	1:123:A:PHE:H	16	0.4
(1,1594)	1:97:A:LEU:HD23	1:123:A:PHE:H	16	0.4
(1,1505)	1:66:A:ARG:HG2	1:68:A:LYS:H	3	0.4
(1,1505)	1:66:A:ARG:HG3	1:68:A:LYS:H	3	0.4
(1,1474)	1:59:A:GLN:HG2	1:60:A:PHE:H	3	0.4
(1,1474)	1:59:A:GLN:HG3	1:60:A:PHE:H	3	0.4
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE21	11	0.4
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE22	11	0.4
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB2	20	0.4
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB3	20	0.4
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE2	8	0.4
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE3	8	0.4
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE2	8	0.4
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE3	8	0.4
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB2	13	0.4
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB3	13	0.4
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	2	0.4
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	4	0.4
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	19	0.4
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	9	0.4
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	17	0.4
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	6	0.4
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	6	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	6	0.4
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	5	0.4
(1,1116)	1:92:A:LEU:HD11	1:93:A:GLY:H	20	0.4
(1,1116)	1:92:A:LEU:HD12	1:93:A:GLY:H	20	0.4
(1,1116)	1:92:A:LEU:HD13	1:93:A:GLY:H	20	0.4
(1,1111)	1:38:A:THR:HG21	1:92:A:LEU:H	19	0.4
(1,1111)	1:38:A:THR:HG22	1:92:A:LEU:H	19	0.4
(1,1111)	1:38:A:THR:HG23	1:92:A:LEU:H	19	0.4
(1,1029)	1:82:A:GLY:H	1:104:A:LEU:HB3	19	0.4
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	2	0.4
(1,1004)	1:73:A:THR:HG21	1:76:A:ALA:H	10	0.4
(1,1004)	1:73:A:THR:HG22	1:76:A:ALA:H	10	0.4
(1,1004)	1:73:A:THR:HG23	1:76:A:ALA:H	10	0.4
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	18	0.4
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	10	0.4
(1,859)	1:50:A:TYR:HD2	1:51:A:ASP:H	14	0.4
(1,859)	1:50:A:TYR:HD2	1:51:A:ASP:H	19	0.4
(1,787)	1:37:A:VAL:HB	1:38:A:THR:H	4	0.4
(1,749)	1:27:A:GLU:H	1:27:A:GLU:HG3	3	0.4
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	15	0.4
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	15	0.4
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	15	0.4
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	20	0.4
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	20	0.4
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	20	0.4
(1,630)	1:127:A:LEU:HG	1:129:A:ALA:HA	18	0.4
(1,547)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	6	0.4
(1,536)	1:102:A:TYR:HE2	1:108:A:GLU:HB2	11	0.4
(1,516)	1:81:A:LYS:H	1:105:A:ALA:HA	15	0.4
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	20	0.4
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	20	0.4
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	20	0.4
(1,481)	1:100:A:ILE:HG21	1:104:A:LEU:HA	20	0.4
(1,481)	1:100:A:ILE:HG22	1:104:A:LEU:HA	20	0.4
(1,481)	1:100:A:ILE:HG23	1:104:A:LEU:HA	20	0.4
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB1	20	0.4
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB2	20	0.4
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB3	20	0.4
(1,403)	1:89:A:THR:HG21	1:98:A:PHE:HD2	15	0.4
(1,403)	1:89:A:THR:HG22	1:98:A:PHE:HD2	15	0.4
(1,403)	1:89:A:THR:HG23	1:98:A:PHE:HD2	15	0.4
(1,371)	1:81:A:LYS:HD3	1:84:A:ASP:HB2	19	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,343)	1:66:A:ARG:HG3	1:68:A:LYS:H	3	0.4
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD11	11	0.4
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD12	11	0.4
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD13	11	0.4
(1,283)	1:73:A:THR:HG21	1:76:A:ALA:HA	17	0.4
(1,283)	1:73:A:THR:HG22	1:76:A:ALA:HA	17	0.4
(1,283)	1:73:A:THR:HG23	1:76:A:ALA:HA	17	0.4
(1,185)	1:53:A:ARG:HB3	1:57:A:GLY:HA2	5	0.4
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG21	11	0.4
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG22	11	0.4
(1,173)	1:55:A:PRO:HA	1:120:A:THR:HG23	11	0.4
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	4	0.4
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG11	13	0.4
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG12	13	0.4
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG13	13	0.4
(1,130)	1:48:A:VAL:HG11	1:50:A:TYR:HD1	7	0.4
(1,130)	1:48:A:VAL:HG12	1:50:A:TYR:HD1	7	0.4
(1,130)	1:48:A:VAL:HG13	1:50:A:TYR:HD1	7	0.4
(1,130)	1:48:A:VAL:HG11	1:50:A:TYR:HD1	13	0.4
(1,130)	1:48:A:VAL:HG12	1:50:A:TYR:HD1	13	0.4
(1,130)	1:48:A:VAL:HG13	1:50:A:TYR:HD1	13	0.4
(1,103)	1:45:A:LYS:HG2	1:46:A:VAL:H	20	0.4
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	12	0.39
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	12	0.39
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	12	0.39
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	12	0.39
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	12	0.39
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	12	0.39
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	20	0.39
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	20	0.39
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	20	0.39
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	20	0.39
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	20	0.39
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	20	0.39
(1,1594)	1:97:A:LEU:HD11	1:123:A:PHE:H	12	0.39
(1,1594)	1:97:A:LEU:HD12	1:123:A:PHE:H	12	0.39
(1,1594)	1:97:A:LEU:HD13	1:123:A:PHE:H	12	0.39
(1,1594)	1:97:A:LEU:HD21	1:123:A:PHE:H	12	0.39
(1,1594)	1:97:A:LEU:HD22	1:123:A:PHE:H	12	0.39
(1,1594)	1:97:A:LEU:HD23	1:123:A:PHE:H	12	0.39
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	5	0.39
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	5	0.39
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	5	0.39
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	5	0.39
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	5	0.39
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG11	8	0.39
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG12	8	0.39
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG13	8	0.39
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG21	8	0.39
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG22	8	0.39
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG23	8	0.39
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG11	8	0.39
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG12	8	0.39
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG13	8	0.39
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG21	8	0.39
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG22	8	0.39
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG23	8	0.39
(1,1433)	1:51:A:ASP:HB2	1:124:A:GLU:HB3	3	0.39
(1,1433)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	3	0.39
(1,1397)	1:43:A:GLY:HA2	1:44:A:LYS:HG2	19	0.39
(1,1397)	1:43:A:GLY:HA2	1:44:A:LYS:HG3	19	0.39
(1,1397)	1:43:A:GLY:HA3	1:44:A:LYS:HG2	19	0.39
(1,1397)	1:43:A:GLY:HA3	1:44:A:LYS:HG3	19	0.39
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE2	12	0.39
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE3	12	0.39
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE2	12	0.39
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE3	12	0.39
(1,1346)	1:28:A:LYS:HG2	1:30:A:VAL:H	16	0.39
(1,1346)	1:28:A:LYS:HG3	1:30:A:VAL:H	16	0.39
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	20	0.39
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	11	0.39
(1,1193)	1:105:A:ALA:H	1:107:A:GLY:H	20	0.39
(1,1069)	1:86:A:GLY:H	1:98:A:PHE:HD2	9	0.39
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	15	0.39
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	15	0.39
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	15	0.39
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	19	0.39
(1,950)	1:64:A:ARG:HA	1:67:A:GLY:H	13	0.39
(1,897)	1:59:A:GLN:HE21	1:62:A:SER:HB3	13	0.39
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	1	0.39
(1,881)	1:54:A:PHE:H	1:54:A:PHE:HD1	11	0.39
(1,820)	1:44:A:LYS:H	1:44:A:LYS:HG3	16	0.39
(1,786)	1:38:A:THR:H	1:91:A:THR:HA	13	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,781)	1:37:A:VAL:H	1:91:A:THR:HB	19	0.39
(1,747)	1:27:A:GLU:H	1:98:A:PHE:HA	6	0.39
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	8	0.39
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	8	0.39
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	8	0.39
(1,716)	1:13:A:GLU:HG3	1:14:A:ALA:H	13	0.39
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	20	0.39
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	20	0.39
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	20	0.39
(1,631)	1:92:A:LEU:H	1:127:A:LEU:HG	19	0.39
(1,623)	1:95:A:LYS:HB2	1:126:A:GLU:HA	7	0.39
(1,611)	1:123:A:PHE:H	1:124:A:GLU:HG3	5	0.39
(1,602)	1:100:A:ILE:HD11	1:123:A:PHE:HB3	5	0.39
(1,602)	1:100:A:ILE:HD12	1:123:A:PHE:HB3	5	0.39
(1,602)	1:100:A:ILE:HD13	1:123:A:PHE:HB3	5	0.39
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	4	0.39
(1,557)	1:110:A:GLY:HA3	1:115:A:ILE:HB	7	0.39
(1,542)	1:108:A:GLU:HA	1:118:A:LYS:HG3	3	0.39
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG21	5	0.39
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG22	5	0.39
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG23	5	0.39
(1,459)	1:97:A:LEU:HG	1:99:A:THR:H	9	0.39
(1,383)	1:66:A:ARG:HG2	1:68:A:LYS:H	1	0.39
(1,346)	1:81:A:LYS:HB3	1:82:A:GLY:HA3	19	0.39
(1,265)	1:42:A:ALA:H	1:74:A:LEU:HB3	4	0.39
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	16	0.39
(1,192)	1:59:A:GLN:HA	1:61:A:ASP:H	20	0.39
(1,185)	1:53:A:ARG:HB3	1:57:A:GLY:HA2	20	0.39
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	6	0.39
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	12	0.39
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG21	15	0.39
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG22	15	0.39
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG23	15	0.39
(1,89)	1:42:A:ALA:HB1	1:74:A:LEU:HA	16	0.39
(1,89)	1:42:A:ALA:HB2	1:74:A:LEU:HA	16	0.39
(1,89)	1:42:A:ALA:HB3	1:74:A:LEU:HA	16	0.39
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG21	20	0.39
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG22	20	0.39
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG23	20	0.39
(1,64)	1:38:A:THR:HG21	1:39:A:LYS:H	6	0.39
(1,64)	1:38:A:THR:HG22	1:39:A:LYS:H	6	0.39
(1,64)	1:38:A:THR:HG23	1:39:A:LYS:H	6	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	1:38:A:THR:HG21	1:39:A:LYS:H	12	0.39
(1,64)	1:38:A:THR:HG22	1:39:A:LYS:H	12	0.39
(1,64)	1:38:A:THR:HG23	1:39:A:LYS:H	12	0.39
(1,2)	1:28:A:LYS:HB2	1:30:A:VAL:H	4	0.39
(1,1613)	1:102:A:TYR:HE2	1:118:A:LYS:HB2	9	0.38
(1,1613)	1:102:A:TYR:HE2	1:118:A:LYS:HB3	9	0.38
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	13	0.38
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	13	0.38
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	13	0.38
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	13	0.38
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	13	0.38
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	13	0.38
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG2	12	0.38
(1,1452)	1:54:A:PHE:HD1	1:58:A:LYS:HG3	12	0.38
(1,1441)	1:53:A:ARG:HD2	1:57:A:GLY:HA2	16	0.38
(1,1441)	1:53:A:ARG:HD3	1:57:A:GLY:HA2	16	0.38
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	12	0.38
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	12	0.38
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	12	0.38
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	12	0.38
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	12	0.38
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	12	0.38
(1,1397)	1:43:A:GLY:HA2	1:44:A:LYS:HG2	17	0.38
(1,1397)	1:43:A:GLY:HA2	1:44:A:LYS:HG3	17	0.38
(1,1397)	1:43:A:GLY:HA3	1:44:A:LYS:HG2	17	0.38
(1,1397)	1:43:A:GLY:HA3	1:44:A:LYS:HG3	17	0.38
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	19	0.38
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	19	0.38
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	19	0.38
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	19	0.38
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	19	0.38
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	19	0.38
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	19	0.38
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	19	0.38
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	19	0.38
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	19	0.38
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	19	0.38
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	19	0.38
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	19	0.38
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	19	0.38
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	19	0.38
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	19	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	19	0.38
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	19	0.38
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD11	18	0.38
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD12	18	0.38
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD13	18	0.38
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD21	18	0.38
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD22	18	0.38
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD23	18	0.38
(1,1281)	1:95:A:LYS:HB2	1:127:A:LEU:H	7	0.38
(1,1195)	1:80:A:ILE:HB	1:105:A:ALA:H	5	0.38
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	2	0.38
(1,1162)	1:27:A:GLU:HB2	1:99:A:THR:H	19	0.38
(1,1130)	1:90:A:MET:HE1	1:95:A:LYS:H	7	0.38
(1,1130)	1:90:A:MET:HE2	1:95:A:LYS:H	7	0.38
(1,1130)	1:90:A:MET:HE3	1:95:A:LYS:H	7	0.38
(1,1111)	1:38:A:THR:HG21	1:92:A:LEU:H	10	0.38
(1,1111)	1:38:A:THR:HG22	1:92:A:LEU:H	10	0.38
(1,1111)	1:38:A:THR:HG23	1:92:A:LEU:H	10	0.38
(1,1104)	1:91:A:THR:H	1:127:A:LEU:HG	20	0.38
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	3	0.38
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	3	0.38
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	3	0.38
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	15	0.38
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	15	0.38
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	15	0.38
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	5	0.38
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	8	0.38
(1,910)	1:55:A:PRO:HA	1:57:A:GLY:H	18	0.38
(1,828)	1:46:A:VAL:H	1:71:A:GLN:HA	15	0.38
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	18	0.38
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	18	0.38
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	18	0.38
(1,744)	1:26:A:LEU:H	1:27:A:GLU:HG3	14	0.38
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	7	0.38
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	7	0.38
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	7	0.38
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG21	2	0.38
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG22	2	0.38
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG23	2	0.38
(1,708)	1:11:A:THR:HA	1:12:A:LEU:H	17	0.38
(1,682)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	1	0.38
(1,630)	1:127:A:LEU:HG	1:129:A:ALA:HA	7	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	10	0.38
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	15	0.38
(1,528)	1:80:A:ILE:HG21	1:106:A:TYR:HA	16	0.38
(1,528)	1:80:A:ILE:HG22	1:106:A:TYR:HA	16	0.38
(1,528)	1:80:A:ILE:HG23	1:106:A:TYR:HA	16	0.38
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	2	0.38
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	6	0.38
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	6	0.38
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	6	0.38
(1,459)	1:97:A:LEU:HG	1:99:A:THR:H	4	0.38
(1,422)	1:38:A:THR:HG21	1:91:A:THR:HA	5	0.38
(1,422)	1:38:A:THR:HG22	1:91:A:THR:HA	5	0.38
(1,422)	1:38:A:THR:HG23	1:91:A:THR:HA	5	0.38
(1,343)	1:66:A:ARG:HG3	1:68:A:LYS:H	11	0.38
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	14	0.38
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG21	14	0.38
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG22	14	0.38
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG23	14	0.38
(1,242)	1:68:A:LYS:H	1:69:A:PRO:HD2	16	0.38
(1,242)	1:68:A:LYS:H	1:69:A:PRO:HD2	19	0.38
(1,209)	1:64:A:ARG:HA	1:68:A:LYS:H	12	0.38
(1,103)	1:45:A:LYS:HG2	1:46:A:VAL:H	15	0.38
(1,89)	1:42:A:ALA:HB1	1:74:A:LEU:HA	9	0.38
(1,89)	1:42:A:ALA:HB2	1:74:A:LEU:HA	9	0.38
(1,89)	1:42:A:ALA:HB3	1:74:A:LEU:HA	9	0.38
(1,85)	1:42:A:ALA:HA	1:74:A:LEU:HD21	17	0.38
(1,85)	1:42:A:ALA:HA	1:74:A:LEU:HD22	17	0.38
(1,85)	1:42:A:ALA:HA	1:74:A:LEU:HD23	17	0.38
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG21	8	0.38
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG22	8	0.38
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG23	8	0.38
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	3	0.38
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG21	9	0.38
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG22	9	0.38
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG23	9	0.38
(1,68)	1:38:A:THR:HG21	1:92:A:LEU:HA	16	0.38
(1,68)	1:38:A:THR:HG22	1:92:A:LEU:HA	16	0.38
(1,68)	1:38:A:THR:HG23	1:92:A:LEU:HA	16	0.38
(1,64)	1:38:A:THR:HG21	1:39:A:LYS:H	10	0.38
(1,64)	1:38:A:THR:HG22	1:39:A:LYS:H	10	0.38
(1,64)	1:38:A:THR:HG23	1:39:A:LYS:H	10	0.38
(1,42)	1:33:A:PRO:HA	1:94:A:GLU:HG2	18	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD2	18	0.37
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD3	18	0.37
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE21	16	0.37
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	16	0.37
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	1	0.37
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	1	0.37
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	1	0.37
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	1	0.37
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	1	0.37
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	1	0.37
(1,1433)	1:51:A:ASP:HB2	1:124:A:GLU:HB3	16	0.37
(1,1433)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	16	0.37
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	11	0.37
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	19	0.37
(1,1265)	1:124:A:GLU:HB3	1:125:A:VAL:H	8	0.37
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	8	0.37
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	16	0.37
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB1	7	0.37
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB2	7	0.37
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB3	7	0.37
(1,1172)	1:102:A:TYR:H	1:105:A:ALA:H	7	0.37
(1,1111)	1:38:A:THR:HG21	1:92:A:LEU:H	1	0.37
(1,1111)	1:38:A:THR:HG22	1:92:A:LEU:H	1	0.37
(1,1111)	1:38:A:THR:HG23	1:92:A:LEU:H	1	0.37
(1,1050)	1:80:A:ILE:HG12	1:84:A:ASP:H	16	0.37
(1,1041)	1:80:A:ILE:HG21	1:83:A:TRP:H	16	0.37
(1,1041)	1:80:A:ILE:HG22	1:83:A:TRP:H	16	0.37
(1,1041)	1:80:A:ILE:HG23	1:83:A:TRP:H	16	0.37
(1,1035)	1:80:A:ILE:HB	1:83:A:TRP:H	9	0.37
(1,1023)	1:81:A:LYS:H	1:81:A:LYS:HG3	7	0.37
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	9	0.37
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	9	0.37
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	9	0.37
(1,1001)	1:73:A:THR:HB	1:76:A:ALA:H	2	0.37
(1,912)	1:53:A:ARG:HD3	1:57:A:GLY:H	14	0.37
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	13	0.37
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	15	0.37
(1,863)	1:50:A:TYR:HB2	1:51:A:ASP:H	15	0.37
(1,857)	1:49:A:HIS:HD2	1:51:A:ASP:H	1	0.37
(1,857)	1:49:A:HIS:HD2	1:51:A:ASP:H	11	0.37
(1,813)	1:43:A:GLY:H	1:74:A:LEU:HG	16	0.37
(1,797)	1:41:A:GLN:H	1:41:A:GLN:HG2	19	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB1	16	0.37
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB2	16	0.37
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB3	16	0.37
(1,630)	1:127:A:LEU:HG	1:129:A:ALA:HA	20	0.37
(1,629)	1:92:A:LEU:HA	1:127:A:LEU:HG	19	0.37
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	5	0.37
(1,581)	1:55:A:PRO:HG3	1:120:A:THR:HB	6	0.37
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD21	20	0.37
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD22	20	0.37
(1,512)	1:81:A:LYS:HD2	1:104:A:LEU:HD23	20	0.37
(1,419)	1:34:A:GLY:HA3	1:91:A:THR:HA	17	0.37
(1,417)	1:90:A:MET:HE1	1:94:A:GLU:HG2	10	0.37
(1,417)	1:90:A:MET:HE2	1:94:A:GLU:HG2	10	0.37
(1,417)	1:90:A:MET:HE3	1:94:A:GLU:HG2	10	0.37
(1,364)	1:80:A:ILE:HD11	1:83:A:TRP:HA	15	0.37
(1,364)	1:80:A:ILE:HD12	1:83:A:TRP:HA	15	0.37
(1,364)	1:80:A:ILE:HD13	1:83:A:TRP:HA	15	0.37
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	11	0.37
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	11	0.37
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	11	0.37
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	11	0.37
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	11	0.37
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	11	0.37
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	11	0.37
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	11	0.37
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	11	0.37
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG21	1	0.37
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG22	1	0.37
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG23	1	0.37
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD21	9	0.37
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD22	9	0.37
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD23	9	0.37
(1,209)	1:64:A:ARG:HA	1:68:A:LYS:H	18	0.37
(1,179)	1:54:A:PHE:HB2	1:55:A:PRO:HD3	3	0.37
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	10	0.37
(1,166)	1:53:A:ARG:HG3	1:60:A:PHE:H	10	0.37
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	15	0.37
(1,155)	1:51:A:ASP:HB3	1:124:A:GLU:H	4	0.37
(1,146)	1:49:A:HIS:HD2	1:50:A:TYR:HA	9	0.37
(1,105)	1:45:A:LYS:H	1:45:A:LYS:HE2	5	0.37
(1,105)	1:45:A:LYS:H	1:45:A:LYS:HE2	11	0.37
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	11	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:38:A:THR:HB	1:40:A:PRO:HD3	1	0.37
(1,76)	1:38:A:THR:HB	1:40:A:PRO:HD3	17	0.37
(1,28)	1:27:A:GLU:HG2	1:99:A:THR:HB	2	0.37
(1,1599)	1:97:A:LEU:HD11	1:124:A:GLU:HB3	4	0.36
(1,1599)	1:97:A:LEU:HD12	1:124:A:GLU:HB3	4	0.36
(1,1599)	1:97:A:LEU:HD13	1:124:A:GLU:HB3	4	0.36
(1,1599)	1:97:A:LEU:HD21	1:124:A:GLU:HB3	4	0.36
(1,1599)	1:97:A:LEU:HD22	1:124:A:GLU:HB3	4	0.36
(1,1599)	1:97:A:LEU:HD23	1:124:A:GLU:HB3	4	0.36
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	12	0.36
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	12	0.36
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	12	0.36
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	12	0.36
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	12	0.36
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	12	0.36
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB2	8	0.36
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB3	8	0.36
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	10	0.36
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	10	0.36
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	10	0.36
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	10	0.36
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	10	0.36
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	10	0.36
(1,1474)	1:59:A:GLN:HG2	1:60:A:PHE:H	16	0.36
(1,1474)	1:59:A:GLN:HG3	1:60:A:PHE:H	16	0.36
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG11	2	0.36
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG12	2	0.36
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG13	2	0.36
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG21	2	0.36
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG22	2	0.36
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG23	2	0.36
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG11	2	0.36
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG12	2	0.36
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG13	2	0.36
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG21	2	0.36
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG22	2	0.36
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG23	2	0.36
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB2	10	0.36
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB3	10	0.36
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	7	0.36
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	16	0.36
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	10	0.36
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	10	0.36
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	18	0.36
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	18	0.36
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	18	0.36
(1,1298)	1:92:A:LEU:HG	1:130:A:VAL:H	1	0.36
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	7	0.36
(1,1195)	1:80:A:ILE:HB	1:105:A:ALA:H	14	0.36
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	15	0.36
(1,1116)	1:92:A:LEU:HD11	1:93:A:GLY:H	9	0.36
(1,1116)	1:92:A:LEU:HD12	1:93:A:GLY:H	9	0.36
(1,1116)	1:92:A:LEU:HD13	1:93:A:GLY:H	9	0.36
(1,1004)	1:73:A:THR:HG21	1:76:A:ALA:H	6	0.36
(1,1004)	1:73:A:THR:HG22	1:76:A:ALA:H	6	0.36
(1,1004)	1:73:A:THR:HG23	1:76:A:ALA:H	6	0.36
(1,1004)	1:73:A:THR:HG21	1:76:A:ALA:H	11	0.36
(1,1004)	1:73:A:THR:HG22	1:76:A:ALA:H	11	0.36
(1,1004)	1:73:A:THR:HG23	1:76:A:ALA:H	11	0.36
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG11	2	0.36
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG12	2	0.36
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG13	2	0.36
(1,859)	1:50:A:TYR:HD2	1:51:A:ASP:H	12	0.36
(1,786)	1:38:A:THR:H	1:91:A:THR:HA	12	0.36
(1,751)	1:27:A:GLU:HG2	1:28:A:LYS:H	20	0.36
(1,747)	1:27:A:GLU:H	1:98:A:PHE:HA	10	0.36
(1,686)	1:102:A:TYR:HE2	1:118:A:LYS:HA	2	0.36
(1,685)	1:102:A:TYR:HE2	1:108:A:GLU:HG2	6	0.36
(1,630)	1:127:A:LEU:HG	1:129:A:ALA:HA	6	0.36
(1,608)	1:97:A:LEU:HG	1:124:A:GLU:HG3	14	0.36
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	1	0.36
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	11	0.36
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	12	0.36
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	13	0.36
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	17	0.36
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	18	0.36
(1,578)	1:119:A:ALA:HB1	1:120:A:THR:HB	18	0.36
(1,578)	1:119:A:ALA:HB2	1:120:A:THR:HB	18	0.36
(1,578)	1:119:A:ALA:HB3	1:120:A:THR:HB	18	0.36
(1,548)	1:102:A:TYR:HE2	1:108:A:GLU:HG3	1	0.36
(1,518)	1:80:A:ILE:HA	1:105:A:ALA:HA	11	0.36
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	11	0.36
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	11	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	11	0.36
(1,422)	1:38:A:THR:HG21	1:91:A:THR:HA	17	0.36
(1,422)	1:38:A:THR:HG22	1:91:A:THR:HA	17	0.36
(1,422)	1:38:A:THR:HG23	1:91:A:THR:HA	17	0.36
(1,385)	1:82:A:GLY:HA2	1:85:A:GLN:HB3	4	0.36
(1,316)	1:80:A:ILE:HB	1:104:A:LEU:HB3	16	0.36
(1,265)	1:42:A:ALA:H	1:74:A:LEU:HB3	10	0.36
(1,242)	1:68:A:LYS:H	1:69:A:PRO:HD2	6	0.36
(1,239)	1:49:A:HIS:HE1	1:69:A:PRO:HG2	13	0.36
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	15	0.36
(1,89)	1:42:A:ALA:HB1	1:74:A:LEU:HA	15	0.36
(1,89)	1:42:A:ALA:HB2	1:74:A:LEU:HA	15	0.36
(1,89)	1:42:A:ALA:HB3	1:74:A:LEU:HA	15	0.36
(1,64)	1:38:A:THR:HG21	1:39:A:LYS:H	5	0.36
(1,64)	1:38:A:THR:HG22	1:39:A:LYS:H	5	0.36
(1,64)	1:38:A:THR:HG23	1:39:A:LYS:H	5	0.36
(1,64)	1:38:A:THR:HG21	1:39:A:LYS:H	16	0.36
(1,64)	1:38:A:THR:HG22	1:39:A:LYS:H	16	0.36
(1,64)	1:38:A:THR:HG23	1:39:A:LYS:H	16	0.36
(1,25)	1:27:A:GLU:HG3	1:28:A:LYS:H	15	0.36
(1,1648)	1:121:A:LEU:HD11	1:123:A:PHE:HD1	3	0.35
(1,1648)	1:121:A:LEU:HD12	1:123:A:PHE:HD1	3	0.35
(1,1648)	1:121:A:LEU:HD13	1:123:A:PHE:HD1	3	0.35
(1,1648)	1:121:A:LEU:HD21	1:123:A:PHE:HD1	3	0.35
(1,1648)	1:121:A:LEU:HD22	1:123:A:PHE:HD1	3	0.35
(1,1648)	1:121:A:LEU:HD23	1:123:A:PHE:HD1	3	0.35
(1,1648)	1:121:A:LEU:HD11	1:123:A:PHE:HD1	9	0.35
(1,1648)	1:121:A:LEU:HD12	1:123:A:PHE:HD1	9	0.35
(1,1648)	1:121:A:LEU:HD13	1:123:A:PHE:HD1	9	0.35
(1,1648)	1:121:A:LEU:HD21	1:123:A:PHE:HD1	9	0.35
(1,1648)	1:121:A:LEU:HD22	1:123:A:PHE:HD1	9	0.35
(1,1648)	1:121:A:LEU:HD23	1:123:A:PHE:HD1	9	0.35
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	5	0.35
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	5	0.35
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	5	0.35
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	5	0.35
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	5	0.35
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	5	0.35
(1,1594)	1:97:A:LEU:HD11	1:123:A:PHE:H	14	0.35
(1,1594)	1:97:A:LEU:HD12	1:123:A:PHE:H	14	0.35
(1,1594)	1:97:A:LEU:HD13	1:123:A:PHE:H	14	0.35
(1,1594)	1:97:A:LEU:HD21	1:123:A:PHE:H	14	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1594)	1:97:A:LEU:HD22	1:123:A:PHE:H	14	0.35
(1,1594)	1:97:A:LEU:HD23	1:123:A:PHE:H	14	0.35
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	10	0.35
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	10	0.35
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB2	16	0.35
(1,1451)	1:54:A:PHE:HD1	1:58:A:LYS:HB3	16	0.35
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA2	7	0.35
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	7	0.35
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	20	0.35
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	20	0.35
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD2	9	0.35
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD3	9	0.35
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD2	9	0.35
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD3	9	0.35
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	4	0.35
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	4	0.35
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	4	0.35
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	18	0.35
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	20	0.35
(1,1195)	1:80:A:ILE:HB	1:105:A:ALA:H	11	0.35
(1,1185)	1:24:A:ALA:HB1	1:103:A:GLN:H	7	0.35
(1,1185)	1:24:A:ALA:HB2	1:103:A:GLN:H	7	0.35
(1,1185)	1:24:A:ALA:HB3	1:103:A:GLN:H	7	0.35
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	6	0.35
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	20	0.35
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	15	0.35
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	15	0.35
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	15	0.35
(1,1116)	1:92:A:LEU:HD11	1:93:A:GLY:H	8	0.35
(1,1116)	1:92:A:LEU:HD12	1:93:A:GLY:H	8	0.35
(1,1116)	1:92:A:LEU:HD13	1:93:A:GLY:H	8	0.35
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	16	0.35
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	16	0.35
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	16	0.35
(1,1003)	1:74:A:LEU:HB3	1:76:A:ALA:H	11	0.35
(1,952)	1:67:A:GLY:H	1:68:A:LYS:HB2	11	0.35
(1,923)	1:71:A:GLN:HE21	1:72:A:PHE:H	9	0.35
(1,862)	1:50:A:TYR:HB3	1:51:A:ASP:H	9	0.35
(1,859)	1:50:A:TYR:HD2	1:51:A:ASP:H	6	0.35
(1,857)	1:49:A:HIS:HD2	1:51:A:ASP:H	9	0.35
(1,824)	1:44:A:LYS:HB3	1:45:A:LYS:H	16	0.35
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG21	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG22	7	0.35
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG23	7	0.35
(1,695)	1:83:A:TRP:HZ2	1:123:A:PHE:HD1	4	0.35
(1,654)	1:47:A:THR:H	1:130:A:VAL:HG11	20	0.35
(1,654)	1:47:A:THR:H	1:130:A:VAL:HG12	20	0.35
(1,654)	1:47:A:THR:H	1:130:A:VAL:HG13	20	0.35
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD11	4	0.35
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD12	4	0.35
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD13	4	0.35
(1,632)	1:93:A:GLY:H	1:127:A:LEU:HG	8	0.35
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	3	0.35
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	14	0.35
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	20	0.35
(1,564)	1:114:A:VAL:HB	1:115:A:ILE:H	7	0.35
(1,491)	1:102:A:TYR:HB3	1:105:A:ALA:HB1	13	0.35
(1,491)	1:102:A:TYR:HB3	1:105:A:ALA:HB2	13	0.35
(1,491)	1:102:A:TYR:HB3	1:105:A:ALA:HB3	13	0.35
(1,490)	1:102:A:TYR:HB3	1:102:A:TYR:HE1	7	0.35
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB1	17	0.35
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB2	17	0.35
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB3	17	0.35
(1,415)	1:90:A:MET:HE1	1:94:A:GLU:HA	20	0.35
(1,415)	1:90:A:MET:HE2	1:94:A:GLU:HA	20	0.35
(1,415)	1:90:A:MET:HE3	1:94:A:GLU:HA	20	0.35
(1,386)	1:86:A:GLY:HA3	1:98:A:PHE:HD2	17	0.35
(1,385)	1:82:A:GLY:HA2	1:85:A:GLN:HB3	12	0.35
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD21	20	0.35
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD22	20	0.35
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD23	20	0.35
(1,329)	1:72:A:PHE:HD2	1:79:A:VAL:HG21	4	0.35
(1,329)	1:72:A:PHE:HD2	1:79:A:VAL:HG22	4	0.35
(1,329)	1:72:A:PHE:HD2	1:79:A:VAL:HG23	4	0.35
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	4	0.35
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	4	0.35
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	4	0.35
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	4	0.35
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	4	0.35
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	4	0.35
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	4	0.35
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	4	0.35
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	4	0.35
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG21	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG22	5	0.35
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG23	5	0.35
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD11	19	0.35
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD12	19	0.35
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD13	19	0.35
(1,274)	1:74:A:LEU:HD11	1:87:A:VAL:H	4	0.35
(1,274)	1:74:A:LEU:HD12	1:87:A:VAL:H	4	0.35
(1,274)	1:74:A:LEU:HD13	1:87:A:VAL:H	4	0.35
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD21	4	0.35
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD22	4	0.35
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD23	4	0.35
(1,265)	1:42:A:ALA:H	1:74:A:LEU:HB3	6	0.35
(1,231)	1:68:A:LYS:H	1:69:A:PRO:HA	19	0.35
(1,194)	1:53:A:ARG:HG2	1:59:A:GLN:HA	6	0.35
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	9	0.35
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	18	0.35
(1,105)	1:45:A:LYS:H	1:45:A:LYS:HE2	3	0.35
(1,105)	1:45:A:LYS:H	1:45:A:LYS:HE2	17	0.35
(1,103)	1:45:A:LYS:HG2	1:46:A:VAL:H	11	0.35
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG21	12	0.35
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG22	12	0.35
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG23	12	0.35
(1,89)	1:42:A:ALA:HB1	1:74:A:LEU:HA	11	0.35
(1,89)	1:42:A:ALA:HB2	1:74:A:LEU:HA	11	0.35
(1,89)	1:42:A:ALA:HB3	1:74:A:LEU:HA	11	0.35
(1,81)	1:42:A:ALA:HA	1:74:A:LEU:H	5	0.35
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	20	0.35
(1,76)	1:38:A:THR:HB	1:40:A:PRO:HD3	12	0.35
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG21	1	0.35
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG22	1	0.35
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG23	1	0.35
(1,68)	1:38:A:THR:HG21	1:92:A:LEU:HA	5	0.35
(1,68)	1:38:A:THR:HG22	1:92:A:LEU:HA	5	0.35
(1,68)	1:38:A:THR:HG23	1:92:A:LEU:HA	5	0.35
(1,68)	1:38:A:THR:HG21	1:92:A:LEU:HA	17	0.35
(1,68)	1:38:A:THR:HG22	1:92:A:LEU:HA	17	0.35
(1,68)	1:38:A:THR:HG23	1:92:A:LEU:HA	17	0.35
(1,42)	1:33:A:PRO:HA	1:94:A:GLU:HG2	15	0.35
(1,39)	1:32:A:THR:HB	1:95:A:LYS:HB2	8	0.35
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	9	0.35
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	10	0.34
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	10	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	10	0.34
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	10	0.34
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	10	0.34
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	10	0.34
(1,1506)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	17	0.34
(1,1506)	1:67:A:GLY:HA3	1:68:A:LYS:HB2	17	0.34
(1,1474)	1:59:A:GLN:HG2	1:60:A:PHE:H	15	0.34
(1,1474)	1:59:A:GLN:HG3	1:60:A:PHE:H	15	0.34
(1,1433)	1:51:A:ASP:HB2	1:124:A:GLU:HB3	17	0.34
(1,1433)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	17	0.34
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB2	16	0.34
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB3	16	0.34
(1,1323)	1:19:A:PRO:HG2	1:55:A:PRO:HB2	13	0.34
(1,1323)	1:19:A:PRO:HG3	1:55:A:PRO:HB2	13	0.34
(1,1205)	1:106:A:TYR:H	1:121:A:LEU:HG	9	0.34
(1,1185)	1:24:A:ALA:HB1	1:103:A:GLN:H	1	0.34
(1,1185)	1:24:A:ALA:HB2	1:103:A:GLN:H	1	0.34
(1,1185)	1:24:A:ALA:HB3	1:103:A:GLN:H	1	0.34
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	12	0.34
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	12	0.34
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	12	0.34
(1,1116)	1:92:A:LEU:HD11	1:93:A:GLY:H	5	0.34
(1,1116)	1:92:A:LEU:HD12	1:93:A:GLY:H	5	0.34
(1,1116)	1:92:A:LEU:HD13	1:93:A:GLY:H	5	0.34
(1,1106)	1:37:A:VAL:H	1:92:A:LEU:H	2	0.34
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	9	0.34
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	9	0.34
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	9	0.34
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	20	0.34
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	20	0.34
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	20	0.34
(1,1006)	1:77:A:GLY:H	1:78:A:GLU:HB2	5	0.34
(1,965)	1:69:A:PRO:HG3	1:70:A:PHE:H	1	0.34
(1,919)	1:60:A:PHE:HD1	1:61:A:ASP:H	4	0.34
(1,897)	1:59:A:GLN:HE21	1:62:A:SER:HB3	3	0.34
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG11	1	0.34
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG12	1	0.34
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG13	1	0.34
(1,787)	1:37:A:VAL:HB	1:38:A:THR:H	11	0.34
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	16	0.34
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	16	0.34
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	16	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,747)	1:27:A:GLU:H	1:98:A:PHE:HA	1	0.34
(1,660)	1:72:A:PHE:HB2	1:79:A:VAL:HG11	8	0.34
(1,660)	1:72:A:PHE:HB2	1:79:A:VAL:HG12	8	0.34
(1,660)	1:72:A:PHE:HB2	1:79:A:VAL:HG13	8	0.34
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD11	20	0.34
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD12	20	0.34
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD13	20	0.34
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	6	0.34
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	7	0.34
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	9	0.34
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	19	0.34
(1,581)	1:55:A:PRO:HG3	1:120:A:THR:HB	20	0.34
(1,553)	1:110:A:GLY:HA2	1:115:A:ILE:HB	4	0.34
(1,542)	1:108:A:GLU:HA	1:118:A:LYS:HG3	18	0.34
(1,536)	1:102:A:TYR:HE2	1:108:A:GLU:HB2	15	0.34
(1,519)	1:80:A:ILE:HB	1:105:A:ALA:HA	14	0.34
(1,490)	1:102:A:TYR:HB3	1:102:A:TYR:HE1	17	0.34
(1,490)	1:102:A:TYR:HB3	1:102:A:TYR:HE1	18	0.34
(1,461)	1:97:A:LEU:HD11	1:123:A:PHE:H	17	0.34
(1,461)	1:97:A:LEU:HD12	1:123:A:PHE:H	17	0.34
(1,461)	1:97:A:LEU:HD13	1:123:A:PHE:H	17	0.34
(1,456)	1:28:A:LYS:HB2	1:96:A:ALA:HB1	3	0.34
(1,456)	1:28:A:LYS:HB2	1:96:A:ALA:HB2	3	0.34
(1,456)	1:28:A:LYS:HB2	1:96:A:ALA:HB3	3	0.34
(1,418)	1:90:A:MET:HE1	1:96:A:ALA:HB1	1	0.34
(1,418)	1:90:A:MET:HE1	1:96:A:ALA:HB2	1	0.34
(1,418)	1:90:A:MET:HE1	1:96:A:ALA:HB3	1	0.34
(1,418)	1:90:A:MET:HE2	1:96:A:ALA:HB1	1	0.34
(1,418)	1:90:A:MET:HE2	1:96:A:ALA:HB2	1	0.34
(1,418)	1:90:A:MET:HE2	1:96:A:ALA:HB3	1	0.34
(1,418)	1:90:A:MET:HE3	1:96:A:ALA:HB1	1	0.34
(1,418)	1:90:A:MET:HE3	1:96:A:ALA:HB2	1	0.34
(1,418)	1:90:A:MET:HE3	1:96:A:ALA:HB3	1	0.34
(1,415)	1:90:A:MET:HE1	1:94:A:GLU:HA	5	0.34
(1,415)	1:90:A:MET:HE2	1:94:A:GLU:HA	5	0.34
(1,415)	1:90:A:MET:HE3	1:94:A:GLU:HA	5	0.34
(1,356)	1:80:A:ILE:HG12	1:83:A:TRP:HB2	9	0.34
(1,350)	1:82:A:GLY:HA3	1:104:A:LEU:HD11	8	0.34
(1,350)	1:82:A:GLY:HA3	1:104:A:LEU:HD12	8	0.34
(1,350)	1:82:A:GLY:HA3	1:104:A:LEU:HD13	8	0.34
(1,346)	1:81:A:LYS:HB3	1:82:A:GLY:HA3	2	0.34
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD11	13	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD12	13	0.34
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD13	13	0.34
(1,145)	1:49:A:HIS:HB2	1:126:A:GLU:HG2	3	0.34
(1,130)	1:48:A:VAL:HG11	1:50:A:TYR:HD1	10	0.34
(1,130)	1:48:A:VAL:HG12	1:50:A:TYR:HD1	10	0.34
(1,130)	1:48:A:VAL:HG13	1:50:A:TYR:HD1	10	0.34
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	6	0.34
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	6	0.34
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	6	0.34
(1,105)	1:45:A:LYS:H	1:45:A:LYS:HE2	10	0.34
(1,103)	1:45:A:LYS:HG2	1:46:A:VAL:H	14	0.34
(1,64)	1:38:A:THR:HG21	1:39:A:LYS:H	14	0.34
(1,64)	1:38:A:THR:HG22	1:39:A:LYS:H	14	0.34
(1,64)	1:38:A:THR:HG23	1:39:A:LYS:H	14	0.34
(1,26)	1:27:A:GLU:HG3	1:99:A:THR:H	10	0.34
(1,1599)	1:97:A:LEU:HD11	1:124:A:GLU:HB3	6	0.33
(1,1599)	1:97:A:LEU:HD12	1:124:A:GLU:HB3	6	0.33
(1,1599)	1:97:A:LEU:HD13	1:124:A:GLU:HB3	6	0.33
(1,1599)	1:97:A:LEU:HD21	1:124:A:GLU:HB3	6	0.33
(1,1599)	1:97:A:LEU:HD22	1:124:A:GLU:HB3	6	0.33
(1,1599)	1:97:A:LEU:HD23	1:124:A:GLU:HB3	6	0.33
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	20	0.33
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	20	0.33
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	20	0.33
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	20	0.33
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	20	0.33
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	20	0.33
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD11	9	0.33
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD12	9	0.33
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD13	9	0.33
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD21	9	0.33
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD22	9	0.33
(1,1509)	1:69:A:PRO:HG3	1:128:A:LEU:HD23	9	0.33
(1,1506)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	19	0.33
(1,1506)	1:67:A:GLY:HA3	1:68:A:LYS:HB2	19	0.33
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB2	4	0.33
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB3	4	0.33
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	10	0.33
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	10	0.33
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	10	0.33
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	10	0.33
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	10	0.33
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	16	0.33
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	16	0.33
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	16	0.33
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	16	0.33
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	16	0.33
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	16	0.33
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	14	0.33
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	14	0.33
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG11	1	0.33
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG12	1	0.33
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG13	1	0.33
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG21	1	0.33
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG22	1	0.33
(1,1340)	1:25:A:GLN:HB2	1:122:A:VAL:HG23	1	0.33
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG11	1	0.33
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG12	1	0.33
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG13	1	0.33
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG21	1	0.33
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG22	1	0.33
(1,1340)	1:25:A:GLN:HB3	1:122:A:VAL:HG23	1	0.33
(1,1310)	1:81:A:LYS:HE2	1:85:A:GLN:HE22	13	0.33
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	8	0.33
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	9	0.33
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	9	0.33
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	9	0.33
(1,1252)	1:100:A:ILE:HD11	1:123:A:PHE:H	1	0.33
(1,1252)	1:100:A:ILE:HD12	1:123:A:PHE:H	1	0.33
(1,1252)	1:100:A:ILE:HD13	1:123:A:PHE:H	1	0.33
(1,1235)	1:55:A:PRO:HG3	1:120:A:THR:H	10	0.33
(1,1219)	1:111:A:TYR:H	1:115:A:ILE:HB	16	0.33
(1,1211)	1:106:A:TYR:HB3	1:110:A:GLY:H	10	0.33
(1,1204)	1:100:A:ILE:HG21	1:106:A:TYR:H	2	0.33
(1,1204)	1:100:A:ILE:HG22	1:106:A:TYR:H	2	0.33
(1,1204)	1:100:A:ILE:HG23	1:106:A:TYR:H	2	0.33
(1,1096)	1:91:A:THR:H	1:94:A:GLU:H	7	0.33
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	13	0.33
(1,1069)	1:86:A:GLY:H	1:98:A:PHE:HD2	7	0.33
(1,1051)	1:80:A:ILE:HD11	1:84:A:ASP:H	9	0.33
(1,1051)	1:80:A:ILE:HD12	1:84:A:ASP:H	9	0.33
(1,1051)	1:80:A:ILE:HD13	1:84:A:ASP:H	9	0.33
(1,1036)	1:79:A:VAL:HB	1:83:A:TRP:H	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,863)	1:50:A:TYR:HB2	1:51:A:ASP:H	13	0.33
(1,862)	1:50:A:TYR:HB3	1:51:A:ASP:H	16	0.33
(1,700)	1:79:A:VAL:HB	1:83:A:TRP:HE3	1	0.33
(1,683)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	2	0.33
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG21	2	0.33
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG22	2	0.33
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG23	2	0.33
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	19	0.33
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	19	0.33
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	19	0.33
(1,629)	1:92:A:LEU:HA	1:127:A:LEU:HG	20	0.33
(1,616)	1:50:A:TYR:HA	1:125:A:VAL:HG11	11	0.33
(1,616)	1:50:A:TYR:HA	1:125:A:VAL:HG12	11	0.33
(1,616)	1:50:A:TYR:HA	1:125:A:VAL:HG13	11	0.33
(1,602)	1:100:A:ILE:HD11	1:123:A:PHE:HB3	6	0.33
(1,602)	1:100:A:ILE:HD12	1:123:A:PHE:HB3	6	0.33
(1,602)	1:100:A:ILE:HD13	1:123:A:PHE:HB3	6	0.33
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	8	0.33
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	6	0.33
(1,554)	1:106:A:TYR:HB2	1:110:A:GLY:HA2	18	0.33
(1,546)	1:108:A:GLU:HG3	1:118:A:LYS:HG2	5	0.33
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB1	8	0.33
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB2	8	0.33
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB3	8	0.33
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB1	8	0.33
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB2	8	0.33
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB3	8	0.33
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB1	8	0.33
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB2	8	0.33
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB3	8	0.33
(1,519)	1:80:A:ILE:HB	1:105:A:ALA:HA	11	0.33
(1,491)	1:102:A:TYR:HB3	1:105:A:ALA:HB1	14	0.33
(1,491)	1:102:A:TYR:HB3	1:105:A:ALA:HB2	14	0.33
(1,491)	1:102:A:TYR:HB3	1:105:A:ALA:HB3	14	0.33
(1,490)	1:102:A:TYR:HB3	1:102:A:TYR:HE1	4	0.33
(1,424)	1:34:A:GLY:HA3	1:91:A:THR:HB	11	0.33
(1,424)	1:34:A:GLY:HA3	1:91:A:THR:HB	15	0.33
(1,422)	1:38:A:THR:HG21	1:91:A:THR:HA	9	0.33
(1,422)	1:38:A:THR:HG22	1:91:A:THR:HA	9	0.33
(1,422)	1:38:A:THR:HG23	1:91:A:THR:HA	9	0.33
(1,389)	1:87:A:VAL:HA	1:90:A:MET:HG3	6	0.33
(1,364)	1:80:A:ILE:HD11	1:83:A:TRP:HA	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	1:80:A:ILE:HD12	1:83:A:TRP:HA	3	0.33
(1,364)	1:80:A:ILE:HD13	1:83:A:TRP:HA	3	0.33
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG21	18	0.33
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG22	18	0.33
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG23	18	0.33
(1,242)	1:68:A:LYS:H	1:69:A:PRO:HD2	13	0.33
(1,242)	1:68:A:LYS:H	1:69:A:PRO:HD2	15	0.33
(1,240)	1:47:A:THR:HG21	1:69:A:PRO:HG3	1	0.33
(1,240)	1:47:A:THR:HG22	1:69:A:PRO:HG3	1	0.33
(1,240)	1:47:A:THR:HG23	1:69:A:PRO:HG3	1	0.33
(1,197)	1:59:A:GLN:HG2	1:60:A:PHE:H	6	0.33
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	2	0.33
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	5	0.33
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	8	0.33
(1,155)	1:51:A:ASP:HB3	1:124:A:GLU:H	5	0.33
(1,153)	1:51:A:ASP:HB2	1:124:A:GLU:HB3	18	0.33
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG11	15	0.33
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG12	15	0.33
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG13	15	0.33
(1,121)	1:46:A:VAL:HG11	1:130:A:VAL:H	11	0.33
(1,121)	1:46:A:VAL:HG12	1:130:A:VAL:H	11	0.33
(1,121)	1:46:A:VAL:HG13	1:130:A:VAL:H	11	0.33
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	20	0.33
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	20	0.33
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	20	0.33
(1,109)	1:46:A:VAL:HB	1:129:A:ALA:H	8	0.33
(1,103)	1:45:A:LYS:HG2	1:46:A:VAL:H	17	0.33
(1,68)	1:38:A:THR:HG21	1:92:A:LEU:HA	14	0.33
(1,68)	1:38:A:THR:HG22	1:92:A:LEU:HA	14	0.33
(1,68)	1:38:A:THR:HG23	1:92:A:LEU:HA	14	0.33
(1,26)	1:27:A:GLU:HG3	1:99:A:THR:H	6	0.33
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	12	0.33
(1,2)	1:28:A:LYS:HB2	1:30:A:VAL:H	10	0.33
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	5	0.32
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	5	0.32
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	5	0.32
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	5	0.32
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	5	0.32
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	5	0.32
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	9	0.32
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	9	0.32
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	9	0.32
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	9	0.32
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	9	0.32
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	8	0.32
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	8	0.32
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	8	0.32
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	8	0.32
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	8	0.32
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	8	0.32
(1,1575)	1:92:A:LEU:HD11	1:130:A:VAL:H	8	0.32
(1,1575)	1:92:A:LEU:HD12	1:130:A:VAL:H	8	0.32
(1,1575)	1:92:A:LEU:HD13	1:130:A:VAL:H	8	0.32
(1,1575)	1:92:A:LEU:HD21	1:130:A:VAL:H	8	0.32
(1,1575)	1:92:A:LEU:HD22	1:130:A:VAL:H	8	0.32
(1,1575)	1:92:A:LEU:HD23	1:130:A:VAL:H	8	0.32
(1,1442)	1:53:A:ARG:HD2	1:59:A:GLN:HA	8	0.32
(1,1442)	1:53:A:ARG:HD3	1:59:A:GLN:HA	8	0.32
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG2	6	0.32
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG3	6	0.32
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD11	10	0.32
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD12	10	0.32
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD13	10	0.32
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD21	10	0.32
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD22	10	0.32
(1,1372)	1:38:A:THR:HA	1:92:A:LEU:HD23	10	0.32
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG2	7	0.32
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG3	7	0.32
(1,1309)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	7	0.32
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	5	0.32
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	20	0.32
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	20	0.32
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	20	0.32
(1,1252)	1:100:A:ILE:HD11	1:123:A:PHE:H	14	0.32
(1,1252)	1:100:A:ILE:HD12	1:123:A:PHE:H	14	0.32
(1,1252)	1:100:A:ILE:HD13	1:123:A:PHE:H	14	0.32
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	13	0.32
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	8	0.32
(1,1116)	1:92:A:LEU:HD11	1:93:A:GLY:H	3	0.32
(1,1116)	1:92:A:LEU:HD12	1:93:A:GLY:H	3	0.32
(1,1116)	1:92:A:LEU:HD13	1:93:A:GLY:H	3	0.32
(1,1111)	1:38:A:THR:HG21	1:92:A:LEU:H	16	0.32
(1,1111)	1:38:A:THR:HG22	1:92:A:LEU:H	16	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1111)	1:38:A:THR:HG23	1:92:A:LEU:H	16	0.32
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	8	0.32
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	8	0.32
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	8	0.32
(1,1001)	1:73:A:THR:HB	1:76:A:ALA:H	13	0.32
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB1	6	0.32
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB2	6	0.32
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB3	6	0.32
(1,923)	1:71:A:GLN:HE21	1:72:A:PHE:H	17	0.32
(1,912)	1:53:A:ARG:HD3	1:57:A:GLY:H	3	0.32
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG21	6	0.32
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG22	6	0.32
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG23	6	0.32
(1,751)	1:27:A:GLU:HG2	1:28:A:LYS:H	8	0.32
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG21	3	0.32
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG22	3	0.32
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG23	3	0.32
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	10	0.32
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	10	0.32
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	10	0.32
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB1	10	0.32
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB2	10	0.32
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB3	10	0.32
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	16	0.32
(1,585)	1:121:A:LEU:HG	1:123:A:PHE:HD1	8	0.32
(1,582)	1:55:A:PRO:HG2	1:120:A:THR:HB	20	0.32
(1,578)	1:119:A:ALA:HB1	1:120:A:THR:HB	14	0.32
(1,578)	1:119:A:ALA:HB2	1:120:A:THR:HB	14	0.32
(1,578)	1:119:A:ALA:HB3	1:120:A:THR:HB	14	0.32
(1,564)	1:114:A:VAL:HB	1:115:A:ILE:H	11	0.32
(1,421)	1:91:A:THR:HA	1:127:A:LEU:HG	15	0.32
(1,415)	1:90:A:MET:HE1	1:94:A:GLU:HA	16	0.32
(1,415)	1:90:A:MET:HE2	1:94:A:GLU:HA	16	0.32
(1,415)	1:90:A:MET:HE3	1:94:A:GLU:HA	16	0.32
(1,385)	1:82:A:GLY:HA2	1:85:A:GLN:HB3	18	0.32
(1,383)	1:66:A:ARG:HG2	1:68:A:LYS:H	3	0.32
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG21	8	0.32
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG22	8	0.32
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG23	8	0.32
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	8	0.32
(1,265)	1:42:A:ALA:H	1:74:A:LEU:HB3	7	0.32
(1,242)	1:68:A:LYS:H	1:69:A:PRO:HD2	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	1	0.32
(1,224)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	18	0.32
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	11	0.32
(1,145)	1:49:A:HIS:HB2	1:126:A:GLU:HG2	14	0.32
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	4	0.32
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	4	0.32
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	4	0.32
(1,103)	1:45:A:LYS:HG2	1:46:A:VAL:H	1	0.32
(1,103)	1:45:A:LYS:HG2	1:46:A:VAL:H	2	0.32
(1,103)	1:45:A:LYS:HG2	1:46:A:VAL:H	12	0.32
(1,92)	1:41:A:GLN:HG2	1:44:A:LYS:HG2	6	0.32
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG21	6	0.32
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG22	6	0.32
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG23	6	0.32
(1,76)	1:38:A:THR:HB	1:40:A:PRO:HD3	3	0.32
(1,48)	1:34:A:GLY:HA2	1:94:A:GLU:HB3	11	0.32
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	6	0.32
(1,3)	1:28:A:LYS:HG3	1:30:A:VAL:H	17	0.32
(1,2)	1:28:A:LYS:HB2	1:30:A:VAL:H	3	0.32
(1,2)	1:28:A:LYS:HB2	1:30:A:VAL:H	6	0.32
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG11	17	0.31
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG12	17	0.31
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG13	17	0.31
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG21	17	0.31
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG22	17	0.31
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG23	17	0.31
(1,1594)	1:97:A:LEU:HD11	1:123:A:PHE:H	3	0.31
(1,1594)	1:97:A:LEU:HD12	1:123:A:PHE:H	3	0.31
(1,1594)	1:97:A:LEU:HD13	1:123:A:PHE:H	3	0.31
(1,1594)	1:97:A:LEU:HD21	1:123:A:PHE:H	3	0.31
(1,1594)	1:97:A:LEU:HD22	1:123:A:PHE:H	3	0.31
(1,1594)	1:97:A:LEU:HD23	1:123:A:PHE:H	3	0.31
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB2	9	0.31
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB3	9	0.31
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	12	0.31
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	12	0.31
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	12	0.31
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	12	0.31
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	12	0.31
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	12	0.31
(1,1440)	1:53:A:ARG:HD2	1:57:A:GLY:H	9	0.31
(1,1440)	1:53:A:ARG:HD3	1:57:A:GLY:H	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD11	8	0.31
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD12	8	0.31
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD13	8	0.31
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD21	8	0.31
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD22	8	0.31
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD23	8	0.31
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD11	17	0.31
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD12	17	0.31
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD13	17	0.31
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD21	17	0.31
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD22	17	0.31
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD23	17	0.31
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	12	0.31
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	12	0.31
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA2	16	0.31
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	16	0.31
(1,1405)	1:44:A:LYS:HE2	1:45:A:LYS:H	3	0.31
(1,1405)	1:44:A:LYS:HE3	1:45:A:LYS:H	3	0.31
(1,1308)	1:81:A:LYS:HD2	1:85:A:GLN:HE21	16	0.31
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	13	0.31
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	13	0.31
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	13	0.31
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	5	0.31
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	14	0.31
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	17	0.31
(1,1197)	1:100:A:ILE:HG21	1:105:A:ALA:H	7	0.31
(1,1197)	1:100:A:ILE:HG22	1:105:A:ALA:H	7	0.31
(1,1197)	1:100:A:ILE:HG23	1:105:A:ALA:H	7	0.31
(1,1106)	1:37:A:VAL:H	1:92:A:LEU:H	6	0.31
(1,1069)	1:86:A:GLY:H	1:98:A:PHE:HD2	12	0.31
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	19	0.31
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	19	0.31
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	19	0.31
(1,1006)	1:77:A:GLY:H	1:78:A:GLU:HB2	1	0.31
(1,960)	1:50:A:TYR:HE2	1:70:A:PHE:H	11	0.31
(1,923)	1:71:A:GLN:HE21	1:72:A:PHE:H	10	0.31
(1,919)	1:60:A:PHE:HD1	1:61:A:ASP:H	3	0.31
(1,897)	1:59:A:GLN:HE21	1:62:A:SER:HB3	10	0.31
(1,830)	1:46:A:VAL:H	1:72:A:PHE:HA	4	0.31
(1,828)	1:46:A:VAL:H	1:71:A:GLN:HA	10	0.31
(1,820)	1:44:A:LYS:H	1:44:A:LYS:HG3	12	0.31
(1,819)	1:44:A:LYS:H	1:44:A:LYS:HG2	17	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG21	20	0.31
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG22	20	0.31
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG23	20	0.31
(1,787)	1:37:A:VAL:HB	1:38:A:THR:H	15	0.31
(1,749)	1:27:A:GLU:H	1:27:A:GLU:HG3	1	0.31
(1,696)	1:83:A:TRP:HZ2	1:123:A:PHE:HB3	14	0.31
(1,694)	1:80:A:ILE:HD11	1:83:A:TRP:HD1	3	0.31
(1,694)	1:80:A:ILE:HD12	1:83:A:TRP:HD1	3	0.31
(1,694)	1:80:A:ILE:HD13	1:83:A:TRP:HD1	3	0.31
(1,681)	1:50:A:TYR:H	1:50:A:TYR:HD2	9	0.31
(1,644)	1:49:A:HIS:HB2	1:128:A:LEU:HG	13	0.31
(1,629)	1:92:A:LEU:HA	1:127:A:LEU:HG	17	0.31
(1,611)	1:123:A:PHE:H	1:124:A:GLU:HG3	13	0.31
(1,582)	1:55:A:PRO:HG2	1:120:A:THR:HB	9	0.31
(1,580)	1:115:A:ILE:HD11	1:119:A:ALA:HB1	8	0.31
(1,580)	1:115:A:ILE:HD11	1:119:A:ALA:HB2	8	0.31
(1,580)	1:115:A:ILE:HD11	1:119:A:ALA:HB3	8	0.31
(1,580)	1:115:A:ILE:HD12	1:119:A:ALA:HB1	8	0.31
(1,580)	1:115:A:ILE:HD12	1:119:A:ALA:HB2	8	0.31
(1,580)	1:115:A:ILE:HD12	1:119:A:ALA:HB3	8	0.31
(1,580)	1:115:A:ILE:HD13	1:119:A:ALA:HB1	8	0.31
(1,580)	1:115:A:ILE:HD13	1:119:A:ALA:HB2	8	0.31
(1,580)	1:115:A:ILE:HD13	1:119:A:ALA:HB3	8	0.31
(1,564)	1:114:A:VAL:HB	1:115:A:ILE:H	9	0.31
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB1	2	0.31
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB2	2	0.31
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB3	2	0.31
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB1	2	0.31
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB2	2	0.31
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB3	2	0.31
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB1	2	0.31
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB2	2	0.31
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB3	2	0.31
(1,520)	1:100:A:ILE:HG21	1:105:A:ALA:HA	7	0.31
(1,520)	1:100:A:ILE:HG22	1:105:A:ALA:HA	7	0.31
(1,520)	1:100:A:ILE:HG23	1:105:A:ALA:HA	7	0.31
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG21	4	0.31
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG22	4	0.31
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG23	4	0.31
(1,459)	1:97:A:LEU:HG	1:99:A:THR:H	13	0.31
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB1	5	0.31
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB2	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB3	5	0.31
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD21	20	0.31
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD22	20	0.31
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD23	20	0.31
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	15	0.31
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG21	15	0.31
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG22	15	0.31
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG23	15	0.31
(1,289)	1:76:A:ALA:HB1	1:78:A:GLU:HB2	3	0.31
(1,289)	1:76:A:ALA:HB2	1:78:A:GLU:HB2	3	0.31
(1,289)	1:76:A:ALA:HB3	1:78:A:GLU:HB2	3	0.31
(1,192)	1:59:A:GLN:HA	1:61:A:ASP:H	16	0.31
(1,154)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	10	0.31
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	16	0.31
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	16	0.31
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	16	0.31
(1,103)	1:45:A:LYS:HG2	1:46:A:VAL:H	10	0.31
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG21	6	0.31
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG22	6	0.31
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG23	6	0.31
(1,76)	1:38:A:THR:HB	1:40:A:PRO:HD3	7	0.31
(1,71)	1:38:A:THR:HG21	1:92:A:LEU:HD21	14	0.31
(1,71)	1:38:A:THR:HG21	1:92:A:LEU:HD22	14	0.31
(1,71)	1:38:A:THR:HG21	1:92:A:LEU:HD23	14	0.31
(1,71)	1:38:A:THR:HG22	1:92:A:LEU:HD21	14	0.31
(1,71)	1:38:A:THR:HG22	1:92:A:LEU:HD22	14	0.31
(1,71)	1:38:A:THR:HG22	1:92:A:LEU:HD23	14	0.31
(1,71)	1:38:A:THR:HG23	1:92:A:LEU:HD21	14	0.31
(1,71)	1:38:A:THR:HG23	1:92:A:LEU:HD22	14	0.31
(1,71)	1:38:A:THR:HG23	1:92:A:LEU:HD23	14	0.31
(1,21)	1:25:A:GLN:H	1:26:A:LEU:HB3	8	0.31
(1,18)	1:41:A:GLN:HA	1:74:A:LEU:HD21	6	0.31
(1,18)	1:41:A:GLN:HA	1:74:A:LEU:HD22	6	0.31
(1,18)	1:41:A:GLN:HA	1:74:A:LEU:HD23	6	0.31
(1,1619)	1:103:A:GLN:HG2	1:104:A:LEU:H	4	0.3
(1,1619)	1:103:A:GLN:HG3	1:104:A:LEU:H	4	0.3
(1,1612)	1:102:A:TYR:HB2	1:108:A:GLU:HG2	16	0.3
(1,1612)	1:102:A:TYR:HB2	1:108:A:GLU:HG3	16	0.3
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	15	0.3
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	15	0.3
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	15	0.3
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	15	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	15	0.3
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	15	0.3
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	9	0.3
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	9	0.3
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	9	0.3
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	9	0.3
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	9	0.3
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	9	0.3
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB2	4	0.3
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB3	4	0.3
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB2	12	0.3
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB3	12	0.3
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	18	0.3
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	18	0.3
(1,1475)	1:59:A:GLN:HG2	1:61:A:ASP:H	14	0.3
(1,1475)	1:59:A:GLN:HG3	1:61:A:ASP:H	14	0.3
(1,1475)	1:59:A:GLN:HG2	1:61:A:ASP:H	18	0.3
(1,1475)	1:59:A:GLN:HG3	1:61:A:ASP:H	18	0.3
(1,1470)	1:59:A:GLN:H	1:59:A:GLN:HG2	2	0.3
(1,1470)	1:59:A:GLN:H	1:59:A:GLN:HG3	2	0.3
(1,1442)	1:53:A:ARG:HD2	1:59:A:GLN:HA	7	0.3
(1,1442)	1:53:A:ARG:HD3	1:59:A:GLN:HA	7	0.3
(1,1441)	1:53:A:ARG:HD2	1:57:A:GLY:HA2	2	0.3
(1,1441)	1:53:A:ARG:HD3	1:57:A:GLY:HA2	2	0.3
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG2	16	0.3
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG3	16	0.3
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD11	2	0.3
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD12	2	0.3
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD13	2	0.3
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD21	2	0.3
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD22	2	0.3
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD23	2	0.3
(1,1433)	1:51:A:ASP:HB2	1:124:A:GLU:HB3	9	0.3
(1,1433)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	9	0.3
(1,1433)	1:51:A:ASP:HB2	1:124:A:GLU:HB3	18	0.3
(1,1433)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	18	0.3
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	2	0.3
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	2	0.3
(1,1405)	1:44:A:LYS:HE2	1:45:A:LYS:H	9	0.3
(1,1405)	1:44:A:LYS:HE3	1:45:A:LYS:H	9	0.3
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE2	3	0.3
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE3	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE2	3	0.3
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE3	3	0.3
(1,1346)	1:28:A:LYS:HG2	1:30:A:VAL:H	4	0.3
(1,1346)	1:28:A:LYS:HG3	1:30:A:VAL:H	4	0.3
(1,1346)	1:28:A:LYS:HG2	1:30:A:VAL:H	7	0.3
(1,1346)	1:28:A:LYS:HG3	1:30:A:VAL:H	7	0.3
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG2	5	0.3
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG3	5	0.3
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG2	11	0.3
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG3	11	0.3
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	6	0.3
(1,1236)	1:119:A:ALA:HB1	1:120:A:THR:H	7	0.3
(1,1236)	1:119:A:ALA:HB2	1:120:A:THR:H	7	0.3
(1,1236)	1:119:A:ALA:HB3	1:120:A:THR:H	7	0.3
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	9	0.3
(1,1111)	1:38:A:THR:HG21	1:92:A:LEU:H	5	0.3
(1,1111)	1:38:A:THR:HG22	1:92:A:LEU:H	5	0.3
(1,1111)	1:38:A:THR:HG23	1:92:A:LEU:H	5	0.3
(1,1105)	1:38:A:THR:H	1:92:A:LEU:H	2	0.3
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	14	0.3
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	14	0.3
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	14	0.3
(1,1041)	1:80:A:ILE:HG21	1:83:A:TRP:H	3	0.3
(1,1041)	1:80:A:ILE:HG22	1:83:A:TRP:H	3	0.3
(1,1041)	1:80:A:ILE:HG23	1:83:A:TRP:H	3	0.3
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB1	2	0.3
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB2	2	0.3
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB3	2	0.3
(1,972)	1:70:A:PHE:HD2	1:71:A:GLN:H	3	0.3
(1,953)	1:49:A:HIS:HE1	1:68:A:LYS:H	10	0.3
(1,919)	1:60:A:PHE:HD1	1:61:A:ASP:H	17	0.3
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	14	0.3
(1,881)	1:54:A:PHE:H	1:54:A:PHE:HD1	10	0.3
(1,881)	1:54:A:PHE:H	1:54:A:PHE:HD1	20	0.3
(1,866)	1:51:A:ASP:H	1:124:A:GLU:HB3	12	0.3
(1,859)	1:50:A:TYR:HD2	1:51:A:ASP:H	4	0.3
(1,859)	1:50:A:TYR:HD2	1:51:A:ASP:H	8	0.3
(1,858)	1:50:A:TYR:HD1	1:51:A:ASP:H	16	0.3
(1,824)	1:44:A:LYS:HB3	1:45:A:LYS:H	14	0.3
(1,820)	1:44:A:LYS:H	1:44:A:LYS:HG3	5	0.3
(1,787)	1:37:A:VAL:HB	1:38:A:THR:H	6	0.3
(1,777)	1:34:A:GLY:H	1:91:A:THR:HG21	17	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,777)	1:34:A:GLY:H	1:91:A:THR:HG22	17	0.3
(1,777)	1:34:A:GLY:H	1:91:A:THR:HG23	17	0.3
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	8	0.3
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	8	0.3
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	8	0.3
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	5	0.3
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	5	0.3
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	5	0.3
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	13	0.3
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	13	0.3
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	13	0.3
(1,629)	1:92:A:LEU:HA	1:127:A:LEU:HG	15	0.3
(1,611)	1:123:A:PHE:H	1:124:A:GLU:HG3	7	0.3
(1,602)	1:100:A:ILE:HD11	1:123:A:PHE:HB3	18	0.3
(1,602)	1:100:A:ILE:HD12	1:123:A:PHE:HB3	18	0.3
(1,602)	1:100:A:ILE:HD13	1:123:A:PHE:HB3	18	0.3
(1,593)	1:122:A:VAL:HA	1:123:A:PHE:HB3	2	0.3
(1,578)	1:119:A:ALA:HB1	1:120:A:THR:HB	16	0.3
(1,578)	1:119:A:ALA:HB2	1:120:A:THR:HB	16	0.3
(1,578)	1:119:A:ALA:HB3	1:120:A:THR:HB	16	0.3
(1,564)	1:114:A:VAL:HB	1:115:A:ILE:H	13	0.3
(1,557)	1:110:A:GLY:HA3	1:115:A:ILE:HB	3	0.3
(1,534)	1:106:A:TYR:HB2	1:111:A:TYR:HD2	4	0.3
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB1	15	0.3
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB2	15	0.3
(1,525)	1:80:A:ILE:HG21	1:105:A:ALA:HB3	15	0.3
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB1	15	0.3
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB2	15	0.3
(1,525)	1:80:A:ILE:HG22	1:105:A:ALA:HB3	15	0.3
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB1	15	0.3
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB2	15	0.3
(1,525)	1:80:A:ILE:HG23	1:105:A:ALA:HB3	15	0.3
(1,460)	1:97:A:LEU:HD11	1:98:A:PHE:H	5	0.3
(1,460)	1:97:A:LEU:HD12	1:98:A:PHE:H	5	0.3
(1,460)	1:97:A:LEU:HD13	1:98:A:PHE:H	5	0.3
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB1	3	0.3
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB2	3	0.3
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB3	3	0.3
(1,422)	1:38:A:THR:HG21	1:91:A:THR:HA	14	0.3
(1,422)	1:38:A:THR:HG22	1:91:A:THR:HA	14	0.3
(1,422)	1:38:A:THR:HG23	1:91:A:THR:HA	14	0.3
(1,369)	1:83:A:TRP:H	1:84:A:ASP:HB2	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,283)	1:73:A:THR:HG21	1:76:A:ALA:HA	19	0.3
(1,283)	1:73:A:THR:HG22	1:76:A:ALA:HA	19	0.3
(1,283)	1:73:A:THR:HG23	1:76:A:ALA:HA	19	0.3
(1,265)	1:42:A:ALA:H	1:74:A:LEU:HB3	15	0.3
(1,238)	1:69:A:PRO:HG2	1:128:A:LEU:HG	10	0.3
(1,237)	1:69:A:PRO:HB2	1:70:A:PHE:H	19	0.3
(1,231)	1:68:A:LYS:H	1:69:A:PRO:HA	17	0.3
(1,194)	1:53:A:ARG:HG2	1:59:A:GLN:HA	16	0.3
(1,179)	1:54:A:PHE:HB2	1:55:A:PRO:HD3	16	0.3
(1,154)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	9	0.3
(1,130)	1:48:A:VAL:HG11	1:50:A:TYR:HD1	12	0.3
(1,130)	1:48:A:VAL:HG12	1:50:A:TYR:HD1	12	0.3
(1,130)	1:48:A:VAL:HG13	1:50:A:TYR:HD1	12	0.3
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG21	15	0.3
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG22	15	0.3
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG23	15	0.3
(1,72)	1:40:A:PRO:HB3	1:41:A:GLN:H	12	0.3
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	20	0.3
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	20	0.3
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	20	0.3
(1,27)	1:27:A:GLU:HG3	1:99:A:THR:HB	19	0.3
(1,2)	1:28:A:LYS:HB2	1:30:A:VAL:H	15	0.3
(1,1601)	1:97:A:LEU:HD11	1:124:A:GLU:HG3	20	0.29
(1,1601)	1:97:A:LEU:HD12	1:124:A:GLU:HG3	20	0.29
(1,1601)	1:97:A:LEU:HD13	1:124:A:GLU:HG3	20	0.29
(1,1601)	1:97:A:LEU:HD21	1:124:A:GLU:HG3	20	0.29
(1,1601)	1:97:A:LEU:HD22	1:124:A:GLU:HG3	20	0.29
(1,1601)	1:97:A:LEU:HD23	1:124:A:GLU:HG3	20	0.29
(1,1594)	1:97:A:LEU:HD11	1:123:A:PHE:H	19	0.29
(1,1594)	1:97:A:LEU:HD12	1:123:A:PHE:H	19	0.29
(1,1594)	1:97:A:LEU:HD13	1:123:A:PHE:H	19	0.29
(1,1594)	1:97:A:LEU:HD21	1:123:A:PHE:H	19	0.29
(1,1594)	1:97:A:LEU:HD22	1:123:A:PHE:H	19	0.29
(1,1594)	1:97:A:LEU:HD23	1:123:A:PHE:H	19	0.29
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	2	0.29
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	2	0.29
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	2	0.29
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	2	0.29
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	2	0.29
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	2	0.29
(1,1558)	1:89:A:THR:H	1:90:A:MET:HG2	6	0.29
(1,1558)	1:89:A:THR:H	1:90:A:MET:HG3	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1543)	1:85:A:GLN:HB2	1:98:A:PHE:HD2	1	0.29
(1,1543)	1:85:A:GLN:HB3	1:98:A:PHE:HD2	1	0.29
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG11	16	0.29
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG12	16	0.29
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG13	16	0.29
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG21	16	0.29
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG22	16	0.29
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG23	16	0.29
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD11	20	0.29
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD12	20	0.29
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD13	20	0.29
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD21	20	0.29
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD22	20	0.29
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD23	20	0.29
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	3	0.29
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	3	0.29
(1,1405)	1:44:A:LYS:HE2	1:45:A:LYS:H	18	0.29
(1,1405)	1:44:A:LYS:HE3	1:45:A:LYS:H	18	0.29
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD2	18	0.29
(1,1395)	1:41:A:GLN:HE21	1:44:A:LYS:HD3	18	0.29
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD2	18	0.29
(1,1395)	1:41:A:GLN:HE22	1:44:A:LYS:HD3	18	0.29
(1,1382)	1:40:A:PRO:HB2	1:74:A:LEU:HD21	7	0.29
(1,1382)	1:40:A:PRO:HB2	1:74:A:LEU:HD22	7	0.29
(1,1382)	1:40:A:PRO:HB2	1:74:A:LEU:HD23	7	0.29
(1,1382)	1:40:A:PRO:HB3	1:74:A:LEU:HD21	7	0.29
(1,1382)	1:40:A:PRO:HB3	1:74:A:LEU:HD22	7	0.29
(1,1382)	1:40:A:PRO:HB3	1:74:A:LEU:HD23	7	0.29
(1,1301)	1:71:A:GLN:HA	1:71:A:GLN:HE21	18	0.29
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	17	0.29
(1,1197)	1:100:A:ILE:HG21	1:105:A:ALA:H	4	0.29
(1,1197)	1:100:A:ILE:HG22	1:105:A:ALA:H	4	0.29
(1,1197)	1:100:A:ILE:HG23	1:105:A:ALA:H	4	0.29
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	16	0.29
(1,1118)	1:34:A:GLY:H	1:94:A:GLU:H	7	0.29
(1,1104)	1:91:A:THR:H	1:127:A:LEU:HG	6	0.29
(1,1104)	1:91:A:THR:H	1:127:A:LEU:HG	16	0.29
(1,1097)	1:34:A:GLY:HA3	1:91:A:THR:H	7	0.29
(1,1065)	1:79:A:VAL:HG21	1:85:A:GLN:H	11	0.29
(1,1065)	1:79:A:VAL:HG22	1:85:A:GLN:H	11	0.29
(1,1065)	1:79:A:VAL:HG23	1:85:A:GLN:H	11	0.29
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	3	0.29
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	3	0.29
(1,1003)	1:74:A:LEU:HB3	1:76:A:ALA:H	10	0.29
(1,972)	1:70:A:PHE:HD2	1:71:A:GLN:H	6	0.29
(1,972)	1:70:A:PHE:HD2	1:71:A:GLN:H	16	0.29
(1,929)	1:63:A:SER:H	1:64:A:ARG:HG3	11	0.29
(1,881)	1:54:A:PHE:H	1:54:A:PHE:HD1	5	0.29
(1,881)	1:54:A:PHE:H	1:54:A:PHE:HD1	15	0.29
(1,859)	1:50:A:TYR:HD2	1:51:A:ASP:H	1	0.29
(1,820)	1:44:A:LYS:H	1:44:A:LYS:HG3	7	0.29
(1,813)	1:43:A:GLY:H	1:74:A:LEU:HG	18	0.29
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG11	9	0.29
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG12	9	0.29
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG13	9	0.29
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	18	0.29
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	18	0.29
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	18	0.29
(1,702)	1:80:A:ILE:HG21	1:83:A:TRP:HE3	3	0.29
(1,702)	1:80:A:ILE:HG22	1:83:A:TRP:HE3	3	0.29
(1,702)	1:80:A:ILE:HG23	1:83:A:TRP:HE3	3	0.29
(1,690)	1:83:A:TRP:HD1	1:123:A:PHE:HD2	11	0.29
(1,681)	1:50:A:TYR:H	1:50:A:TYR:HD2	3	0.29
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	17	0.29
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	17	0.29
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	17	0.29
(1,629)	1:92:A:LEU:HA	1:127:A:LEU:HG	1	0.29
(1,611)	1:123:A:PHE:H	1:124:A:GLU:HG3	6	0.29
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	1	0.29
(1,578)	1:119:A:ALA:HB1	1:120:A:THR:HB	12	0.29
(1,578)	1:119:A:ALA:HB2	1:120:A:THR:HB	12	0.29
(1,578)	1:119:A:ALA:HB3	1:120:A:THR:HB	12	0.29
(1,546)	1:108:A:GLU:HG3	1:118:A:LYS:HG2	6	0.29
(1,541)	1:108:A:GLU:HA	1:118:A:LYS:HA	15	0.29
(1,520)	1:100:A:ILE:HG21	1:105:A:ALA:HA	4	0.29
(1,520)	1:100:A:ILE:HG22	1:105:A:ALA:HA	4	0.29
(1,520)	1:100:A:ILE:HG23	1:105:A:ALA:HA	4	0.29
(1,504)	1:82:A:GLY:H	1:104:A:LEU:HD11	13	0.29
(1,504)	1:82:A:GLY:H	1:104:A:LEU:HD12	13	0.29
(1,504)	1:82:A:GLY:H	1:104:A:LEU:HD13	13	0.29
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG21	11	0.29
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG22	11	0.29
(1,469)	1:27:A:GLU:HB2	1:99:A:THR:HG23	11	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,430)	1:92:A:LEU:HD21	1:129:A:ALA:HA	3	0.29
(1,430)	1:92:A:LEU:HD22	1:129:A:ALA:HA	3	0.29
(1,430)	1:92:A:LEU:HD23	1:129:A:ALA:HA	3	0.29
(1,417)	1:90:A:MET:HE1	1:94:A:GLU:HG2	15	0.29
(1,417)	1:90:A:MET:HE2	1:94:A:GLU:HG2	15	0.29
(1,417)	1:90:A:MET:HE3	1:94:A:GLU:HG2	15	0.29
(1,395)	1:40:A:PRO:HG2	1:88:A:ALA:HA	18	0.29
(1,336)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	19	0.29
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD11	1	0.29
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD12	1	0.29
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD13	1	0.29
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD11	7	0.29
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD12	7	0.29
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD13	7	0.29
(1,286)	1:74:A:LEU:HA	1:76:A:ALA:HB1	14	0.29
(1,286)	1:74:A:LEU:HA	1:76:A:ALA:HB2	14	0.29
(1,286)	1:74:A:LEU:HA	1:76:A:ALA:HB3	14	0.29
(1,242)	1:68:A:LYS:H	1:69:A:PRO:HD2	11	0.29
(1,227)	1:67:A:GLY:HA3	1:68:A:LYS:HB2	17	0.29
(1,220)	1:66:A:ARG:HA	1:66:A:ARG:HD2	6	0.29
(1,208)	1:63:A:SER:H	1:64:A:ARG:HA	4	0.29
(1,165)	1:53:A:ARG:HG2	1:60:A:PHE:H	15	0.29
(1,158)	1:52:A:GLY:HA2	1:123:A:PHE:HD1	8	0.29
(1,121)	1:46:A:VAL:HG11	1:130:A:VAL:H	7	0.29
(1,121)	1:46:A:VAL:HG12	1:130:A:VAL:H	7	0.29
(1,121)	1:46:A:VAL:HG13	1:130:A:VAL:H	7	0.29
(1,119)	1:46:A:VAL:HG21	1:74:A:LEU:HD11	11	0.29
(1,119)	1:46:A:VAL:HG21	1:74:A:LEU:HD12	11	0.29
(1,119)	1:46:A:VAL:HG21	1:74:A:LEU:HD13	11	0.29
(1,119)	1:46:A:VAL:HG22	1:74:A:LEU:HD11	11	0.29
(1,119)	1:46:A:VAL:HG22	1:74:A:LEU:HD12	11	0.29
(1,119)	1:46:A:VAL:HG22	1:74:A:LEU:HD13	11	0.29
(1,119)	1:46:A:VAL:HG23	1:74:A:LEU:HD11	11	0.29
(1,119)	1:46:A:VAL:HG23	1:74:A:LEU:HD12	11	0.29
(1,119)	1:46:A:VAL:HG23	1:74:A:LEU:HD13	11	0.29
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG21	2	0.29
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG22	2	0.29
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG23	2	0.29
(1,81)	1:42:A:ALA:HA	1:74:A:LEU:H	15	0.29
(1,64)	1:38:A:THR:HG21	1:39:A:LYS:H	11	0.29
(1,64)	1:38:A:THR:HG22	1:39:A:LYS:H	11	0.29
(1,64)	1:38:A:THR:HG23	1:39:A:LYS:H	11	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	4	0.29
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	4	0.29
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	4	0.29
(1,1612)	1:102:A:TYR:HB2	1:108:A:GLU:HG2	18	0.28
(1,1612)	1:102:A:TYR:HB2	1:108:A:GLU:HG3	18	0.28
(1,1592)	1:97:A:LEU:HD11	1:98:A:PHE:HD1	18	0.28
(1,1592)	1:97:A:LEU:HD12	1:98:A:PHE:HD1	18	0.28
(1,1592)	1:97:A:LEU:HD13	1:98:A:PHE:HD1	18	0.28
(1,1592)	1:97:A:LEU:HD21	1:98:A:PHE:HD1	18	0.28
(1,1592)	1:97:A:LEU:HD22	1:98:A:PHE:HD1	18	0.28
(1,1592)	1:97:A:LEU:HD23	1:98:A:PHE:HD1	18	0.28
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG11	19	0.28
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG12	19	0.28
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG13	19	0.28
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG21	19	0.28
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG22	19	0.28
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG23	19	0.28
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE21	14	0.28
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	14	0.28
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	19	0.28
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	19	0.28
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	19	0.28
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	19	0.28
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	19	0.28
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	19	0.28
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE21	20	0.28
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE22	20	0.28
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	3	0.28
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	3	0.28
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	3	0.28
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	3	0.28
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	3	0.28
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	3	0.28
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	16	0.28
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	16	0.28
(1,1346)	1:28:A:LYS:HG2	1:30:A:VAL:H	12	0.28
(1,1346)	1:28:A:LYS:HG3	1:30:A:VAL:H	12	0.28
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG2	12	0.28
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG3	12	0.28
(1,1323)	1:19:A:PRO:HG2	1:55:A:PRO:HB2	11	0.28
(1,1323)	1:19:A:PRO:HG3	1:55:A:PRO:HB2	11	0.28
(1,1314)	1:13:A:GLU:H	1:13:A:GLU:HB2	19	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1314)	1:13:A:GLU:H	1:13:A:GLU:HB3	19	0.28
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	19	0.28
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	19	0.28
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	19	0.28
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	11	0.28
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	11	0.28
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	11	0.28
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	9	0.28
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	13	0.28
(1,1219)	1:111:A:TYR:H	1:115:A:ILE:HB	18	0.28
(1,1215)	1:110:A:GLY:HA3	1:111:A:TYR:H	8	0.28
(1,1213)	1:109:A:ARG:HB3	1:110:A:GLY:H	15	0.28
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB1	9	0.28
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB2	9	0.28
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB3	9	0.28
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	10	0.28
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	10	0.28
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	10	0.28
(1,1156)	1:97:A:LEU:HD21	1:98:A:PHE:H	14	0.28
(1,1156)	1:97:A:LEU:HD22	1:98:A:PHE:H	14	0.28
(1,1156)	1:97:A:LEU:HD23	1:98:A:PHE:H	14	0.28
(1,1116)	1:92:A:LEU:HD11	1:93:A:GLY:H	12	0.28
(1,1116)	1:92:A:LEU:HD12	1:93:A:GLY:H	12	0.28
(1,1116)	1:92:A:LEU:HD13	1:93:A:GLY:H	12	0.28
(1,1111)	1:38:A:THR:HG21	1:92:A:LEU:H	17	0.28
(1,1111)	1:38:A:THR:HG22	1:92:A:LEU:H	17	0.28
(1,1111)	1:38:A:THR:HG23	1:92:A:LEU:H	17	0.28
(1,1106)	1:37:A:VAL:H	1:92:A:LEU:H	5	0.28
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	15	0.28
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	15	0.28
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	15	0.28
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	17	0.28
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	17	0.28
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	17	0.28
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	18	0.28
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	18	0.28
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	18	0.28
(1,1041)	1:80:A:ILE:HG21	1:83:A:TRP:H	15	0.28
(1,1041)	1:80:A:ILE:HG22	1:83:A:TRP:H	15	0.28
(1,1041)	1:80:A:ILE:HG23	1:83:A:TRP:H	15	0.28
(1,862)	1:50:A:TYR:HB3	1:51:A:ASP:H	3	0.28
(1,858)	1:50:A:TYR:HD1	1:51:A:ASP:H	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,830)	1:46:A:VAL:H	1:72:A:PHE:HA	9	0.28
(1,830)	1:46:A:VAL:H	1:72:A:PHE:HA	14	0.28
(1,820)	1:44:A:LYS:H	1:44:A:LYS:HG3	15	0.28
(1,806)	1:42:A:ALA:H	1:74:A:LEU:HG	3	0.28
(1,630)	1:127:A:LEU:HG	1:129:A:ALA:HA	15	0.28
(1,629)	1:92:A:LEU:HA	1:127:A:LEU:HG	18	0.28
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG21	10	0.28
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG22	10	0.28
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG23	10	0.28
(1,547)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	20	0.28
(1,545)	1:108:A:GLU:HG2	1:118:A:LYS:HG2	11	0.28
(1,542)	1:108:A:GLU:HA	1:118:A:LYS:HG3	6	0.28
(1,542)	1:108:A:GLU:HA	1:118:A:LYS:HG3	14	0.28
(1,537)	1:108:A:GLU:HB2	1:118:A:LYS:HG2	18	0.28
(1,536)	1:102:A:TYR:HE2	1:108:A:GLU:HB2	1	0.28
(1,528)	1:80:A:ILE:HG21	1:106:A:TYR:HA	2	0.28
(1,528)	1:80:A:ILE:HG22	1:106:A:TYR:HA	2	0.28
(1,528)	1:80:A:ILE:HG23	1:106:A:TYR:HA	2	0.28
(1,518)	1:80:A:ILE:HA	1:105:A:ALA:HA	13	0.28
(1,491)	1:102:A:TYR:HB3	1:105:A:ALA:HB1	2	0.28
(1,491)	1:102:A:TYR:HB3	1:105:A:ALA:HB2	2	0.28
(1,491)	1:102:A:TYR:HB3	1:105:A:ALA:HB3	2	0.28
(1,465)	1:99:A:THR:HB	1:122:A:VAL:HG11	20	0.28
(1,465)	1:99:A:THR:HB	1:122:A:VAL:HG12	20	0.28
(1,465)	1:99:A:THR:HB	1:122:A:VAL:HG13	20	0.28
(1,460)	1:97:A:LEU:HD11	1:98:A:PHE:H	13	0.28
(1,460)	1:97:A:LEU:HD12	1:98:A:PHE:H	13	0.28
(1,460)	1:97:A:LEU:HD13	1:98:A:PHE:H	13	0.28
(1,460)	1:97:A:LEU:HD11	1:98:A:PHE:H	20	0.28
(1,460)	1:97:A:LEU:HD12	1:98:A:PHE:H	20	0.28
(1,460)	1:97:A:LEU:HD13	1:98:A:PHE:H	20	0.28
(1,411)	1:90:A:MET:HE1	1:127:A:LEU:H	3	0.28
(1,411)	1:90:A:MET:HE2	1:127:A:LEU:H	3	0.28
(1,411)	1:90:A:MET:HE3	1:127:A:LEU:H	3	0.28
(1,336)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	8	0.28
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD21	12	0.28
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD22	12	0.28
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD23	12	0.28
(1,212)	1:64:A:ARG:HA	1:64:A:ARG:HD2	12	0.28
(1,209)	1:64:A:ARG:HA	1:68:A:LYS:H	5	0.28
(1,194)	1:53:A:ARG:HG2	1:59:A:GLN:HA	17	0.28
(1,192)	1:59:A:GLN:HA	1:61:A:ASP:H	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,179)	1:54:A:PHE:HB2	1:55:A:PRO:HD3	1	0.28
(1,166)	1:53:A:ARG:HG3	1:60:A:PHE:H	8	0.28
(1,161)	1:53:A:ARG:HA	1:60:A:PHE:H	4	0.28
(1,150)	1:50:A:TYR:HB3	1:125:A:VAL:HG11	11	0.28
(1,150)	1:50:A:TYR:HB3	1:125:A:VAL:HG12	11	0.28
(1,150)	1:50:A:TYR:HB3	1:125:A:VAL:HG13	11	0.28
(1,117)	1:46:A:VAL:HG21	1:48:A:VAL:HA	8	0.28
(1,117)	1:46:A:VAL:HG22	1:48:A:VAL:HA	8	0.28
(1,117)	1:46:A:VAL:HG23	1:48:A:VAL:HA	8	0.28
(1,105)	1:45:A:LYS:H	1:45:A:LYS:HE2	16	0.28
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG21	7	0.28
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG22	7	0.28
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG23	7	0.28
(1,78)	1:40:A:PRO:HD3	1:91:A:THR:HG21	15	0.28
(1,78)	1:40:A:PRO:HD3	1:91:A:THR:HG22	15	0.28
(1,78)	1:40:A:PRO:HD3	1:91:A:THR:HG23	15	0.28
(1,68)	1:38:A:THR:HG21	1:92:A:LEU:HA	1	0.28
(1,68)	1:38:A:THR:HG22	1:92:A:LEU:HA	1	0.28
(1,68)	1:38:A:THR:HG23	1:92:A:LEU:HA	1	0.28
(1,68)	1:38:A:THR:HG21	1:92:A:LEU:HA	9	0.28
(1,68)	1:38:A:THR:HG22	1:92:A:LEU:HA	9	0.28
(1,68)	1:38:A:THR:HG23	1:92:A:LEU:HA	9	0.28
(1,48)	1:34:A:GLY:HA2	1:94:A:GLU:HB3	16	0.28
(1,9)	1:23:A:SER:HB2	1:24:A:ALA:HB1	3	0.28
(1,9)	1:23:A:SER:HB2	1:24:A:ALA:HB2	3	0.28
(1,9)	1:23:A:SER:HB2	1:24:A:ALA:HB3	3	0.28
(1,3)	1:28:A:LYS:HG3	1:30:A:VAL:H	10	0.28
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG11	17	0.27
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG12	17	0.27
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG13	17	0.27
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG21	17	0.27
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG22	17	0.27
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG23	17	0.27
(1,1506)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	6	0.27
(1,1506)	1:67:A:GLY:HA3	1:68:A:LYS:HB2	6	0.27
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	13	0.27
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	13	0.27
(1,1461)	1:55:A:PRO:HD2	1:120:A:THR:HG21	20	0.27
(1,1461)	1:55:A:PRO:HD2	1:120:A:THR:HG22	20	0.27
(1,1461)	1:55:A:PRO:HD2	1:120:A:THR:HG23	20	0.27
(1,1461)	1:55:A:PRO:HD3	1:120:A:THR:HG21	20	0.27
(1,1461)	1:55:A:PRO:HD3	1:120:A:THR:HG22	20	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1461)	1:55:A:PRO:HD3	1:120:A:THR:HG23	20	0.27
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG2	13	0.27
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG3	13	0.27
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG11	18	0.27
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG12	18	0.27
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG13	18	0.27
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG11	18	0.27
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG12	18	0.27
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG13	18	0.27
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD11	15	0.27
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD12	15	0.27
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD13	15	0.27
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD21	15	0.27
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD22	15	0.27
(1,1376)	1:38:A:THR:HG21	1:92:A:LEU:HD23	15	0.27
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD11	15	0.27
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD12	15	0.27
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD13	15	0.27
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD21	15	0.27
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD22	15	0.27
(1,1376)	1:38:A:THR:HG22	1:92:A:LEU:HD23	15	0.27
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD11	15	0.27
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD12	15	0.27
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD13	15	0.27
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD21	15	0.27
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD22	15	0.27
(1,1376)	1:38:A:THR:HG23	1:92:A:LEU:HD23	15	0.27
(1,1309)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	2	0.27
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	2	0.27
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	2	0.27
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	2	0.27
(1,1276)	1:96:A:ALA:H	1:127:A:LEU:H	14	0.27
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	3	0.27
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	8	0.27
(1,1245)	1:120:A:THR:HG21	1:122:A:VAL:H	11	0.27
(1,1245)	1:120:A:THR:HG22	1:122:A:VAL:H	11	0.27
(1,1245)	1:120:A:THR:HG23	1:122:A:VAL:H	11	0.27
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG21	8	0.27
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG22	8	0.27
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG23	8	0.27
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG21	10	0.27
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG22	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG23	10	0.27
(1,1215)	1:110:A:GLY:HA3	1:111:A:TYR:H	9	0.27
(1,1197)	1:100:A:ILE:HG21	1:105:A:ALA:H	20	0.27
(1,1197)	1:100:A:ILE:HG22	1:105:A:ALA:H	20	0.27
(1,1197)	1:100:A:ILE:HG23	1:105:A:ALA:H	20	0.27
(1,1172)	1:102:A:TYR:H	1:105:A:ALA:H	14	0.27
(1,1118)	1:34:A:GLY:H	1:94:A:GLU:H	12	0.27
(1,1111)	1:38:A:THR:HG21	1:92:A:LEU:H	14	0.27
(1,1111)	1:38:A:THR:HG22	1:92:A:LEU:H	14	0.27
(1,1111)	1:38:A:THR:HG23	1:92:A:LEU:H	14	0.27
(1,1106)	1:37:A:VAL:H	1:92:A:LEU:H	17	0.27
(1,1093)	1:87:A:VAL:HG11	1:90:A:MET:H	14	0.27
(1,1093)	1:87:A:VAL:HG12	1:90:A:MET:H	14	0.27
(1,1093)	1:87:A:VAL:HG13	1:90:A:MET:H	14	0.27
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	6	0.27
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	6	0.27
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	6	0.27
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	11	0.27
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	11	0.27
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	11	0.27
(1,1006)	1:77:A:GLY:H	1:78:A:GLU:HB2	4	0.27
(1,983)	1:73:A:THR:H	1:78:A:GLU:HB2	1	0.27
(1,812)	1:43:A:GLY:H	1:44:A:LYS:HB2	1	0.27
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD21	14	0.27
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD22	14	0.27
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD23	14	0.27
(1,786)	1:38:A:THR:H	1:91:A:THR:HA	1	0.27
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	9	0.27
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	9	0.27
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	9	0.27
(1,781)	1:37:A:VAL:H	1:91:A:THR:HB	5	0.27
(1,775)	1:34:A:GLY:H	1:94:A:GLU:HB3	4	0.27
(1,749)	1:27:A:GLU:H	1:27:A:GLU:HG3	15	0.27
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	19	0.27
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	19	0.27
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	19	0.27
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG21	11	0.27
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG22	11	0.27
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG23	11	0.27
(1,686)	1:102:A:TYR:HE2	1:118:A:LYS:HA	20	0.27
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG21	9	0.27
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG22	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,621)	1:50:A:TYR:HB3	1:125:A:VAL:HG23	9	0.27
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	9	0.27
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	13	0.27
(1,579)	1:102:A:TYR:HB2	1:119:A:ALA:HB1	11	0.27
(1,579)	1:102:A:TYR:HB2	1:119:A:ALA:HB2	11	0.27
(1,579)	1:102:A:TYR:HB2	1:119:A:ALA:HB3	11	0.27
(1,547)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	16	0.27
(1,544)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	14	0.27
(1,542)	1:108:A:GLU:HA	1:118:A:LYS:HG3	16	0.27
(1,516)	1:81:A:LYS:H	1:105:A:ALA:HA	19	0.27
(1,460)	1:97:A:LEU:HD11	1:98:A:PHE:H	4	0.27
(1,460)	1:97:A:LEU:HD12	1:98:A:PHE:H	4	0.27
(1,460)	1:97:A:LEU:HD13	1:98:A:PHE:H	4	0.27
(1,425)	1:92:A:LEU:HG	1:93:A:GLY:H	18	0.27
(1,421)	1:91:A:THR:HA	1:127:A:LEU:HG	1	0.27
(1,391)	1:46:A:VAL:HG21	1:87:A:VAL:HB	6	0.27
(1,391)	1:46:A:VAL:HG22	1:87:A:VAL:HB	6	0.27
(1,391)	1:46:A:VAL:HG23	1:87:A:VAL:HB	6	0.27
(1,378)	1:81:A:LYS:HA	1:84:A:ASP:HB3	8	0.27
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD11	18	0.27
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD12	18	0.27
(1,338)	1:81:A:LYS:HB3	1:104:A:LEU:HD13	18	0.27
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD21	20	0.27
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD22	20	0.27
(1,335)	1:81:A:LYS:HA	1:104:A:LEU:HD23	20	0.27
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	1	0.27
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	1	0.27
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	1	0.27
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	1	0.27
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	1	0.27
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	1	0.27
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	1	0.27
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	1	0.27
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	1	0.27
(1,309)	1:80:A:ILE:HA	1:81:A:LYS:HB2	2	0.27
(1,289)	1:76:A:ALA:HB1	1:78:A:GLU:HB2	14	0.27
(1,289)	1:76:A:ALA:HB2	1:78:A:GLU:HB2	14	0.27
(1,289)	1:76:A:ALA:HB3	1:78:A:GLU:HB2	14	0.27
(1,278)	1:74:A:LEU:HD11	1:87:A:VAL:HB	17	0.27
(1,278)	1:74:A:LEU:HD12	1:87:A:VAL:HB	17	0.27
(1,278)	1:74:A:LEU:HD13	1:87:A:VAL:HB	17	0.27
(1,216)	1:64:A:ARG:HA	1:64:A:ARG:HD3	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,216)	1:64:A:ARG:HA	1:64:A:ARG:HD3	19	0.27
(1,193)	1:53:A:ARG:HB3	1:59:A:GLN:HA	16	0.27
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	3	0.27
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	17	0.27
(1,105)	1:45:A:LYS:H	1:45:A:LYS:HE2	1	0.27
(1,93)	1:41:A:GLN:HG3	1:44:A:LYS:HG2	12	0.27
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	7	0.27
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG21	3	0.27
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG22	3	0.27
(1,79)	1:40:A:PRO:HD2	1:91:A:THR:HG23	3	0.27
(1,69)	1:38:A:THR:HG21	1:130:A:VAL:HB	5	0.27
(1,69)	1:38:A:THR:HG22	1:130:A:VAL:HB	5	0.27
(1,69)	1:38:A:THR:HG23	1:130:A:VAL:HB	5	0.27
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG21	18	0.27
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG22	18	0.27
(1,63)	1:38:A:THR:HB	1:91:A:THR:HG23	18	0.27
(1,48)	1:34:A:GLY:HA2	1:94:A:GLU:HB3	6	0.27
(1,1648)	1:121:A:LEU:HD11	1:123:A:PHE:HD1	14	0.26
(1,1648)	1:121:A:LEU:HD12	1:123:A:PHE:HD1	14	0.26
(1,1648)	1:121:A:LEU:HD13	1:123:A:PHE:HD1	14	0.26
(1,1648)	1:121:A:LEU:HD21	1:123:A:PHE:HD1	14	0.26
(1,1648)	1:121:A:LEU:HD22	1:123:A:PHE:HD1	14	0.26
(1,1648)	1:121:A:LEU:HD23	1:123:A:PHE:HD1	14	0.26
(1,1631)	1:109:A:ARG:HB2	1:110:A:GLY:H	17	0.26
(1,1631)	1:109:A:ARG:HB3	1:110:A:GLY:H	17	0.26
(1,1624)	1:108:A:GLU:HG2	1:118:A:LYS:HG2	14	0.26
(1,1624)	1:108:A:GLU:HG3	1:118:A:LYS:HG2	14	0.26
(1,1606)	1:98:A:PHE:HB2	1:100:A:ILE:HD11	4	0.26
(1,1606)	1:98:A:PHE:HB2	1:100:A:ILE:HD12	4	0.26
(1,1606)	1:98:A:PHE:HB2	1:100:A:ILE:HD13	4	0.26
(1,1606)	1:98:A:PHE:HB3	1:100:A:ILE:HD11	4	0.26
(1,1606)	1:98:A:PHE:HB3	1:100:A:ILE:HD12	4	0.26
(1,1606)	1:98:A:PHE:HB3	1:100:A:ILE:HD13	4	0.26
(1,1599)	1:97:A:LEU:HD11	1:124:A:GLU:HB3	17	0.26
(1,1599)	1:97:A:LEU:HD12	1:124:A:GLU:HB3	17	0.26
(1,1599)	1:97:A:LEU:HD13	1:124:A:GLU:HB3	17	0.26
(1,1599)	1:97:A:LEU:HD21	1:124:A:GLU:HB3	17	0.26
(1,1599)	1:97:A:LEU:HD22	1:124:A:GLU:HB3	17	0.26
(1,1599)	1:97:A:LEU:HD23	1:124:A:GLU:HB3	17	0.26
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	2	0.26
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	2	0.26
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	2	0.26
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	2	0.26
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	2	0.26
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG11	12	0.26
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG12	12	0.26
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG13	12	0.26
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG21	12	0.26
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG22	12	0.26
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG23	12	0.26
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE21	6	0.26
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE22	6	0.26
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	6	0.26
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	6	0.26
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	6	0.26
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	6	0.26
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	6	0.26
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	6	0.26
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	18	0.26
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	18	0.26
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	18	0.26
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	18	0.26
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	18	0.26
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	18	0.26
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	18	0.26
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	18	0.26
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	18	0.26
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	18	0.26
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	18	0.26
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	18	0.26
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	18	0.26
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	18	0.26
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	18	0.26
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	18	0.26
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	18	0.26
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	18	0.26
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	10	0.26
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	10	0.26
(1,1311)	1:81:A:LYS:HE3	1:85:A:GLN:HE22	17	0.26
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	10	0.26
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	10	0.26
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	10	0.26
(1,1301)	1:71:A:GLN:HA	1:71:A:GLN:HE21	14	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	1	0.26
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	1	0.26
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	1	0.26
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	7	0.26
(1,1236)	1:119:A:ALA:HB1	1:120:A:THR:H	6	0.26
(1,1236)	1:119:A:ALA:HB2	1:120:A:THR:H	6	0.26
(1,1236)	1:119:A:ALA:HB3	1:120:A:THR:H	6	0.26
(1,1197)	1:100:A:ILE:HG21	1:105:A:ALA:H	6	0.26
(1,1197)	1:100:A:ILE:HG22	1:105:A:ALA:H	6	0.26
(1,1197)	1:100:A:ILE:HG23	1:105:A:ALA:H	6	0.26
(1,1174)	1:102:A:TYR:H	1:120:A:THR:HB	2	0.26
(1,1111)	1:38:A:THR:HG21	1:92:A:LEU:H	15	0.26
(1,1111)	1:38:A:THR:HG22	1:92:A:LEU:H	15	0.26
(1,1111)	1:38:A:THR:HG23	1:92:A:LEU:H	15	0.26
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	5	0.26
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	5	0.26
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	5	0.26
(1,1050)	1:80:A:ILE:HG12	1:84:A:ASP:H	17	0.26
(1,1050)	1:80:A:ILE:HG12	1:84:A:ASP:H	18	0.26
(1,1006)	1:77:A:GLY:H	1:78:A:GLU:HB2	9	0.26
(1,1001)	1:73:A:THR:HB	1:76:A:ALA:H	10	0.26
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG11	14	0.26
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG12	14	0.26
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG13	14	0.26
(1,972)	1:70:A:PHE:HD2	1:71:A:GLN:H	15	0.26
(1,960)	1:50:A:TYR:HE2	1:70:A:PHE:H	7	0.26
(1,919)	1:60:A:PHE:HD1	1:61:A:ASP:H	1	0.26
(1,919)	1:60:A:PHE:HD1	1:61:A:ASP:H	2	0.26
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	9	0.26
(1,863)	1:50:A:TYR:HB2	1:51:A:ASP:H	2	0.26
(1,859)	1:50:A:TYR:HD2	1:51:A:ASP:H	11	0.26
(1,859)	1:50:A:TYR:HD2	1:51:A:ASP:H	17	0.26
(1,828)	1:46:A:VAL:H	1:71:A:GLN:HA	6	0.26
(1,828)	1:46:A:VAL:H	1:71:A:GLN:HA	16	0.26
(1,820)	1:44:A:LYS:H	1:44:A:LYS:HG3	8	0.26
(1,779)	1:36:A:GLY:H	1:91:A:THR:HG21	7	0.26
(1,779)	1:36:A:GLY:H	1:91:A:THR:HG22	7	0.26
(1,779)	1:36:A:GLY:H	1:91:A:THR:HG23	7	0.26
(1,704)	1:49:A:HIS:HE1	1:69:A:PRO:HA	16	0.26
(1,702)	1:80:A:ILE:HG21	1:83:A:TRP:HE3	18	0.26
(1,702)	1:80:A:ILE:HG22	1:83:A:TRP:HE3	18	0.26
(1,702)	1:80:A:ILE:HG23	1:83:A:TRP:HE3	18	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,681)	1:50:A:TYR:H	1:50:A:TYR:HD2	20	0.26
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB1	7	0.26
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB2	7	0.26
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB3	7	0.26
(1,630)	1:127:A:LEU:HG	1:129:A:ALA:HA	5	0.26
(1,630)	1:127:A:LEU:HG	1:129:A:ALA:HA	9	0.26
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	11	0.26
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG21	12	0.26
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG22	12	0.26
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG23	12	0.26
(1,582)	1:55:A:PRO:HG2	1:120:A:THR:HB	10	0.26
(1,578)	1:119:A:ALA:HB1	1:120:A:THR:HB	3	0.26
(1,578)	1:119:A:ALA:HB2	1:120:A:THR:HB	3	0.26
(1,578)	1:119:A:ALA:HB3	1:120:A:THR:HB	3	0.26
(1,564)	1:114:A:VAL:HB	1:115:A:ILE:H	20	0.26
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD21	5	0.26
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD22	5	0.26
(1,509)	1:81:A:LYS:HE2	1:104:A:LEU:HD23	5	0.26
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB1	11	0.26
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB2	11	0.26
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB3	11	0.26
(1,487)	1:102:A:TYR:HA	1:105:A:ALA:HB1	13	0.26
(1,487)	1:102:A:TYR:HA	1:105:A:ALA:HB2	13	0.26
(1,487)	1:102:A:TYR:HA	1:105:A:ALA:HB3	13	0.26
(1,464)	1:27:A:GLU:HB2	1:99:A:THR:HB	1	0.26
(1,459)	1:97:A:LEU:HG	1:99:A:THR:H	7	0.26
(1,419)	1:34:A:GLY:HA3	1:91:A:THR:HA	2	0.26
(1,414)	1:90:A:MET:HE1	1:126:A:GLU:HA	4	0.26
(1,414)	1:90:A:MET:HE2	1:126:A:GLU:HA	4	0.26
(1,414)	1:90:A:MET:HE3	1:126:A:GLU:HA	4	0.26
(1,405)	1:85:A:GLN:HA	1:89:A:THR:HG21	19	0.26
(1,405)	1:85:A:GLN:HA	1:89:A:THR:HG22	19	0.26
(1,405)	1:85:A:GLN:HA	1:89:A:THR:HG23	19	0.26
(1,375)	1:74:A:LEU:HD11	1:84:A:ASP:HB3	6	0.26
(1,375)	1:74:A:LEU:HD12	1:84:A:ASP:HB3	6	0.26
(1,375)	1:74:A:LEU:HD13	1:84:A:ASP:HB3	6	0.26
(1,369)	1:83:A:TRP:H	1:84:A:ASP:HB2	6	0.26
(1,350)	1:82:A:GLY:HA3	1:104:A:LEU:HD11	10	0.26
(1,350)	1:82:A:GLY:HA3	1:104:A:LEU:HD12	10	0.26
(1,350)	1:82:A:GLY:HA3	1:104:A:LEU:HD13	10	0.26
(1,276)	1:74:A:LEU:HD11	1:88:A:ALA:H	9	0.26
(1,276)	1:74:A:LEU:HD12	1:88:A:ALA:H	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:74:A:LEU:HD13	1:88:A:ALA:H	9	0.26
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD21	10	0.26
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD22	10	0.26
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD23	10	0.26
(1,266)	1:74:A:LEU:HD21	1:75:A:GLY:H	16	0.26
(1,266)	1:74:A:LEU:HD22	1:75:A:GLY:H	16	0.26
(1,266)	1:74:A:LEU:HD23	1:75:A:GLY:H	16	0.26
(1,242)	1:68:A:LYS:H	1:69:A:PRO:HD2	20	0.26
(1,240)	1:47:A:THR:HG21	1:69:A:PRO:HG3	11	0.26
(1,240)	1:47:A:THR:HG22	1:69:A:PRO:HG3	11	0.26
(1,240)	1:47:A:THR:HG23	1:69:A:PRO:HG3	11	0.26
(1,232)	1:48:A:VAL:H	1:69:A:PRO:HB3	3	0.26
(1,231)	1:68:A:LYS:H	1:69:A:PRO:HA	4	0.26
(1,231)	1:68:A:LYS:H	1:69:A:PRO:HA	12	0.26
(1,231)	1:68:A:LYS:H	1:69:A:PRO:HA	16	0.26
(1,225)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	18	0.26
(1,216)	1:64:A:ARG:HA	1:64:A:ARG:HD3	9	0.26
(1,212)	1:64:A:ARG:HA	1:64:A:ARG:HD2	4	0.26
(1,212)	1:64:A:ARG:HA	1:64:A:ARG:HD2	11	0.26
(1,212)	1:64:A:ARG:HA	1:64:A:ARG:HD2	18	0.26
(1,212)	1:64:A:ARG:HA	1:64:A:ARG:HD2	20	0.26
(1,211)	1:49:A:HIS:HB3	1:64:A:ARG:HA	7	0.26
(1,208)	1:63:A:SER:H	1:64:A:ARG:HA	7	0.26
(1,197)	1:59:A:GLN:HG2	1:60:A:PHE:H	11	0.26
(1,196)	1:59:A:GLN:H	1:59:A:GLN:HG2	17	0.26
(1,179)	1:54:A:PHE:HB2	1:55:A:PRO:HD3	9	0.26
(1,165)	1:53:A:ARG:HG2	1:60:A:PHE:H	11	0.26
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	16	0.26
(1,147)	1:50:A:TYR:HA	1:124:A:GLU:HB3	16	0.26
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	12	0.26
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	12	0.26
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	12	0.26
(1,106)	1:45:A:LYS:H	1:45:A:LYS:HE3	2	0.26
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	1	0.26
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	20	0.26
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG21	9	0.26
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG22	9	0.26
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG23	9	0.26
(1,42)	1:33:A:PRO:HA	1:94:A:GLU:HG2	3	0.26
(1,38)	1:31:A:LEU:HG	1:32:A:THR:H	15	0.26
(1,29)	1:27:A:GLU:H	1:27:A:GLU:HG2	14	0.26
(1,26)	1:27:A:GLU:HG3	1:99:A:THR:H	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	8	0.26
(1,2)	1:28:A:LYS:HB2	1:30:A:VAL:H	19	0.26
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD2	17	0.25
(1,1614)	1:102:A:TYR:HE2	1:118:A:LYS:HD3	17	0.25
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	17	0.25
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	17	0.25
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	17	0.25
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	17	0.25
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	17	0.25
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	17	0.25
(1,1575)	1:92:A:LEU:HD11	1:130:A:VAL:H	15	0.25
(1,1575)	1:92:A:LEU:HD12	1:130:A:VAL:H	15	0.25
(1,1575)	1:92:A:LEU:HD13	1:130:A:VAL:H	15	0.25
(1,1575)	1:92:A:LEU:HD21	1:130:A:VAL:H	15	0.25
(1,1575)	1:92:A:LEU:HD22	1:130:A:VAL:H	15	0.25
(1,1575)	1:92:A:LEU:HD23	1:130:A:VAL:H	15	0.25
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG11	3	0.25
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG12	3	0.25
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG13	3	0.25
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG21	3	0.25
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG22	3	0.25
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG23	3	0.25
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG11	15	0.25
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG12	15	0.25
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG13	15	0.25
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG21	15	0.25
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG22	15	0.25
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG23	15	0.25
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB2	18	0.25
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB3	18	0.25
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE21	12	0.25
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	12	0.25
(1,1441)	1:53:A:ARG:HD2	1:57:A:GLY:HA2	1	0.25
(1,1441)	1:53:A:ARG:HD3	1:57:A:GLY:HA2	1	0.25
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	5	0.25
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	5	0.25
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	5	0.25
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	5	0.25
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	5	0.25
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	5	0.25
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	13	0.25
(1,1430)	1:50:A:TYR:HE2	1:70:A:PHE:HB3	13	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	7	0.25
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	7	0.25
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	10	0.25
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	10	0.25
(1,1405)	1:44:A:LYS:HE2	1:45:A:LYS:H	7	0.25
(1,1405)	1:44:A:LYS:HE3	1:45:A:LYS:H	7	0.25
(1,1399)	1:44:A:LYS:HB2	1:44:A:LYS:HE2	1	0.25
(1,1399)	1:44:A:LYS:HB2	1:44:A:LYS:HE3	1	0.25
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG2	1	0.25
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG3	1	0.25
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG2	20	0.25
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG3	20	0.25
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	3	0.25
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	3	0.25
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	3	0.25
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	19	0.25
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	19	0.25
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	19	0.25
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	11	0.25
(1,1213)	1:109:A:ARG:HB3	1:110:A:GLY:H	17	0.25
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	8	0.25
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	10	0.25
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	1	0.25
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	2	0.25
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB1	1	0.25
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB2	1	0.25
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB3	1	0.25
(1,1172)	1:102:A:TYR:H	1:105:A:ALA:H	13	0.25
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	7	0.25
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	7	0.25
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	7	0.25
(1,1111)	1:38:A:THR:HG21	1:92:A:LEU:H	20	0.25
(1,1111)	1:38:A:THR:HG22	1:92:A:LEU:H	20	0.25
(1,1111)	1:38:A:THR:HG23	1:92:A:LEU:H	20	0.25
(1,1104)	1:91:A:THR:H	1:127:A:LEU:HG	19	0.25
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	12	0.25
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	8	0.25
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	8	0.25
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	8	0.25
(1,1041)	1:80:A:ILE:HG21	1:83:A:TRP:H	2	0.25
(1,1041)	1:80:A:ILE:HG22	1:83:A:TRP:H	2	0.25
(1,1041)	1:80:A:ILE:HG23	1:83:A:TRP:H	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1006)	1:77:A:GLY:H	1:78:A:GLU:HB2	20	0.25
(1,952)	1:67:A:GLY:H	1:68:A:LYS:HB2	2	0.25
(1,951)	1:67:A:GLY:H	1:68:A:LYS:HB3	9	0.25
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	20	0.25
(1,912)	1:53:A:ARG:HD3	1:57:A:GLY:H	6	0.25
(1,911)	1:53:A:ARG:HD2	1:57:A:GLY:H	5	0.25
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	8	0.25
(1,787)	1:37:A:VAL:HB	1:38:A:THR:H	18	0.25
(1,744)	1:26:A:LEU:H	1:27:A:GLU:HG3	4	0.25
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	4	0.25
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	4	0.25
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	4	0.25
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	16	0.25
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	16	0.25
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	16	0.25
(1,696)	1:83:A:TRP:HZ2	1:123:A:PHE:HB3	20	0.25
(1,695)	1:83:A:TRP:HZ2	1:123:A:PHE:HD1	14	0.25
(1,686)	1:102:A:TYR:HE2	1:118:A:LYS:HA	13	0.25
(1,682)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	11	0.25
(1,643)	1:49:A:HIS:HD1	1:128:A:LEU:HG	1	0.25
(1,629)	1:92:A:LEU:HA	1:127:A:LEU:HG	6	0.25
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG21	1	0.25
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG22	1	0.25
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG23	1	0.25
(1,578)	1:119:A:ALA:HB1	1:120:A:THR:HB	10	0.25
(1,578)	1:119:A:ALA:HB2	1:120:A:THR:HB	10	0.25
(1,578)	1:119:A:ALA:HB3	1:120:A:THR:HB	10	0.25
(1,544)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	12	0.25
(1,502)	1:82:A:GLY:H	1:104:A:LEU:HG	7	0.25
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD11	18	0.25
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD12	18	0.25
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD13	18	0.25
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD11	18	0.25
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD12	18	0.25
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD13	18	0.25
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD11	18	0.25
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD12	18	0.25
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD13	18	0.25
(1,482)	1:100:A:ILE:HG21	1:104:A:LEU:HB2	4	0.25
(1,482)	1:100:A:ILE:HG22	1:104:A:LEU:HB2	4	0.25
(1,482)	1:100:A:ILE:HG23	1:104:A:LEU:HB2	4	0.25
(1,425)	1:92:A:LEU:HG	1:93:A:GLY:H	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:90:A:MET:HE1	1:91:A:THR:H	7	0.25
(1,413)	1:90:A:MET:HE2	1:91:A:THR:H	7	0.25
(1,413)	1:90:A:MET:HE3	1:91:A:THR:H	7	0.25
(1,378)	1:81:A:LYS:HA	1:84:A:ASP:HB3	19	0.25
(1,364)	1:80:A:ILE:HD11	1:83:A:TRP:HA	5	0.25
(1,364)	1:80:A:ILE:HD12	1:83:A:TRP:HA	5	0.25
(1,364)	1:80:A:ILE:HD13	1:83:A:TRP:HA	5	0.25
(1,289)	1:76:A:ALA:HB1	1:78:A:GLU:HB2	10	0.25
(1,289)	1:76:A:ALA:HB2	1:78:A:GLU:HB2	10	0.25
(1,289)	1:76:A:ALA:HB3	1:78:A:GLU:HB2	10	0.25
(1,284)	1:73:A:THR:HG21	1:76:A:ALA:HB1	2	0.25
(1,284)	1:73:A:THR:HG21	1:76:A:ALA:HB2	2	0.25
(1,284)	1:73:A:THR:HG21	1:76:A:ALA:HB3	2	0.25
(1,284)	1:73:A:THR:HG22	1:76:A:ALA:HB1	2	0.25
(1,284)	1:73:A:THR:HG22	1:76:A:ALA:HB2	2	0.25
(1,284)	1:73:A:THR:HG22	1:76:A:ALA:HB3	2	0.25
(1,284)	1:73:A:THR:HG23	1:76:A:ALA:HB1	2	0.25
(1,284)	1:73:A:THR:HG23	1:76:A:ALA:HB2	2	0.25
(1,284)	1:73:A:THR:HG23	1:76:A:ALA:HB3	2	0.25
(1,284)	1:73:A:THR:HG21	1:76:A:ALA:HB1	12	0.25
(1,284)	1:73:A:THR:HG21	1:76:A:ALA:HB2	12	0.25
(1,284)	1:73:A:THR:HG21	1:76:A:ALA:HB3	12	0.25
(1,284)	1:73:A:THR:HG22	1:76:A:ALA:HB1	12	0.25
(1,284)	1:73:A:THR:HG22	1:76:A:ALA:HB2	12	0.25
(1,284)	1:73:A:THR:HG22	1:76:A:ALA:HB3	12	0.25
(1,284)	1:73:A:THR:HG23	1:76:A:ALA:HB1	12	0.25
(1,284)	1:73:A:THR:HG23	1:76:A:ALA:HB2	12	0.25
(1,284)	1:73:A:THR:HG23	1:76:A:ALA:HB3	12	0.25
(1,265)	1:42:A:ALA:H	1:74:A:LEU:HB3	3	0.25
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	9	0.25
(1,224)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	16	0.25
(1,212)	1:64:A:ARG:HA	1:64:A:ARG:HD2	8	0.25
(1,193)	1:53:A:ARG:HB3	1:59:A:GLN:HA	6	0.25
(1,81)	1:42:A:ALA:HA	1:74:A:LEU:H	4	0.25
(1,81)	1:42:A:ALA:HA	1:74:A:LEU:H	8	0.25
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	10	0.25
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	10	0.25
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	10	0.25
(1,1599)	1:97:A:LEU:HD11	1:124:A:GLU:HB3	5	0.24
(1,1599)	1:97:A:LEU:HD12	1:124:A:GLU:HB3	5	0.24
(1,1599)	1:97:A:LEU:HD13	1:124:A:GLU:HB3	5	0.24
(1,1599)	1:97:A:LEU:HD21	1:124:A:GLU:HB3	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1599)	1:97:A:LEU:HD22	1:124:A:GLU:HB3	5	0.24
(1,1599)	1:97:A:LEU:HD23	1:124:A:GLU:HB3	5	0.24
(1,1598)	1:97:A:LEU:HD11	1:124:A:GLU:HB2	19	0.24
(1,1598)	1:97:A:LEU:HD12	1:124:A:GLU:HB2	19	0.24
(1,1598)	1:97:A:LEU:HD13	1:124:A:GLU:HB2	19	0.24
(1,1598)	1:97:A:LEU:HD21	1:124:A:GLU:HB2	19	0.24
(1,1598)	1:97:A:LEU:HD22	1:124:A:GLU:HB2	19	0.24
(1,1598)	1:97:A:LEU:HD23	1:124:A:GLU:HB2	19	0.24
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG11	2	0.24
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG12	2	0.24
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG13	2	0.24
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG21	2	0.24
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG22	2	0.24
(1,1566)	1:92:A:LEU:H	1:130:A:VAL:HG23	2	0.24
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG11	6	0.24
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG12	6	0.24
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG13	6	0.24
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG21	6	0.24
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG22	6	0.24
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG23	6	0.24
(1,1474)	1:59:A:GLN:HG2	1:60:A:PHE:H	14	0.24
(1,1474)	1:59:A:GLN:HG3	1:60:A:PHE:H	14	0.24
(1,1461)	1:55:A:PRO:HD2	1:120:A:THR:HG21	17	0.24
(1,1461)	1:55:A:PRO:HD2	1:120:A:THR:HG22	17	0.24
(1,1461)	1:55:A:PRO:HD2	1:120:A:THR:HG23	17	0.24
(1,1461)	1:55:A:PRO:HD3	1:120:A:THR:HG21	17	0.24
(1,1461)	1:55:A:PRO:HD3	1:120:A:THR:HG22	17	0.24
(1,1461)	1:55:A:PRO:HD3	1:120:A:THR:HG23	17	0.24
(1,1346)	1:28:A:LYS:HG2	1:30:A:VAL:H	8	0.24
(1,1346)	1:28:A:LYS:HG3	1:30:A:VAL:H	8	0.24
(1,1328)	1:19:A:PRO:HG2	1:56:A:ASP:HA	6	0.24
(1,1328)	1:19:A:PRO:HG3	1:56:A:ASP:HA	6	0.24
(1,1301)	1:71:A:GLN:HA	1:71:A:GLN:HE21	4	0.24
(1,1298)	1:92:A:LEU:HG	1:130:A:VAL:H	16	0.24
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	15	0.24
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	15	0.24
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	15	0.24
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	16	0.24
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	16	0.24
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	16	0.24
(1,1252)	1:100:A:ILE:HD11	1:123:A:PHE:H	20	0.24
(1,1252)	1:100:A:ILE:HD12	1:123:A:PHE:H	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1252)	1:100:A:ILE:HD13	1:123:A:PHE:H	20	0.24
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	19	0.24
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	6	0.24
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	12	0.24
(1,1059)	1:84:A:ASP:HB2	1:85:A:GLN:H	14	0.24
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	10	0.24
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	10	0.24
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	10	0.24
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	12	0.24
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	12	0.24
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	12	0.24
(1,1050)	1:80:A:ILE:HG12	1:84:A:ASP:H	3	0.24
(1,1036)	1:79:A:VAL:HB	1:83:A:TRP:H	3	0.24
(1,1025)	1:82:A:GLY:H	1:104:A:LEU:HA	19	0.24
(1,1006)	1:77:A:GLY:H	1:78:A:GLU:HB2	6	0.24
(1,1003)	1:74:A:LEU:HB3	1:76:A:ALA:H	13	0.24
(1,858)	1:50:A:TYR:HD1	1:51:A:ASP:H	3	0.24
(1,828)	1:46:A:VAL:H	1:71:A:GLN:HA	20	0.24
(1,806)	1:42:A:ALA:H	1:74:A:LEU:HG	7	0.24
(1,775)	1:34:A:GLY:H	1:94:A:GLU:HB3	12	0.24
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	12	0.24
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	12	0.24
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	12	0.24
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG21	19	0.24
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG22	19	0.24
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG23	19	0.24
(1,708)	1:11:A:THR:HA	1:12:A:LEU:H	6	0.24
(1,695)	1:83:A:TRP:HZ2	1:123:A:PHE:HD1	20	0.24
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG11	7	0.24
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG12	7	0.24
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG13	7	0.24
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB1	12	0.24
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB2	12	0.24
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB3	12	0.24
(1,630)	1:127:A:LEU:HG	1:129:A:ALA:HA	4	0.24
(1,623)	1:95:A:LYS:HB2	1:126:A:GLU:HA	16	0.24
(1,602)	1:100:A:ILE:HD11	1:123:A:PHE:HB3	19	0.24
(1,602)	1:100:A:ILE:HD12	1:123:A:PHE:HB3	19	0.24
(1,602)	1:100:A:ILE:HD13	1:123:A:PHE:HB3	19	0.24
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	15	0.24
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	16	0.24
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	19	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	20	0.24
(1,582)	1:55:A:PRO:HG2	1:120:A:THR:HB	17	0.24
(1,566)	1:111:A:TYR:HB2	1:115:A:ILE:HB	12	0.24
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB1	9	0.24
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB2	9	0.24
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB3	9	0.24
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB1	13	0.24
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB2	13	0.24
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB3	13	0.24
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD11	5	0.24
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD12	5	0.24
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD13	5	0.24
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD11	5	0.24
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD12	5	0.24
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD13	5	0.24
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD11	5	0.24
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD12	5	0.24
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD13	5	0.24
(1,482)	1:100:A:ILE:HG21	1:104:A:LEU:HB2	8	0.24
(1,482)	1:100:A:ILE:HG22	1:104:A:LEU:HB2	8	0.24
(1,482)	1:100:A:ILE:HG23	1:104:A:LEU:HB2	8	0.24
(1,459)	1:97:A:LEU:HG	1:99:A:THR:H	8	0.24
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB1	8	0.24
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB2	8	0.24
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB3	8	0.24
(1,450)	1:32:A:THR:HB	1:95:A:LYS:HE3	1	0.24
(1,444)	1:31:A:LEU:HG	1:95:A:LYS:HB3	12	0.24
(1,412)	1:90:A:MET:H	1:90:A:MET:HE1	11	0.24
(1,412)	1:90:A:MET:H	1:90:A:MET:HE2	11	0.24
(1,412)	1:90:A:MET:H	1:90:A:MET:HE3	11	0.24
(1,391)	1:46:A:VAL:HG21	1:87:A:VAL:HB	17	0.24
(1,391)	1:46:A:VAL:HG22	1:87:A:VAL:HB	17	0.24
(1,391)	1:46:A:VAL:HG23	1:87:A:VAL:HB	17	0.24
(1,371)	1:81:A:LYS:HD3	1:84:A:ASP:HB2	8	0.24
(1,354)	1:82:A:GLY:HA2	1:104:A:LEU:HB3	4	0.24
(1,346)	1:81:A:LYS:HB3	1:82:A:GLY:HA3	9	0.24
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD21	2	0.24
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD22	2	0.24
(1,340)	1:81:A:LYS:HG2	1:104:A:LEU:HD23	2	0.24
(1,315)	1:80:A:ILE:HD11	1:100:A:ILE:HG21	2	0.24
(1,315)	1:80:A:ILE:HD11	1:100:A:ILE:HG22	2	0.24
(1,315)	1:80:A:ILE:HD11	1:100:A:ILE:HG23	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:80:A:ILE:HD12	1:100:A:ILE:HG21	2	0.24
(1,315)	1:80:A:ILE:HD12	1:100:A:ILE:HG22	2	0.24
(1,315)	1:80:A:ILE:HD12	1:100:A:ILE:HG23	2	0.24
(1,315)	1:80:A:ILE:HD13	1:100:A:ILE:HG21	2	0.24
(1,315)	1:80:A:ILE:HD13	1:100:A:ILE:HG22	2	0.24
(1,315)	1:80:A:ILE:HD13	1:100:A:ILE:HG23	2	0.24
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD11	18	0.24
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD12	18	0.24
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD13	18	0.24
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD11	20	0.24
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD12	20	0.24
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD13	20	0.24
(1,284)	1:73:A:THR:HG21	1:76:A:ALA:HB1	4	0.24
(1,284)	1:73:A:THR:HG21	1:76:A:ALA:HB2	4	0.24
(1,284)	1:73:A:THR:HG21	1:76:A:ALA:HB3	4	0.24
(1,284)	1:73:A:THR:HG22	1:76:A:ALA:HB1	4	0.24
(1,284)	1:73:A:THR:HG22	1:76:A:ALA:HB2	4	0.24
(1,284)	1:73:A:THR:HG22	1:76:A:ALA:HB3	4	0.24
(1,284)	1:73:A:THR:HG23	1:76:A:ALA:HB1	4	0.24
(1,284)	1:73:A:THR:HG23	1:76:A:ALA:HB2	4	0.24
(1,284)	1:73:A:THR:HG23	1:76:A:ALA:HB3	4	0.24
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD21	20	0.24
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD22	20	0.24
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD23	20	0.24
(1,216)	1:64:A:ARG:HA	1:64:A:ARG:HD3	3	0.24
(1,209)	1:64:A:ARG:HA	1:68:A:LYS:H	19	0.24
(1,208)	1:63:A:SER:H	1:64:A:ARG:HA	5	0.24
(1,185)	1:53:A:ARG:HB3	1:57:A:GLY:HA2	11	0.24
(1,184)	1:53:A:ARG:HD3	1:57:A:GLY:HA2	17	0.24
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG21	10	0.24
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG22	10	0.24
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG23	10	0.24
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	7	0.24
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	7	0.24
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	7	0.24
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	5	0.24
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	5	0.24
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	5	0.24
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	6	0.24
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	6	0.24
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	6	0.24
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	17	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	17	0.24
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	17	0.24
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG21	10	0.24
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG22	10	0.24
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG23	10	0.24
(1,82)	1:42:A:ALA:HA	1:74:A:LEU:HB2	12	0.24
(1,77)	1:40:A:PRO:HD3	1:130:A:VAL:HB	19	0.24
(1,64)	1:38:A:THR:HG21	1:39:A:LYS:H	7	0.24
(1,64)	1:38:A:THR:HG22	1:39:A:LYS:H	7	0.24
(1,64)	1:38:A:THR:HG23	1:39:A:LYS:H	7	0.24
(1,49)	1:35:A:ASP:HA	1:37:A:VAL:HG21	19	0.24
(1,49)	1:35:A:ASP:HA	1:37:A:VAL:HG22	19	0.24
(1,49)	1:35:A:ASP:HA	1:37:A:VAL:HG23	19	0.24
(1,42)	1:33:A:PRO:HA	1:94:A:GLU:HG2	5	0.24
(1,1619)	1:103:A:GLN:HG2	1:104:A:LEU:H	3	0.23
(1,1619)	1:103:A:GLN:HG3	1:104:A:LEU:H	3	0.23
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG11	9	0.23
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG12	9	0.23
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG13	9	0.23
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG21	9	0.23
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG22	9	0.23
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG23	9	0.23
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE21	4	0.23
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE22	4	0.23
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB2	15	0.23
(1,1453)	1:54:A:PHE:HE1	1:60:A:PHE:HB3	15	0.23
(1,1442)	1:53:A:ARG:HD2	1:59:A:GLN:HA	18	0.23
(1,1442)	1:53:A:ARG:HD3	1:59:A:GLN:HA	18	0.23
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD2	5	0.23
(1,1428)	1:49:A:HIS:HE1	1:69:A:PRO:HD3	5	0.23
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE2	1	0.23
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE3	1	0.23
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE2	1	0.23
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE3	1	0.23
(1,1380)	1:40:A:PRO:HB2	1:41:A:GLN:H	6	0.23
(1,1380)	1:40:A:PRO:HB3	1:41:A:GLN:H	6	0.23
(1,1309)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	15	0.23
(1,1301)	1:71:A:GLN:HA	1:71:A:GLN:HE21	2	0.23
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	1	0.23
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	20	0.23
(1,1215)	1:110:A:GLY:HA3	1:111:A:TYR:H	16	0.23
(1,1152)	1:98:A:PHE:H	1:123:A:PHE:HB3	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1152)	1:98:A:PHE:H	1:123:A:PHE:HB3	11	0.23
(1,1147)	1:98:A:PHE:H	1:99:A:THR:H	9	0.23
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	11	0.23
(1,1106)	1:37:A:VAL:H	1:92:A:LEU:H	9	0.23
(1,1106)	1:37:A:VAL:H	1:92:A:LEU:H	16	0.23
(1,1097)	1:34:A:GLY:HA3	1:91:A:THR:H	1	0.23
(1,1050)	1:80:A:ILE:HG12	1:84:A:ASP:H	6	0.23
(1,1006)	1:77:A:GLY:H	1:78:A:GLU:HB2	7	0.23
(1,1003)	1:74:A:LEU:HB3	1:76:A:ALA:H	15	0.23
(1,1001)	1:73:A:THR:HB	1:76:A:ALA:H	6	0.23
(1,929)	1:63:A:SER:H	1:64:A:ARG:HG3	19	0.23
(1,923)	1:71:A:GLN:HE21	1:72:A:PHE:H	20	0.23
(1,828)	1:46:A:VAL:H	1:71:A:GLN:HA	4	0.23
(1,820)	1:44:A:LYS:H	1:44:A:LYS:HG3	9	0.23
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG21	2	0.23
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG22	2	0.23
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG23	2	0.23
(1,789)	1:38:A:THR:H	1:91:A:THR:HG21	12	0.23
(1,789)	1:38:A:THR:H	1:91:A:THR:HG22	12	0.23
(1,789)	1:38:A:THR:H	1:91:A:THR:HG23	12	0.23
(1,747)	1:27:A:GLU:H	1:98:A:PHE:HA	11	0.23
(1,747)	1:27:A:GLU:H	1:98:A:PHE:HA	12	0.23
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG21	2	0.23
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG22	2	0.23
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG23	2	0.23
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG21	11	0.23
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG22	11	0.23
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG23	11	0.23
(1,686)	1:102:A:TYR:HE2	1:118:A:LYS:HA	1	0.23
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG21	20	0.23
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG22	20	0.23
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG23	20	0.23
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	16	0.23
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	16	0.23
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	16	0.23
(1,580)	1:115:A:ILE:HD11	1:119:A:ALA:HB1	15	0.23
(1,580)	1:115:A:ILE:HD11	1:119:A:ALA:HB2	15	0.23
(1,580)	1:115:A:ILE:HD11	1:119:A:ALA:HB3	15	0.23
(1,580)	1:115:A:ILE:HD12	1:119:A:ALA:HB1	15	0.23
(1,580)	1:115:A:ILE:HD12	1:119:A:ALA:HB2	15	0.23
(1,580)	1:115:A:ILE:HD12	1:119:A:ALA:HB3	15	0.23
(1,580)	1:115:A:ILE:HD13	1:119:A:ALA:HB1	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,580)	1:115:A:ILE:HD13	1:119:A:ALA:HB2	15	0.23
(1,580)	1:115:A:ILE:HD13	1:119:A:ALA:HB3	15	0.23
(1,578)	1:119:A:ALA:HB1	1:120:A:THR:HB	11	0.23
(1,578)	1:119:A:ALA:HB2	1:120:A:THR:HB	11	0.23
(1,578)	1:119:A:ALA:HB3	1:120:A:THR:HB	11	0.23
(1,554)	1:106:A:TYR:HB2	1:110:A:GLY:HA2	2	0.23
(1,519)	1:80:A:ILE:HB	1:105:A:ALA:HA	2	0.23
(1,516)	1:81:A:LYS:H	1:105:A:ALA:HA	20	0.23
(1,504)	1:82:A:GLY:H	1:104:A:LEU:HD11	17	0.23
(1,504)	1:82:A:GLY:H	1:104:A:LEU:HD12	17	0.23
(1,504)	1:82:A:GLY:H	1:104:A:LEU:HD13	17	0.23
(1,491)	1:102:A:TYR:HB3	1:105:A:ALA:HB1	9	0.23
(1,491)	1:102:A:TYR:HB3	1:105:A:ALA:HB2	9	0.23
(1,491)	1:102:A:TYR:HB3	1:105:A:ALA:HB3	9	0.23
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD11	15	0.23
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD12	15	0.23
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD13	15	0.23
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD11	15	0.23
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD12	15	0.23
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD13	15	0.23
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD11	15	0.23
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD12	15	0.23
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD13	15	0.23
(1,482)	1:100:A:ILE:HG21	1:104:A:LEU:HB2	10	0.23
(1,482)	1:100:A:ILE:HG22	1:104:A:LEU:HB2	10	0.23
(1,482)	1:100:A:ILE:HG23	1:104:A:LEU:HB2	10	0.23
(1,462)	1:97:A:LEU:HD21	1:123:A:PHE:H	18	0.23
(1,462)	1:97:A:LEU:HD22	1:123:A:PHE:H	18	0.23
(1,462)	1:97:A:LEU:HD23	1:123:A:PHE:H	18	0.23
(1,460)	1:97:A:LEU:HD11	1:98:A:PHE:H	7	0.23
(1,460)	1:97:A:LEU:HD12	1:98:A:PHE:H	7	0.23
(1,460)	1:97:A:LEU:HD13	1:98:A:PHE:H	7	0.23
(1,459)	1:97:A:LEU:HG	1:99:A:THR:H	18	0.23
(1,444)	1:31:A:LEU:HG	1:95:A:LYS:HB3	19	0.23
(1,411)	1:90:A:MET:HE1	1:127:A:LEU:H	19	0.23
(1,411)	1:90:A:MET:HE2	1:127:A:LEU:H	19	0.23
(1,411)	1:90:A:MET:HE3	1:127:A:LEU:H	19	0.23
(1,375)	1:74:A:LEU:HD11	1:84:A:ASP:HB3	19	0.23
(1,375)	1:74:A:LEU:HD12	1:84:A:ASP:HB3	19	0.23
(1,375)	1:74:A:LEU:HD13	1:84:A:ASP:HB3	19	0.23
(1,369)	1:83:A:TRP:H	1:84:A:ASP:HB2	11	0.23
(1,357)	1:80:A:ILE:HG13	1:83:A:TRP:HB2	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	5	0.23
(1,310)	1:80:A:ILE:HA	1:81:A:LYS:HG2	7	0.23
(1,305)	1:79:A:VAL:HB	1:80:A:ILE:HD11	4	0.23
(1,305)	1:79:A:VAL:HB	1:80:A:ILE:HD12	4	0.23
(1,305)	1:79:A:VAL:HB	1:80:A:ILE:HD13	4	0.23
(1,265)	1:42:A:ALA:H	1:74:A:LEU:HB3	20	0.23
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	10	0.23
(1,231)	1:68:A:LYS:H	1:69:A:PRO:HA	14	0.23
(1,227)	1:67:A:GLY:HA3	1:68:A:LYS:HB2	19	0.23
(1,224)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	13	0.23
(1,197)	1:59:A:GLN:HG2	1:60:A:PHE:H	19	0.23
(1,152)	1:51:A:ASP:HB2	1:124:A:GLU:H	16	0.23
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG11	8	0.23
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG12	8	0.23
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG13	8	0.23
(1,121)	1:46:A:VAL:HG11	1:130:A:VAL:H	13	0.23
(1,121)	1:46:A:VAL:HG12	1:130:A:VAL:H	13	0.23
(1,121)	1:46:A:VAL:HG13	1:130:A:VAL:H	13	0.23
(1,81)	1:42:A:ALA:HA	1:74:A:LEU:H	10	0.23
(1,29)	1:27:A:GLU:H	1:27:A:GLU:HG2	6	0.23
(1,2)	1:28:A:LYS:HB2	1:30:A:VAL:H	11	0.23
(1,1624)	1:108:A:GLU:HG2	1:118:A:LYS:HG2	11	0.22
(1,1624)	1:108:A:GLU:HG3	1:118:A:LYS:HG2	11	0.22
(1,1619)	1:103:A:GLN:HG2	1:104:A:LEU:H	15	0.22
(1,1619)	1:103:A:GLN:HG3	1:104:A:LEU:H	15	0.22
(1,1612)	1:102:A:TYR:HB2	1:108:A:GLU:HG2	6	0.22
(1,1612)	1:102:A:TYR:HB2	1:108:A:GLU:HG3	6	0.22
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG11	20	0.22
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG12	20	0.22
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG13	20	0.22
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG21	20	0.22
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG22	20	0.22
(1,1608)	1:99:A:THR:HB	1:122:A:VAL:HG23	20	0.22
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	7	0.22
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	7	0.22
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	7	0.22
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	7	0.22
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	7	0.22
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	7	0.22
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG11	4	0.22
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG12	4	0.22
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG13	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG21	4	0.22
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG22	4	0.22
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG23	4	0.22
(1,1506)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	16	0.22
(1,1506)	1:67:A:GLY:HA3	1:68:A:LYS:HB2	16	0.22
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	1	0.22
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	1	0.22
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	2	0.22
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	2	0.22
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	12	0.22
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	12	0.22
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	19	0.22
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	19	0.22
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE21	8	0.22
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE22	8	0.22
(1,1443)	1:53:A:ARG:HD2	1:97:A:LEU:HD11	17	0.22
(1,1443)	1:53:A:ARG:HD2	1:97:A:LEU:HD12	17	0.22
(1,1443)	1:53:A:ARG:HD2	1:97:A:LEU:HD13	17	0.22
(1,1443)	1:53:A:ARG:HD2	1:97:A:LEU:HD21	17	0.22
(1,1443)	1:53:A:ARG:HD2	1:97:A:LEU:HD22	17	0.22
(1,1443)	1:53:A:ARG:HD2	1:97:A:LEU:HD23	17	0.22
(1,1443)	1:53:A:ARG:HD3	1:97:A:LEU:HD11	17	0.22
(1,1443)	1:53:A:ARG:HD3	1:97:A:LEU:HD12	17	0.22
(1,1443)	1:53:A:ARG:HD3	1:97:A:LEU:HD13	17	0.22
(1,1443)	1:53:A:ARG:HD3	1:97:A:LEU:HD21	17	0.22
(1,1443)	1:53:A:ARG:HD3	1:97:A:LEU:HD22	17	0.22
(1,1443)	1:53:A:ARG:HD3	1:97:A:LEU:HD23	17	0.22
(1,1380)	1:40:A:PRO:HB2	1:41:A:GLN:H	13	0.22
(1,1380)	1:40:A:PRO:HB3	1:41:A:GLN:H	13	0.22
(1,1307)	1:81:A:LYS:HE3	1:85:A:GLN:HE21	6	0.22
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	20	0.22
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	20	0.22
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	20	0.22
(1,1301)	1:71:A:GLN:HA	1:71:A:GLN:HE21	3	0.22
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	12	0.22
(1,1235)	1:55:A:PRO:HG3	1:120:A:THR:H	15	0.22
(1,1197)	1:100:A:ILE:HG21	1:105:A:ALA:H	10	0.22
(1,1197)	1:100:A:ILE:HG22	1:105:A:ALA:H	10	0.22
(1,1197)	1:100:A:ILE:HG23	1:105:A:ALA:H	10	0.22
(1,1172)	1:102:A:TYR:H	1:105:A:ALA:H	10	0.22
(1,1152)	1:98:A:PHE:H	1:123:A:PHE:HB3	3	0.22
(1,1152)	1:98:A:PHE:H	1:123:A:PHE:HB3	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1152)	1:98:A:PHE:H	1:123:A:PHE:HB3	18	0.22
(1,1120)	1:34:A:GLY:HA2	1:94:A:GLU:H	11	0.22
(1,1116)	1:92:A:LEU:HD11	1:93:A:GLY:H	16	0.22
(1,1116)	1:92:A:LEU:HD12	1:93:A:GLY:H	16	0.22
(1,1116)	1:92:A:LEU:HD13	1:93:A:GLY:H	16	0.22
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	20	0.22
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	7	0.22
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	7	0.22
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	7	0.22
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	20	0.22
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	20	0.22
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	20	0.22
(1,1050)	1:80:A:ILE:HG12	1:84:A:ASP:H	14	0.22
(1,1047)	1:84:A:ASP:H	1:84:A:ASP:HB2	14	0.22
(1,1041)	1:80:A:ILE:HG21	1:83:A:TRP:H	17	0.22
(1,1041)	1:80:A:ILE:HG22	1:83:A:TRP:H	17	0.22
(1,1041)	1:80:A:ILE:HG23	1:83:A:TRP:H	17	0.22
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	1	0.22
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	1	0.22
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	1	0.22
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	7	0.22
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	7	0.22
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	7	0.22
(1,1003)	1:74:A:LEU:HB3	1:76:A:ALA:H	2	0.22
(1,977)	1:47:A:THR:HG21	1:71:A:GLN:H	1	0.22
(1,977)	1:47:A:THR:HG22	1:71:A:GLN:H	1	0.22
(1,977)	1:47:A:THR:HG23	1:71:A:GLN:H	1	0.22
(1,903)	1:59:A:GLN:HE22	1:62:A:SER:HB2	4	0.22
(1,868)	1:51:A:ASP:H	1:125:A:VAL:HG11	11	0.22
(1,868)	1:51:A:ASP:H	1:125:A:VAL:HG12	11	0.22
(1,868)	1:51:A:ASP:H	1:125:A:VAL:HG13	11	0.22
(1,863)	1:50:A:TYR:HB2	1:51:A:ASP:H	7	0.22
(1,858)	1:50:A:TYR:HD1	1:51:A:ASP:H	20	0.22
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG21	1	0.22
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG22	1	0.22
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG23	1	0.22
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG21	4	0.22
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG22	4	0.22
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG23	4	0.22
(1,789)	1:38:A:THR:H	1:91:A:THR:HG21	13	0.22
(1,789)	1:38:A:THR:H	1:91:A:THR:HG22	13	0.22
(1,789)	1:38:A:THR:H	1:91:A:THR:HG23	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:49:A:HIS:HE1	1:64:A:ARG:HA	5	0.22
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD11	7	0.22
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD12	7	0.22
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD13	7	0.22
(1,632)	1:93:A:GLY:H	1:127:A:LEU:HG	5	0.22
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	12	0.22
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	14	0.22
(1,557)	1:110:A:GLY:HA3	1:115:A:ILE:HB	10	0.22
(1,557)	1:110:A:GLY:HA3	1:115:A:ILE:HB	13	0.22
(1,548)	1:102:A:TYR:HE2	1:108:A:GLU:HG3	12	0.22
(1,541)	1:108:A:GLU:HA	1:118:A:LYS:HA	20	0.22
(1,537)	1:108:A:GLU:HB2	1:118:A:LYS:HG2	5	0.22
(1,536)	1:102:A:TYR:HE2	1:108:A:GLU:HB2	10	0.22
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD11	5	0.22
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD12	5	0.22
(1,511)	1:81:A:LYS:HD2	1:104:A:LEU:HD13	5	0.22
(1,500)	1:81:A:LYS:HB2	1:104:A:LEU:HA	18	0.22
(1,481)	1:100:A:ILE:HG21	1:104:A:LEU:HA	6	0.22
(1,481)	1:100:A:ILE:HG22	1:104:A:LEU:HA	6	0.22
(1,481)	1:100:A:ILE:HG23	1:104:A:LEU:HA	6	0.22
(1,470)	1:100:A:ILE:HB	1:121:A:LEU:HB2	3	0.22
(1,460)	1:97:A:LEU:HD11	1:98:A:PHE:H	8	0.22
(1,460)	1:97:A:LEU:HD12	1:98:A:PHE:H	8	0.22
(1,460)	1:97:A:LEU:HD13	1:98:A:PHE:H	8	0.22
(1,460)	1:97:A:LEU:HD11	1:98:A:PHE:H	15	0.22
(1,460)	1:97:A:LEU:HD12	1:98:A:PHE:H	15	0.22
(1,460)	1:97:A:LEU:HD13	1:98:A:PHE:H	15	0.22
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB1	12	0.22
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB2	12	0.22
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB3	12	0.22
(1,411)	1:90:A:MET:HE1	1:127:A:LEU:H	14	0.22
(1,411)	1:90:A:MET:HE2	1:127:A:LEU:H	14	0.22
(1,411)	1:90:A:MET:HE3	1:127:A:LEU:H	14	0.22
(1,405)	1:85:A:GLN:HA	1:89:A:THR:HG21	16	0.22
(1,405)	1:85:A:GLN:HA	1:89:A:THR:HG22	16	0.22
(1,405)	1:85:A:GLN:HA	1:89:A:THR:HG23	16	0.22
(1,375)	1:74:A:LEU:HD11	1:84:A:ASP:HB3	20	0.22
(1,375)	1:74:A:LEU:HD12	1:84:A:ASP:HB3	20	0.22
(1,375)	1:74:A:LEU:HD13	1:84:A:ASP:HB3	20	0.22
(1,369)	1:83:A:TRP:H	1:84:A:ASP:HB2	18	0.22
(1,364)	1:80:A:ILE:HD11	1:83:A:TRP:HA	8	0.22
(1,364)	1:80:A:ILE:HD12	1:83:A:TRP:HA	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	1:80:A:ILE:HD13	1:83:A:TRP:HA	8	0.22
(1,343)	1:66:A:ARG:HG3	1:68:A:LYS:H	2	0.22
(1,309)	1:80:A:ILE:HA	1:81:A:LYS:HB2	6	0.22
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD11	17	0.22
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD12	17	0.22
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD13	17	0.22
(1,292)	1:76:A:ALA:HB1	1:78:A:GLU:HG2	16	0.22
(1,292)	1:76:A:ALA:HB2	1:78:A:GLU:HG2	16	0.22
(1,292)	1:76:A:ALA:HB3	1:78:A:GLU:HG2	16	0.22
(1,276)	1:74:A:LEU:HD11	1:88:A:ALA:H	11	0.22
(1,276)	1:74:A:LEU:HD12	1:88:A:ALA:H	11	0.22
(1,276)	1:74:A:LEU:HD13	1:88:A:ALA:H	11	0.22
(1,209)	1:64:A:ARG:HA	1:68:A:LYS:H	17	0.22
(1,197)	1:59:A:GLN:HG2	1:60:A:PHE:H	7	0.22
(1,179)	1:54:A:PHE:HB2	1:55:A:PRO:HD3	6	0.22
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG21	7	0.22
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG22	7	0.22
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG23	7	0.22
(1,157)	1:52:A:GLY:HA2	1:124:A:GLU:H	10	0.22
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	6	0.22
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	7	0.22
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	10	0.22
(1,103)	1:45:A:LYS:HG2	1:46:A:VAL:H	6	0.22
(1,103)	1:45:A:LYS:HG2	1:46:A:VAL:H	18	0.22
(1,94)	1:41:A:GLN:HG2	1:44:A:LYS:HG3	12	0.22
(1,16)	1:41:A:GLN:H	1:41:A:GLN:HB2	5	0.22
(1,3)	1:28:A:LYS:HG3	1:30:A:VAL:H	11	0.22
(1,1601)	1:97:A:LEU:HD11	1:124:A:GLU:HG3	1	0.21
(1,1601)	1:97:A:LEU:HD12	1:124:A:GLU:HG3	1	0.21
(1,1601)	1:97:A:LEU:HD13	1:124:A:GLU:HG3	1	0.21
(1,1601)	1:97:A:LEU:HD21	1:124:A:GLU:HG3	1	0.21
(1,1601)	1:97:A:LEU:HD22	1:124:A:GLU:HG3	1	0.21
(1,1601)	1:97:A:LEU:HD23	1:124:A:GLU:HG3	1	0.21
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	15	0.21
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	15	0.21
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	15	0.21
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	15	0.21
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	15	0.21
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	15	0.21
(1,1404)	1:44:A:LYS:HD2	1:45:A:LYS:H	18	0.21
(1,1404)	1:44:A:LYS:HD3	1:45:A:LYS:H	18	0.21
(1,1399)	1:44:A:LYS:HB2	1:44:A:LYS:HE2	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1399)	1:44:A:LYS:HB2	1:44:A:LYS:HE3	2	0.21
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE2	18	0.21
(1,1396)	1:41:A:GLN:HE21	1:44:A:LYS:HE3	18	0.21
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE2	18	0.21
(1,1396)	1:41:A:GLN:HE22	1:44:A:LYS:HE3	18	0.21
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE2	7	0.21
(1,1391)	1:41:A:GLN:HB2	1:44:A:LYS:HE3	7	0.21
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE2	7	0.21
(1,1391)	1:41:A:GLN:HB3	1:44:A:LYS:HE3	7	0.21
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB2	19	0.21
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB3	19	0.21
(1,1332)	1:24:A:ALA:HA	1:103:A:GLN:HG2	8	0.21
(1,1332)	1:24:A:ALA:HA	1:103:A:GLN:HG3	8	0.21
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	16	0.21
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	16	0.21
(1,1309)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	16	0.21
(1,1308)	1:81:A:LYS:HD2	1:85:A:GLN:HE21	14	0.21
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	16	0.21
(1,1152)	1:98:A:PHE:H	1:123:A:PHE:HB3	1	0.21
(1,1147)	1:98:A:PHE:H	1:99:A:THR:H	17	0.21
(1,1106)	1:37:A:VAL:H	1:92:A:LEU:H	13	0.21
(1,1097)	1:34:A:GLY:HA3	1:91:A:THR:H	16	0.21
(1,1069)	1:86:A:GLY:H	1:98:A:PHE:HD2	10	0.21
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	1	0.21
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	1	0.21
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	1	0.21
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	13	0.21
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	13	0.21
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	13	0.21
(1,1050)	1:80:A:ILE:HG12	1:84:A:ASP:H	8	0.21
(1,1041)	1:80:A:ILE:HG21	1:83:A:TRP:H	5	0.21
(1,1041)	1:80:A:ILE:HG22	1:83:A:TRP:H	5	0.21
(1,1041)	1:80:A:ILE:HG23	1:83:A:TRP:H	5	0.21
(1,1029)	1:82:A:GLY:H	1:104:A:LEU:HB3	4	0.21
(1,1023)	1:81:A:LYS:H	1:81:A:LYS:HG3	19	0.21
(1,1009)	1:76:A:ALA:H	1:78:A:GLU:H	16	0.21
(1,1005)	1:77:A:GLY:H	1:78:A:GLU:H	15	0.21
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	12	0.21
(1,906)	1:58:A:LYS:HG2	1:59:A:GLN:H	17	0.21
(1,863)	1:50:A:TYR:HB2	1:51:A:ASP:H	14	0.21
(1,858)	1:50:A:TYR:HD1	1:51:A:ASP:H	9	0.21
(1,830)	1:46:A:VAL:H	1:72:A:PHE:HA	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:46:A:VAL:H	1:71:A:GLN:HA	12	0.21
(1,819)	1:44:A:LYS:H	1:44:A:LYS:HG2	3	0.21
(1,802)	1:41:A:GLN:H	1:74:A:LEU:HB3	9	0.21
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG21	18	0.21
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG22	18	0.21
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG23	18	0.21
(1,787)	1:37:A:VAL:HB	1:38:A:THR:H	20	0.21
(1,775)	1:34:A:GLY:H	1:94:A:GLU:HB3	18	0.21
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	17	0.21
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	17	0.21
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	17	0.21
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG21	17	0.21
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG22	17	0.21
(1,729)	1:35:A:ASP:H	1:91:A:THR:HG23	17	0.21
(1,709)	1:11:A:THR:HG21	1:12:A:LEU:H	11	0.21
(1,709)	1:11:A:THR:HG22	1:12:A:LEU:H	11	0.21
(1,709)	1:11:A:THR:HG23	1:12:A:LEU:H	11	0.21
(1,694)	1:80:A:ILE:HD11	1:83:A:TRP:HD1	5	0.21
(1,694)	1:80:A:ILE:HD12	1:83:A:TRP:HD1	5	0.21
(1,694)	1:80:A:ILE:HD13	1:83:A:TRP:HD1	5	0.21
(1,684)	1:48:A:VAL:HG21	1:50:A:TYR:HE1	15	0.21
(1,684)	1:48:A:VAL:HG22	1:50:A:TYR:HE1	15	0.21
(1,684)	1:48:A:VAL:HG23	1:50:A:TYR:HE1	15	0.21
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG21	9	0.21
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG22	9	0.21
(1,667)	1:106:A:TYR:HE1	1:115:A:ILE:HG23	9	0.21
(1,631)	1:92:A:LEU:H	1:127:A:LEU:HG	14	0.21
(1,619)	1:98:A:PHE:HD1	1:125:A:VAL:HG21	6	0.21
(1,619)	1:98:A:PHE:HD1	1:125:A:VAL:HG22	6	0.21
(1,619)	1:98:A:PHE:HD1	1:125:A:VAL:HG23	6	0.21
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	10	0.21
(1,564)	1:114:A:VAL:HB	1:115:A:ILE:H	18	0.21
(1,530)	1:106:A:TYR:HB3	1:111:A:TYR:HD2	13	0.21
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD11	15	0.21
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD12	15	0.21
(1,474)	1:98:A:PHE:HD2	1:100:A:ILE:HD13	15	0.21
(1,449)	1:32:A:THR:HB	1:95:A:LYS:HE2	1	0.21
(1,416)	1:87:A:VAL:HA	1:90:A:MET:HE1	2	0.21
(1,416)	1:87:A:VAL:HA	1:90:A:MET:HE2	2	0.21
(1,416)	1:87:A:VAL:HA	1:90:A:MET:HE3	2	0.21
(1,413)	1:90:A:MET:HE1	1:91:A:THR:H	3	0.21
(1,413)	1:90:A:MET:HE2	1:91:A:THR:H	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:90:A:MET:HE3	1:91:A:THR:H	3	0.21
(1,413)	1:90:A:MET:HE1	1:91:A:THR:H	14	0.21
(1,413)	1:90:A:MET:HE2	1:91:A:THR:H	14	0.21
(1,413)	1:90:A:MET:HE3	1:91:A:THR:H	14	0.21
(1,405)	1:85:A:GLN:HA	1:89:A:THR:HG21	17	0.21
(1,405)	1:85:A:GLN:HA	1:89:A:THR:HG22	17	0.21
(1,405)	1:85:A:GLN:HA	1:89:A:THR:HG23	17	0.21
(1,369)	1:83:A:TRP:H	1:84:A:ASP:HB2	13	0.21
(1,364)	1:80:A:ILE:HD11	1:83:A:TRP:HA	17	0.21
(1,364)	1:80:A:ILE:HD12	1:83:A:TRP:HA	17	0.21
(1,364)	1:80:A:ILE:HD13	1:83:A:TRP:HA	17	0.21
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD11	12	0.21
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD12	12	0.21
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD13	12	0.21
(1,289)	1:76:A:ALA:HB1	1:78:A:GLU:HB2	2	0.21
(1,289)	1:76:A:ALA:HB2	1:78:A:GLU:HB2	2	0.21
(1,289)	1:76:A:ALA:HB3	1:78:A:GLU:HB2	2	0.21
(1,179)	1:54:A:PHE:HB2	1:55:A:PRO:HD3	8	0.21
(1,166)	1:53:A:ARG:HG3	1:60:A:PHE:H	18	0.21
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	13	0.21
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	19	0.21
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG11	5	0.21
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG12	5	0.21
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG13	5	0.21
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG21	10	0.21
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG22	10	0.21
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG23	10	0.21
(1,64)	1:38:A:THR:HG21	1:39:A:LYS:H	3	0.21
(1,64)	1:38:A:THR:HG22	1:39:A:LYS:H	3	0.21
(1,64)	1:38:A:THR:HG23	1:39:A:LYS:H	3	0.21
(1,42)	1:33:A:PRO:HA	1:94:A:GLU:HG2	19	0.21
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB1	11	0.21
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB2	11	0.21
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB3	11	0.21
(1,16)	1:41:A:GLN:H	1:41:A:GLN:HB2	2	0.21
(1,1605)	1:98:A:PHE:HB2	1:100:A:ILE:H	19	0.2
(1,1605)	1:98:A:PHE:HB3	1:100:A:ILE:H	19	0.2
(1,1599)	1:97:A:LEU:HD11	1:124:A:GLU:HB3	18	0.2
(1,1599)	1:97:A:LEU:HD12	1:124:A:GLU:HB3	18	0.2
(1,1599)	1:97:A:LEU:HD13	1:124:A:GLU:HB3	18	0.2
(1,1599)	1:97:A:LEU:HD21	1:124:A:GLU:HB3	18	0.2
(1,1599)	1:97:A:LEU:HD22	1:124:A:GLU:HB3	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1599)	1:97:A:LEU:HD23	1:124:A:GLU:HB3	18	0.2
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	9	0.2
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	9	0.2
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	9	0.2
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	9	0.2
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	9	0.2
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	9	0.2
(1,1594)	1:97:A:LEU:HD11	1:123:A:PHE:H	9	0.2
(1,1594)	1:97:A:LEU:HD12	1:123:A:PHE:H	9	0.2
(1,1594)	1:97:A:LEU:HD13	1:123:A:PHE:H	9	0.2
(1,1594)	1:97:A:LEU:HD21	1:123:A:PHE:H	9	0.2
(1,1594)	1:97:A:LEU:HD22	1:123:A:PHE:H	9	0.2
(1,1594)	1:97:A:LEU:HD23	1:123:A:PHE:H	9	0.2
(1,1575)	1:92:A:LEU:HD11	1:130:A:VAL:H	16	0.2
(1,1575)	1:92:A:LEU:HD12	1:130:A:VAL:H	16	0.2
(1,1575)	1:92:A:LEU:HD13	1:130:A:VAL:H	16	0.2
(1,1575)	1:92:A:LEU:HD21	1:130:A:VAL:H	16	0.2
(1,1575)	1:92:A:LEU:HD22	1:130:A:VAL:H	16	0.2
(1,1575)	1:92:A:LEU:HD23	1:130:A:VAL:H	16	0.2
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	14	0.2
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	14	0.2
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	4	0.2
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	4	0.2
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	8	0.2
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	8	0.2
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	11	0.2
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	11	0.2
(1,1474)	1:59:A:GLN:HG2	1:60:A:PHE:H	20	0.2
(1,1474)	1:59:A:GLN:HG3	1:60:A:PHE:H	20	0.2
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD11	4	0.2
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD12	4	0.2
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD13	4	0.2
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD21	4	0.2
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD22	4	0.2
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD23	4	0.2
(1,1433)	1:51:A:ASP:HB2	1:124:A:GLU:HB3	19	0.2
(1,1433)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	19	0.2
(1,1425)	1:49:A:HIS:HB3	1:126:A:GLU:HB2	1	0.2
(1,1425)	1:49:A:HIS:HB3	1:126:A:GLU:HB3	1	0.2
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	15	0.2
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	15	0.2
(1,1386)	1:41:A:GLN:H	1:44:A:LYS:HG2	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1386)	1:41:A:GLN:H	1:44:A:LYS:HG3	20	0.2
(1,1384)	1:41:A:GLN:H	1:41:A:GLN:HB2	2	0.2
(1,1384)	1:41:A:GLN:H	1:41:A:GLN:HB3	2	0.2
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG11	7	0.2
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG12	7	0.2
(1,1381)	1:40:A:PRO:HB2	1:46:A:VAL:HG13	7	0.2
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG11	7	0.2
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG12	7	0.2
(1,1381)	1:40:A:PRO:HB3	1:46:A:VAL:HG13	7	0.2
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG11	4	0.2
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG12	4	0.2
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG13	4	0.2
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG21	4	0.2
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG22	4	0.2
(1,1377)	1:38:A:THR:HG21	1:130:A:VAL:HG23	4	0.2
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG11	4	0.2
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG12	4	0.2
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG13	4	0.2
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG21	4	0.2
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG22	4	0.2
(1,1377)	1:38:A:THR:HG22	1:130:A:VAL:HG23	4	0.2
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG11	4	0.2
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG12	4	0.2
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG13	4	0.2
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG21	4	0.2
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG22	4	0.2
(1,1377)	1:38:A:THR:HG23	1:130:A:VAL:HG23	4	0.2
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB2	14	0.2
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB3	14	0.2
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB2	15	0.2
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB3	15	0.2
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	1	0.2
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	14	0.2
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	14	0.2
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	14	0.2
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	7	0.2
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	7	0.2
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	7	0.2
(1,1219)	1:111:A:TYR:H	1:115:A:ILE:HB	6	0.2
(1,1193)	1:105:A:ALA:H	1:107:A:GLY:H	8	0.2
(1,1184)	1:103:A:GLN:H	1:104:A:LEU:HB2	4	0.2
(1,1179)	1:102:A:TYR:HE1	1:103:A:GLN:H	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB1	4	0.2
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB2	4	0.2
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB3	4	0.2
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD11	8	0.2
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD12	8	0.2
(1,1157)	1:98:A:PHE:H	1:100:A:ILE:HD13	8	0.2
(1,1116)	1:92:A:LEU:HD11	1:93:A:GLY:H	6	0.2
(1,1116)	1:92:A:LEU:HD12	1:93:A:GLY:H	6	0.2
(1,1116)	1:92:A:LEU:HD13	1:93:A:GLY:H	6	0.2
(1,1111)	1:38:A:THR:HG21	1:92:A:LEU:H	9	0.2
(1,1111)	1:38:A:THR:HG22	1:92:A:LEU:H	9	0.2
(1,1111)	1:38:A:THR:HG23	1:92:A:LEU:H	9	0.2
(1,1104)	1:91:A:THR:H	1:127:A:LEU:HG	9	0.2
(1,1097)	1:34:A:GLY:HA3	1:91:A:THR:H	2	0.2
(1,1069)	1:86:A:GLY:H	1:98:A:PHE:HD2	19	0.2
(1,1065)	1:79:A:VAL:HG21	1:85:A:GLN:H	16	0.2
(1,1065)	1:79:A:VAL:HG22	1:85:A:GLN:H	16	0.2
(1,1065)	1:79:A:VAL:HG23	1:85:A:GLN:H	16	0.2
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	8	0.2
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	8	0.2
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	8	0.2
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG11	19	0.2
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG12	19	0.2
(1,986)	1:73:A:THR:H	1:79:A:VAL:HG13	19	0.2
(1,935)	1:64:A:ARG:H	1:64:A:ARG:HD2	10	0.2
(1,896)	1:59:A:GLN:HE21	1:62:A:SER:HB2	1	0.2
(1,866)	1:51:A:ASP:H	1:124:A:GLU:HB3	18	0.2
(1,862)	1:50:A:TYR:HB3	1:51:A:ASP:H	17	0.2
(1,830)	1:46:A:VAL:H	1:72:A:PHE:HA	2	0.2
(1,830)	1:46:A:VAL:H	1:72:A:PHE:HA	10	0.2
(1,820)	1:44:A:LYS:H	1:44:A:LYS:HG3	14	0.2
(1,806)	1:42:A:ALA:H	1:74:A:LEU:HG	5	0.2
(1,799)	1:40:A:PRO:HB2	1:41:A:GLN:H	6	0.2
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG21	19	0.2
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG22	19	0.2
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG23	19	0.2
(1,789)	1:38:A:THR:H	1:91:A:THR:HG21	19	0.2
(1,789)	1:38:A:THR:H	1:91:A:THR:HG22	19	0.2
(1,789)	1:38:A:THR:H	1:91:A:THR:HG23	19	0.2
(1,781)	1:37:A:VAL:H	1:91:A:THR:HB	17	0.2
(1,747)	1:27:A:GLU:H	1:98:A:PHE:HA	7	0.2
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG21	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG22	20	0.2
(1,728)	1:35:A:ASP:H	1:38:A:THR:HG23	20	0.2
(1,702)	1:80:A:ILE:HG21	1:83:A:TRP:HE3	14	0.2
(1,702)	1:80:A:ILE:HG22	1:83:A:TRP:HE3	14	0.2
(1,702)	1:80:A:ILE:HG23	1:83:A:TRP:HE3	14	0.2
(1,684)	1:48:A:VAL:HG21	1:50:A:TYR:HE1	2	0.2
(1,684)	1:48:A:VAL:HG22	1:50:A:TYR:HE1	2	0.2
(1,684)	1:48:A:VAL:HG23	1:50:A:TYR:HE1	2	0.2
(1,661)	1:72:A:PHE:HB3	1:79:A:VAL:HG11	8	0.2
(1,661)	1:72:A:PHE:HB3	1:79:A:VAL:HG12	8	0.2
(1,661)	1:72:A:PHE:HB3	1:79:A:VAL:HG13	8	0.2
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	15	0.2
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	15	0.2
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	15	0.2
(1,624)	1:49:A:HIS:HB3	1:126:A:GLU:HB3	1	0.2
(1,602)	1:100:A:ILE:HD11	1:123:A:PHE:HB3	8	0.2
(1,602)	1:100:A:ILE:HD12	1:123:A:PHE:HB3	8	0.2
(1,602)	1:100:A:ILE:HD13	1:123:A:PHE:HB3	8	0.2
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	4	0.2
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	17	0.2
(1,557)	1:110:A:GLY:HA3	1:115:A:ILE:HB	20	0.2
(1,554)	1:106:A:TYR:HB2	1:110:A:GLY:HA2	15	0.2
(1,537)	1:108:A:GLU:HB2	1:118:A:LYS:HG2	9	0.2
(1,528)	1:80:A:ILE:HG21	1:106:A:TYR:HA	1	0.2
(1,528)	1:80:A:ILE:HG22	1:106:A:TYR:HA	1	0.2
(1,528)	1:80:A:ILE:HG23	1:106:A:TYR:HA	1	0.2
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	17	0.2
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	17	0.2
(1,507)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	17	0.2
(1,443)	1:32:A:THR:HG21	1:95:A:LYS:HB3	8	0.2
(1,443)	1:32:A:THR:HG22	1:95:A:LYS:HB3	8	0.2
(1,443)	1:32:A:THR:HG23	1:95:A:LYS:HB3	8	0.2
(1,425)	1:92:A:LEU:HG	1:93:A:GLY:H	15	0.2
(1,418)	1:90:A:MET:HE1	1:96:A:ALA:HB1	4	0.2
(1,418)	1:90:A:MET:HE1	1:96:A:ALA:HB2	4	0.2
(1,418)	1:90:A:MET:HE1	1:96:A:ALA:HB3	4	0.2
(1,418)	1:90:A:MET:HE2	1:96:A:ALA:HB1	4	0.2
(1,418)	1:90:A:MET:HE2	1:96:A:ALA:HB2	4	0.2
(1,418)	1:90:A:MET:HE2	1:96:A:ALA:HB3	4	0.2
(1,418)	1:90:A:MET:HE3	1:96:A:ALA:HB1	4	0.2
(1,418)	1:90:A:MET:HE3	1:96:A:ALA:HB2	4	0.2
(1,418)	1:90:A:MET:HE3	1:96:A:ALA:HB3	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	1:86:A:GLY:HA2	1:98:A:PHE:HD2	1	0.2
(1,375)	1:74:A:LEU:HD11	1:84:A:ASP:HB3	8	0.2
(1,375)	1:74:A:LEU:HD12	1:84:A:ASP:HB3	8	0.2
(1,375)	1:74:A:LEU:HD13	1:84:A:ASP:HB3	8	0.2
(1,369)	1:83:A:TRP:H	1:84:A:ASP:HB2	5	0.2
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG21	11	0.2
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG22	11	0.2
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG23	11	0.2
(1,266)	1:74:A:LEU:HD21	1:75:A:GLY:H	7	0.2
(1,266)	1:74:A:LEU:HD22	1:75:A:GLY:H	7	0.2
(1,266)	1:74:A:LEU:HD23	1:75:A:GLY:H	7	0.2
(1,229)	1:69:A:PRO:HA	1:128:A:LEU:HG	15	0.2
(1,197)	1:59:A:GLN:HG2	1:60:A:PHE:H	10	0.2
(1,193)	1:53:A:ARG:HB3	1:59:A:GLN:HA	9	0.2
(1,179)	1:54:A:PHE:HB2	1:55:A:PRO:HD3	18	0.2
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	9	0.2
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	8	0.2
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	8	0.2
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	8	0.2
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	14	0.2
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	14	0.2
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	14	0.2
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	17	0.2
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	17	0.2
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	17	0.2
(1,121)	1:46:A:VAL:HG11	1:130:A:VAL:H	14	0.2
(1,121)	1:46:A:VAL:HG12	1:130:A:VAL:H	14	0.2
(1,121)	1:46:A:VAL:HG13	1:130:A:VAL:H	14	0.2
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	4	0.2
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	4	0.2
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	4	0.2
(1,103)	1:45:A:LYS:HG2	1:46:A:VAL:H	7	0.2
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG21	8	0.2
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG22	8	0.2
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG23	8	0.2
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG21	17	0.2
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG22	17	0.2
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG23	17	0.2
(1,81)	1:42:A:ALA:HA	1:74:A:LEU:H	3	0.2
(1,28)	1:27:A:GLU:HG2	1:99:A:THR:HB	8	0.2
(1,26)	1:27:A:GLU:HG3	1:99:A:THR:H	20	0.2
(1,2)	1:28:A:LYS:HB2	1:30:A:VAL:H	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1629)	1:109:A:ARG:HA	1:117:A:PRO:HB2	17	0.19
(1,1629)	1:109:A:ARG:HA	1:117:A:PRO:HB3	17	0.19
(1,1613)	1:102:A:TYR:HE2	1:118:A:LYS:HB2	2	0.19
(1,1613)	1:102:A:TYR:HE2	1:118:A:LYS:HB3	2	0.19
(1,1601)	1:97:A:LEU:HD11	1:124:A:GLU:HG3	3	0.19
(1,1601)	1:97:A:LEU:HD12	1:124:A:GLU:HG3	3	0.19
(1,1601)	1:97:A:LEU:HD13	1:124:A:GLU:HG3	3	0.19
(1,1601)	1:97:A:LEU:HD21	1:124:A:GLU:HG3	3	0.19
(1,1601)	1:97:A:LEU:HD22	1:124:A:GLU:HG3	3	0.19
(1,1601)	1:97:A:LEU:HD23	1:124:A:GLU:HG3	3	0.19
(1,1575)	1:92:A:LEU:HD11	1:130:A:VAL:H	1	0.19
(1,1575)	1:92:A:LEU:HD12	1:130:A:VAL:H	1	0.19
(1,1575)	1:92:A:LEU:HD13	1:130:A:VAL:H	1	0.19
(1,1575)	1:92:A:LEU:HD21	1:130:A:VAL:H	1	0.19
(1,1575)	1:92:A:LEU:HD22	1:130:A:VAL:H	1	0.19
(1,1575)	1:92:A:LEU:HD23	1:130:A:VAL:H	1	0.19
(1,1543)	1:85:A:GLN:HB2	1:98:A:PHE:HD2	13	0.19
(1,1543)	1:85:A:GLN:HB3	1:98:A:PHE:HD2	13	0.19
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE21	7	0.19
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	7	0.19
(1,1505)	1:66:A:ARG:HG2	1:68:A:LYS:H	8	0.19
(1,1505)	1:66:A:ARG:HG3	1:68:A:LYS:H	8	0.19
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD11	9	0.19
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD12	9	0.19
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD13	9	0.19
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD21	9	0.19
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD22	9	0.19
(1,1434)	1:53:A:ARG:HB2	1:97:A:LEU:HD23	9	0.19
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	19	0.19
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	19	0.19
(1,1384)	1:41:A:GLN:H	1:41:A:GLN:HB2	5	0.19
(1,1384)	1:41:A:GLN:H	1:41:A:GLN:HB3	5	0.19
(1,1380)	1:40:A:PRO:HB2	1:41:A:GLN:H	12	0.19
(1,1380)	1:40:A:PRO:HB3	1:41:A:GLN:H	12	0.19
(1,1346)	1:28:A:LYS:HG2	1:30:A:VAL:H	5	0.19
(1,1346)	1:28:A:LYS:HG3	1:30:A:VAL:H	5	0.19
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB2	1	0.19
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB3	1	0.19
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG2	18	0.19
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG3	18	0.19
(1,1311)	1:81:A:LYS:HE3	1:85:A:GLN:HE22	11	0.19
(1,1301)	1:71:A:GLN:HA	1:71:A:GLN:HE21	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD21	7	0.19
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD22	7	0.19
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD23	7	0.19
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	2	0.19
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	16	0.19
(1,1235)	1:55:A:PRO:HG3	1:120:A:THR:H	17	0.19
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG21	16	0.19
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG22	16	0.19
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG23	16	0.19
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB1	19	0.19
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB2	19	0.19
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB3	19	0.19
(1,1162)	1:27:A:GLU:HB2	1:99:A:THR:H	1	0.19
(1,1116)	1:92:A:LEU:HD11	1:93:A:GLY:H	7	0.19
(1,1116)	1:92:A:LEU:HD12	1:93:A:GLY:H	7	0.19
(1,1116)	1:92:A:LEU:HD13	1:93:A:GLY:H	7	0.19
(1,1113)	1:91:A:THR:HG21	1:92:A:LEU:H	5	0.19
(1,1113)	1:91:A:THR:HG22	1:92:A:LEU:H	5	0.19
(1,1113)	1:91:A:THR:HG23	1:92:A:LEU:H	5	0.19
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	4	0.19
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	4	0.19
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	4	0.19
(1,1050)	1:80:A:ILE:HG12	1:84:A:ASP:H	15	0.19
(1,1037)	1:80:A:ILE:HG12	1:83:A:TRP:H	9	0.19
(1,1023)	1:81:A:LYS:H	1:81:A:LYS:HG3	8	0.19
(1,1015)	1:77:A:GLY:H	1:79:A:VAL:H	16	0.19
(1,1003)	1:74:A:LEU:HB3	1:76:A:ALA:H	17	0.19
(1,983)	1:73:A:THR:H	1:78:A:GLU:HB2	13	0.19
(1,977)	1:47:A:THR:HG21	1:71:A:GLN:H	16	0.19
(1,977)	1:47:A:THR:HG22	1:71:A:GLN:H	16	0.19
(1,977)	1:47:A:THR:HG23	1:71:A:GLN:H	16	0.19
(1,968)	1:47:A:THR:HG21	1:70:A:PHE:H	1	0.19
(1,968)	1:47:A:THR:HG22	1:70:A:PHE:H	1	0.19
(1,968)	1:47:A:THR:HG23	1:70:A:PHE:H	1	0.19
(1,863)	1:50:A:TYR:HB2	1:51:A:ASP:H	8	0.19
(1,862)	1:50:A:TYR:HB3	1:51:A:ASP:H	20	0.19
(1,830)	1:46:A:VAL:H	1:72:A:PHE:HA	15	0.19
(1,828)	1:46:A:VAL:H	1:71:A:GLN:HA	2	0.19
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	6	0.19
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	9	0.19
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	12	0.19
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,781)	1:37:A:VAL:H	1:91:A:THR:HB	13	0.19
(1,745)	1:27:A:GLU:H	1:99:A:THR:H	6	0.19
(1,740)	1:24:A:ALA:HB1	1:25:A:GLN:H	2	0.19
(1,740)	1:24:A:ALA:HB2	1:25:A:GLN:H	2	0.19
(1,740)	1:24:A:ALA:HB3	1:25:A:GLN:H	2	0.19
(1,676)	1:106:A:TYR:HE2	1:121:A:LEU:HG	16	0.19
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG21	1	0.19
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG22	1	0.19
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG23	1	0.19
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG11	3	0.19
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG12	3	0.19
(1,659)	1:50:A:TYR:HD1	1:79:A:VAL:HG13	3	0.19
(1,579)	1:102:A:TYR:HB2	1:119:A:ALA:HB1	10	0.19
(1,579)	1:102:A:TYR:HB2	1:119:A:ALA:HB2	10	0.19
(1,579)	1:102:A:TYR:HB2	1:119:A:ALA:HB3	10	0.19
(1,564)	1:114:A:VAL:HB	1:115:A:ILE:H	14	0.19
(1,547)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	11	0.19
(1,541)	1:108:A:GLU:HA	1:118:A:LYS:HA	17	0.19
(1,518)	1:80:A:ILE:HA	1:105:A:ALA:HA	4	0.19
(1,468)	1:27:A:GLU:H	1:99:A:THR:HG21	6	0.19
(1,468)	1:27:A:GLU:H	1:99:A:THR:HG22	6	0.19
(1,468)	1:27:A:GLU:H	1:99:A:THR:HG23	6	0.19
(1,460)	1:97:A:LEU:HD11	1:98:A:PHE:H	1	0.19
(1,460)	1:97:A:LEU:HD12	1:98:A:PHE:H	1	0.19
(1,460)	1:97:A:LEU:HD13	1:98:A:PHE:H	1	0.19
(1,459)	1:97:A:LEU:HG	1:99:A:THR:H	5	0.19
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB1	18	0.19
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB2	18	0.19
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB3	18	0.19
(1,416)	1:87:A:VAL:HA	1:90:A:MET:HE1	11	0.19
(1,416)	1:87:A:VAL:HA	1:90:A:MET:HE2	11	0.19
(1,416)	1:87:A:VAL:HA	1:90:A:MET:HE3	11	0.19
(1,375)	1:74:A:LEU:HD11	1:84:A:ASP:HB3	18	0.19
(1,375)	1:74:A:LEU:HD12	1:84:A:ASP:HB3	18	0.19
(1,375)	1:74:A:LEU:HD13	1:84:A:ASP:HB3	18	0.19
(1,369)	1:83:A:TRP:H	1:84:A:ASP:HB2	20	0.19
(1,355)	1:81:A:LYS:HB3	1:82:A:GLY:HA2	3	0.19
(1,316)	1:80:A:ILE:HB	1:104:A:LEU:HB3	5	0.19
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG21	12	0.19
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG22	12	0.19
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG23	12	0.19
(1,220)	1:66:A:ARG:HA	1:66:A:ARG:HD2	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,208)	1:63:A:SER:H	1:64:A:ARG:HA	20	0.19
(1,183)	1:53:A:ARG:HD2	1:57:A:GLY:HA2	4	0.19
(1,172)	1:53:A:ARG:HD3	1:59:A:GLN:H	8	0.19
(1,163)	1:53:A:ARG:HG3	1:59:A:GLN:H	19	0.19
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	1	0.19
(1,154)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	19	0.19
(1,147)	1:50:A:TYR:HA	1:124:A:GLU:HB3	12	0.19
(1,146)	1:49:A:HIS:HD2	1:50:A:TYR:HA	1	0.19
(1,123)	1:46:A:VAL:HG11	1:130:A:VAL:HB	5	0.19
(1,123)	1:46:A:VAL:HG12	1:130:A:VAL:HB	5	0.19
(1,123)	1:46:A:VAL:HG13	1:130:A:VAL:HB	5	0.19
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG21	19	0.19
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG22	19	0.19
(1,74)	1:40:A:PRO:HB2	1:46:A:VAL:HG23	19	0.19
(1,68)	1:38:A:THR:HG21	1:92:A:LEU:HA	19	0.19
(1,68)	1:38:A:THR:HG22	1:92:A:LEU:HA	19	0.19
(1,68)	1:38:A:THR:HG23	1:92:A:LEU:HA	19	0.19
(1,64)	1:38:A:THR:HG21	1:39:A:LYS:H	2	0.19
(1,64)	1:38:A:THR:HG22	1:39:A:LYS:H	2	0.19
(1,64)	1:38:A:THR:HG23	1:39:A:LYS:H	2	0.19
(1,29)	1:27:A:GLU:H	1:27:A:GLU:HG2	16	0.19
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB1	9	0.19
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB2	9	0.19
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB3	9	0.19
(1,16)	1:41:A:GLN:H	1:41:A:GLN:HB2	18	0.19
(1,1647)	1:121:A:LEU:HD11	1:122:A:VAL:H	15	0.18
(1,1647)	1:121:A:LEU:HD12	1:122:A:VAL:H	15	0.18
(1,1647)	1:121:A:LEU:HD13	1:122:A:VAL:H	15	0.18
(1,1647)	1:121:A:LEU:HD21	1:122:A:VAL:H	15	0.18
(1,1647)	1:121:A:LEU:HD22	1:122:A:VAL:H	15	0.18
(1,1647)	1:121:A:LEU:HD23	1:122:A:VAL:H	15	0.18
(1,1627)	1:109:A:ARG:HA	1:109:A:ARG:HG2	17	0.18
(1,1627)	1:109:A:ARG:HA	1:109:A:ARG:HG3	17	0.18
(1,1627)	1:109:A:ARG:HA	1:109:A:ARG:HG2	19	0.18
(1,1627)	1:109:A:ARG:HA	1:109:A:ARG:HG3	19	0.18
(1,1595)	1:97:A:LEU:HD11	1:123:A:PHE:HA	14	0.18
(1,1595)	1:97:A:LEU:HD12	1:123:A:PHE:HA	14	0.18
(1,1595)	1:97:A:LEU:HD13	1:123:A:PHE:HA	14	0.18
(1,1595)	1:97:A:LEU:HD21	1:123:A:PHE:HA	14	0.18
(1,1595)	1:97:A:LEU:HD22	1:123:A:PHE:HA	14	0.18
(1,1595)	1:97:A:LEU:HD23	1:123:A:PHE:HA	14	0.18
(1,1550)	1:86:A:GLY:HA2	1:98:A:PHE:HD2	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1550)	1:86:A:GLY:HA3	1:98:A:PHE:HD2	17	0.18
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE21	11	0.18
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	11	0.18
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	17	0.18
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	17	0.18
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	17	0.18
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	17	0.18
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	17	0.18
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	17	0.18
(1,1506)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	8	0.18
(1,1506)	1:67:A:GLY:HA3	1:68:A:LYS:HB2	8	0.18
(1,1506)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	12	0.18
(1,1506)	1:67:A:GLY:HA3	1:68:A:LYS:HB2	12	0.18
(1,1506)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	18	0.18
(1,1506)	1:67:A:GLY:HA3	1:68:A:LYS:HB2	18	0.18
(1,1505)	1:66:A:ARG:HG2	1:68:A:LYS:H	18	0.18
(1,1505)	1:66:A:ARG:HG3	1:68:A:LYS:H	18	0.18
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	14	0.18
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	14	0.18
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	17	0.18
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	17	0.18
(1,1474)	1:59:A:GLN:HG2	1:60:A:PHE:H	4	0.18
(1,1474)	1:59:A:GLN:HG3	1:60:A:PHE:H	4	0.18
(1,1461)	1:55:A:PRO:HD2	1:120:A:THR:HG21	10	0.18
(1,1461)	1:55:A:PRO:HD2	1:120:A:THR:HG22	10	0.18
(1,1461)	1:55:A:PRO:HD2	1:120:A:THR:HG23	10	0.18
(1,1461)	1:55:A:PRO:HD3	1:120:A:THR:HG21	10	0.18
(1,1461)	1:55:A:PRO:HD3	1:120:A:THR:HG22	10	0.18
(1,1461)	1:55:A:PRO:HD3	1:120:A:THR:HG23	10	0.18
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	18	0.18
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	18	0.18
(1,1355)	1:30:A:VAL:HG11	1:33:A:PRO:HB3	19	0.18
(1,1355)	1:30:A:VAL:HG12	1:33:A:PRO:HB3	19	0.18
(1,1355)	1:30:A:VAL:HG13	1:33:A:PRO:HB3	19	0.18
(1,1355)	1:30:A:VAL:HG21	1:33:A:PRO:HB3	19	0.18
(1,1355)	1:30:A:VAL:HG22	1:33:A:PRO:HB3	19	0.18
(1,1355)	1:30:A:VAL:HG23	1:33:A:PRO:HB3	19	0.18
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD2	12	0.18
(1,1326)	1:19:A:PRO:HG2	1:55:A:PRO:HD3	12	0.18
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD2	12	0.18
(1,1326)	1:19:A:PRO:HG3	1:55:A:PRO:HD3	12	0.18
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	8	0.18
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	8	0.18
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD21	4	0.18
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD22	4	0.18
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD23	4	0.18
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	5	0.18
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	14	0.18
(1,1204)	1:100:A:ILE:HG21	1:106:A:TYR:H	4	0.18
(1,1204)	1:100:A:ILE:HG22	1:106:A:TYR:H	4	0.18
(1,1204)	1:100:A:ILE:HG23	1:106:A:TYR:H	4	0.18
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	10	0.18
(1,1172)	1:102:A:TYR:H	1:105:A:ALA:H	2	0.18
(1,1172)	1:102:A:TYR:H	1:105:A:ALA:H	9	0.18
(1,1120)	1:34:A:GLY:HA2	1:94:A:GLU:H	7	0.18
(1,1093)	1:87:A:VAL:HG11	1:90:A:MET:H	20	0.18
(1,1093)	1:87:A:VAL:HG12	1:90:A:MET:H	20	0.18
(1,1093)	1:87:A:VAL:HG13	1:90:A:MET:H	20	0.18
(1,1041)	1:80:A:ILE:HG21	1:83:A:TRP:H	6	0.18
(1,1041)	1:80:A:ILE:HG22	1:83:A:TRP:H	6	0.18
(1,1041)	1:80:A:ILE:HG23	1:83:A:TRP:H	6	0.18
(1,1041)	1:80:A:ILE:HG21	1:83:A:TRP:H	8	0.18
(1,1041)	1:80:A:ILE:HG22	1:83:A:TRP:H	8	0.18
(1,1041)	1:80:A:ILE:HG23	1:83:A:TRP:H	8	0.18
(1,1029)	1:82:A:GLY:H	1:104:A:LEU:HB3	13	0.18
(1,1025)	1:82:A:GLY:H	1:104:A:LEU:HA	13	0.18
(1,950)	1:64:A:ARG:HA	1:67:A:GLY:H	7	0.18
(1,911)	1:53:A:ARG:HD2	1:57:A:GLY:H	8	0.18
(1,895)	1:58:A:LYS:H	1:59:A:GLN:H	3	0.18
(1,887)	1:53:A:ARG:HB3	1:54:A:PHE:H	4	0.18
(1,887)	1:53:A:ARG:HB3	1:54:A:PHE:H	10	0.18
(1,863)	1:50:A:TYR:HB2	1:51:A:ASP:H	18	0.18
(1,828)	1:46:A:VAL:H	1:71:A:GLN:HA	14	0.18
(1,812)	1:43:A:GLY:H	1:44:A:LYS:HB2	4	0.18
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	1	0.18
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	5	0.18
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	11	0.18
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	13	0.18
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	14	0.18
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	15	0.18
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD21	10	0.18
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD22	10	0.18
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD23	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,789)	1:38:A:THR:H	1:91:A:THR:HG21	8	0.18
(1,789)	1:38:A:THR:H	1:91:A:THR:HG22	8	0.18
(1,789)	1:38:A:THR:H	1:91:A:THR:HG23	8	0.18
(1,787)	1:37:A:VAL:HB	1:38:A:THR:H	3	0.18
(1,781)	1:37:A:VAL:H	1:91:A:THR:HB	3	0.18
(1,709)	1:11:A:THR:HG21	1:12:A:LEU:H	19	0.18
(1,709)	1:11:A:THR:HG22	1:12:A:LEU:H	19	0.18
(1,709)	1:11:A:THR:HG23	1:12:A:LEU:H	19	0.18
(1,702)	1:80:A:ILE:HG21	1:83:A:TRP:HE3	10	0.18
(1,702)	1:80:A:ILE:HG22	1:83:A:TRP:HE3	10	0.18
(1,702)	1:80:A:ILE:HG23	1:83:A:TRP:HE3	10	0.18
(1,679)	1:50:A:TYR:HB2	1:50:A:TYR:HD2	17	0.18
(1,660)	1:72:A:PHE:HB2	1:79:A:VAL:HG11	13	0.18
(1,660)	1:72:A:PHE:HB2	1:79:A:VAL:HG12	13	0.18
(1,660)	1:72:A:PHE:HB2	1:79:A:VAL:HG13	13	0.18
(1,654)	1:47:A:THR:H	1:130:A:VAL:HG11	5	0.18
(1,654)	1:47:A:THR:H	1:130:A:VAL:HG12	5	0.18
(1,654)	1:47:A:THR:H	1:130:A:VAL:HG13	5	0.18
(1,638)	1:127:A:LEU:HD11	1:129:A:ALA:HB1	7	0.18
(1,638)	1:127:A:LEU:HD11	1:129:A:ALA:HB2	7	0.18
(1,638)	1:127:A:LEU:HD11	1:129:A:ALA:HB3	7	0.18
(1,638)	1:127:A:LEU:HD12	1:129:A:ALA:HB1	7	0.18
(1,638)	1:127:A:LEU:HD12	1:129:A:ALA:HB2	7	0.18
(1,638)	1:127:A:LEU:HD12	1:129:A:ALA:HB3	7	0.18
(1,638)	1:127:A:LEU:HD13	1:129:A:ALA:HB1	7	0.18
(1,638)	1:127:A:LEU:HD13	1:129:A:ALA:HB2	7	0.18
(1,638)	1:127:A:LEU:HD13	1:129:A:ALA:HB3	7	0.18
(1,632)	1:93:A:GLY:H	1:127:A:LEU:HG	7	0.18
(1,629)	1:92:A:LEU:HA	1:127:A:LEU:HG	3	0.18
(1,616)	1:50:A:TYR:HA	1:125:A:VAL:HG11	6	0.18
(1,616)	1:50:A:TYR:HA	1:125:A:VAL:HG12	6	0.18
(1,616)	1:50:A:TYR:HA	1:125:A:VAL:HG13	6	0.18
(1,606)	1:123:A:PHE:HA	1:124:A:GLU:HB2	9	0.18
(1,603)	1:123:A:PHE:H	1:124:A:GLU:HA	14	0.18
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	3	0.18
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	6	0.18
(1,578)	1:119:A:ALA:HB1	1:120:A:THR:HB	19	0.18
(1,578)	1:119:A:ALA:HB2	1:120:A:THR:HB	19	0.18
(1,578)	1:119:A:ALA:HB3	1:120:A:THR:HB	19	0.18
(1,571)	1:117:A:PRO:HA	1:118:A:LYS:HG3	4	0.18
(1,544)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	18	0.18
(1,543)	1:108:A:GLU:HA	1:118:A:LYS:HG2	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,539)	1:102:A:TYR:HE2	1:108:A:GLU:HA	13	0.18
(1,498)	1:103:A:GLN:HA	1:104:A:LEU:HG	13	0.18
(1,460)	1:97:A:LEU:HD11	1:98:A:PHE:H	12	0.18
(1,460)	1:97:A:LEU:HD12	1:98:A:PHE:H	12	0.18
(1,460)	1:97:A:LEU:HD13	1:98:A:PHE:H	12	0.18
(1,449)	1:32:A:THR:HB	1:95:A:LYS:HE2	8	0.18
(1,444)	1:31:A:LEU:HG	1:95:A:LYS:HB3	13	0.18
(1,430)	1:92:A:LEU:HD21	1:129:A:ALA:HA	17	0.18
(1,430)	1:92:A:LEU:HD22	1:129:A:ALA:HA	17	0.18
(1,430)	1:92:A:LEU:HD23	1:129:A:ALA:HA	17	0.18
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD21	3	0.18
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD22	3	0.18
(1,339)	1:81:A:LYS:HB2	1:104:A:LEU:HD23	3	0.18
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	4	0.18
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD11	10	0.18
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD12	10	0.18
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD13	10	0.18
(1,198)	1:59:A:GLN:HG2	1:61:A:ASP:H	19	0.18
(1,185)	1:53:A:ARG:HB3	1:57:A:GLY:HA2	7	0.18
(1,183)	1:53:A:ARG:HD2	1:57:A:GLY:HA2	19	0.18
(1,160)	1:53:A:ARG:HB2	1:59:A:GLN:HA	4	0.18
(1,146)	1:49:A:HIS:HD2	1:50:A:TYR:HA	11	0.18
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	18	0.18
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	18	0.18
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	18	0.18
(1,127)	1:47:A:THR:HB	1:48:A:VAL:HA	3	0.18
(1,127)	1:47:A:THR:HB	1:48:A:VAL:HA	19	0.18
(1,107)	1:46:A:VAL:HA	1:129:A:ALA:HB1	3	0.18
(1,107)	1:46:A:VAL:HA	1:129:A:ALA:HB2	3	0.18
(1,107)	1:46:A:VAL:HA	1:129:A:ALA:HB3	3	0.18
(1,105)	1:45:A:LYS:H	1:45:A:LYS:HE2	20	0.18
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	4	0.18
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	4	0.18
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	4	0.18
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB1	14	0.18
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB2	14	0.18
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB3	14	0.18
(1,16)	1:41:A:GLN:H	1:41:A:GLN:HB2	17	0.18
(1,8)	1:23:A:SER:HA	1:24:A:ALA:HB1	12	0.18
(1,8)	1:23:A:SER:HA	1:24:A:ALA:HB2	12	0.18
(1,8)	1:23:A:SER:HA	1:24:A:ALA:HB3	12	0.18
(1,1647)	1:121:A:LEU:HD11	1:122:A:VAL:H	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1647)	1:121:A:LEU:HD12	1:122:A:VAL:H	20	0.17
(1,1647)	1:121:A:LEU:HD13	1:122:A:VAL:H	20	0.17
(1,1647)	1:121:A:LEU:HD21	1:122:A:VAL:H	20	0.17
(1,1647)	1:121:A:LEU:HD22	1:122:A:VAL:H	20	0.17
(1,1647)	1:121:A:LEU:HD23	1:122:A:VAL:H	20	0.17
(1,1613)	1:102:A:TYR:HE2	1:118:A:LYS:HB2	14	0.17
(1,1613)	1:102:A:TYR:HE2	1:118:A:LYS:HB3	14	0.17
(1,1605)	1:98:A:PHE:HB2	1:100:A:ILE:H	11	0.17
(1,1605)	1:98:A:PHE:HB3	1:100:A:ILE:H	11	0.17
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	11	0.17
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	11	0.17
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	11	0.17
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	11	0.17
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	11	0.17
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	11	0.17
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	11	0.17
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	11	0.17
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	11	0.17
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	11	0.17
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	11	0.17
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	11	0.17
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG11	18	0.17
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG12	18	0.17
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG13	18	0.17
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG21	18	0.17
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG22	18	0.17
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG23	18	0.17
(1,1525)	1:78:A:GLU:HG2	1:79:A:VAL:HG11	11	0.17
(1,1525)	1:78:A:GLU:HG2	1:79:A:VAL:HG12	11	0.17
(1,1525)	1:78:A:GLU:HG2	1:79:A:VAL:HG13	11	0.17
(1,1525)	1:78:A:GLU:HG3	1:79:A:VAL:HG11	11	0.17
(1,1525)	1:78:A:GLU:HG3	1:79:A:VAL:HG12	11	0.17
(1,1525)	1:78:A:GLU:HG3	1:79:A:VAL:HG13	11	0.17
(1,1511)	1:70:A:PHE:HB2	1:71:A:GLN:H	17	0.17
(1,1511)	1:70:A:PHE:HB3	1:71:A:GLN:H	17	0.17
(1,1506)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	4	0.17
(1,1506)	1:67:A:GLY:HA3	1:68:A:LYS:HB2	4	0.17
(1,1490)	1:64:A:ARG:H	1:64:A:ARG:HD2	18	0.17
(1,1490)	1:64:A:ARG:H	1:64:A:ARG:HD3	18	0.17
(1,1475)	1:59:A:GLN:HG2	1:61:A:ASP:H	15	0.17
(1,1475)	1:59:A:GLN:HG3	1:61:A:ASP:H	15	0.17
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	19	0.17
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	19	0.17
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	19	0.17
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	19	0.17
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	19	0.17
(1,1425)	1:49:A:HIS:HB3	1:126:A:GLU:HB2	18	0.17
(1,1425)	1:49:A:HIS:HB3	1:126:A:GLU:HB3	18	0.17
(1,1384)	1:41:A:GLN:H	1:41:A:GLN:HB2	7	0.17
(1,1384)	1:41:A:GLN:H	1:41:A:GLN:HB3	7	0.17
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB2	2	0.17
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB3	2	0.17
(1,1309)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	4	0.17
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	10	0.17
(1,1301)	1:71:A:GLN:HA	1:71:A:GLN:HE21	7	0.17
(1,1301)	1:71:A:GLN:HA	1:71:A:GLN:HE21	19	0.17
(1,1298)	1:92:A:LEU:HG	1:130:A:VAL:H	10	0.17
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	10	0.17
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	10	0.17
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	10	0.17
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	12	0.17
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	12	0.17
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	12	0.17
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD21	1	0.17
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD22	1	0.17
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD23	1	0.17
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	4	0.17
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	15	0.17
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	18	0.17
(1,1236)	1:119:A:ALA:HB1	1:120:A:THR:H	13	0.17
(1,1236)	1:119:A:ALA:HB2	1:120:A:THR:H	13	0.17
(1,1236)	1:119:A:ALA:HB3	1:120:A:THR:H	13	0.17
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG21	3	0.17
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG22	3	0.17
(1,1220)	1:111:A:TYR:H	1:115:A:ILE:HG23	3	0.17
(1,1204)	1:100:A:ILE:HG21	1:106:A:TYR:H	13	0.17
(1,1204)	1:100:A:ILE:HG22	1:106:A:TYR:H	13	0.17
(1,1204)	1:100:A:ILE:HG23	1:106:A:TYR:H	13	0.17
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	15	0.17
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	18	0.17
(1,1193)	1:105:A:ALA:H	1:107:A:GLY:H	5	0.17
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	19	0.17
(1,1118)	1:34:A:GLY:H	1:94:A:GLU:H	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1093)	1:87:A:VAL:HG11	1:90:A:MET:H	18	0.17
(1,1093)	1:87:A:VAL:HG12	1:90:A:MET:H	18	0.17
(1,1093)	1:87:A:VAL:HG13	1:90:A:MET:H	18	0.17
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	19	0.17
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	19	0.17
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	19	0.17
(1,1005)	1:77:A:GLY:H	1:78:A:GLU:H	3	0.17
(1,1003)	1:74:A:LEU:HB3	1:76:A:ALA:H	14	0.17
(1,1001)	1:73:A:THR:HB	1:76:A:ALA:H	17	0.17
(1,977)	1:47:A:THR:HG21	1:71:A:GLN:H	15	0.17
(1,977)	1:47:A:THR:HG22	1:71:A:GLN:H	15	0.17
(1,977)	1:47:A:THR:HG23	1:71:A:GLN:H	15	0.17
(1,919)	1:60:A:PHE:HD1	1:61:A:ASP:H	5	0.17
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	10	0.17
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	11	0.17
(1,902)	1:59:A:GLN:HE22	1:62:A:SER:HB3	6	0.17
(1,808)	1:43:A:GLY:H	1:74:A:LEU:H	14	0.17
(1,808)	1:43:A:GLY:H	1:74:A:LEU:H	15	0.17
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	2	0.17
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD21	6	0.17
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD22	6	0.17
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD23	6	0.17
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG21	3	0.17
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG22	3	0.17
(1,793)	1:39:A:LYS:H	1:91:A:THR:HG23	3	0.17
(1,787)	1:37:A:VAL:HB	1:38:A:THR:H	19	0.17
(1,751)	1:27:A:GLU:HG2	1:28:A:LYS:H	12	0.17
(1,744)	1:26:A:LEU:H	1:27:A:GLU:HG3	19	0.17
(1,730)	1:35:A:ASP:H	1:37:A:VAL:HG21	18	0.17
(1,730)	1:35:A:ASP:H	1:37:A:VAL:HG22	18	0.17
(1,730)	1:35:A:ASP:H	1:37:A:VAL:HG23	18	0.17
(1,702)	1:80:A:ILE:HG21	1:83:A:TRP:HE3	8	0.17
(1,702)	1:80:A:ILE:HG22	1:83:A:TRP:HE3	8	0.17
(1,702)	1:80:A:ILE:HG23	1:83:A:TRP:HE3	8	0.17
(1,700)	1:79:A:VAL:HB	1:83:A:TRP:HE3	20	0.17
(1,680)	1:50:A:TYR:HB3	1:50:A:TYR:HD1	5	0.17
(1,668)	1:110:A:GLY:HA3	1:115:A:ILE:HG21	4	0.17
(1,668)	1:110:A:GLY:HA3	1:115:A:ILE:HG22	4	0.17
(1,668)	1:110:A:GLY:HA3	1:115:A:ILE:HG23	4	0.17
(1,661)	1:72:A:PHE:HB3	1:79:A:VAL:HG11	17	0.17
(1,661)	1:72:A:PHE:HB3	1:79:A:VAL:HG12	17	0.17
(1,661)	1:72:A:PHE:HB3	1:79:A:VAL:HG13	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:127:A:LEU:HD11	1:129:A:ALA:HB1	10	0.17
(1,638)	1:127:A:LEU:HD11	1:129:A:ALA:HB2	10	0.17
(1,638)	1:127:A:LEU:HD11	1:129:A:ALA:HB3	10	0.17
(1,638)	1:127:A:LEU:HD12	1:129:A:ALA:HB1	10	0.17
(1,638)	1:127:A:LEU:HD12	1:129:A:ALA:HB2	10	0.17
(1,638)	1:127:A:LEU:HD12	1:129:A:ALA:HB3	10	0.17
(1,638)	1:127:A:LEU:HD13	1:129:A:ALA:HB1	10	0.17
(1,638)	1:127:A:LEU:HD13	1:129:A:ALA:HB2	10	0.17
(1,638)	1:127:A:LEU:HD13	1:129:A:ALA:HB3	10	0.17
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD11	18	0.17
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD12	18	0.17
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD13	18	0.17
(1,616)	1:50:A:TYR:HA	1:125:A:VAL:HG11	1	0.17
(1,616)	1:50:A:TYR:HA	1:125:A:VAL:HG12	1	0.17
(1,616)	1:50:A:TYR:HA	1:125:A:VAL:HG13	1	0.17
(1,608)	1:97:A:LEU:HG	1:124:A:GLU:HG3	19	0.17
(1,603)	1:123:A:PHE:H	1:124:A:GLU:HA	18	0.17
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	5	0.17
(1,582)	1:55:A:PRO:HG2	1:120:A:THR:HB	8	0.17
(1,519)	1:80:A:ILE:HB	1:105:A:ALA:HA	13	0.17
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	7	0.17
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	7	0.17
(1,506)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	7	0.17
(1,498)	1:103:A:GLN:HA	1:104:A:LEU:HG	14	0.17
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB1	1	0.17
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB2	1	0.17
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB3	1	0.17
(1,482)	1:100:A:ILE:HG21	1:104:A:LEU:HB2	19	0.17
(1,482)	1:100:A:ILE:HG22	1:104:A:LEU:HB2	19	0.17
(1,482)	1:100:A:ILE:HG23	1:104:A:LEU:HB2	19	0.17
(1,481)	1:100:A:ILE:HG21	1:104:A:LEU:HA	1	0.17
(1,481)	1:100:A:ILE:HG22	1:104:A:LEU:HA	1	0.17
(1,481)	1:100:A:ILE:HG23	1:104:A:LEU:HA	1	0.17
(1,460)	1:97:A:LEU:HD11	1:98:A:PHE:H	17	0.17
(1,460)	1:97:A:LEU:HD12	1:98:A:PHE:H	17	0.17
(1,460)	1:97:A:LEU:HD13	1:98:A:PHE:H	17	0.17
(1,460)	1:97:A:LEU:HD11	1:98:A:PHE:H	19	0.17
(1,460)	1:97:A:LEU:HD12	1:98:A:PHE:H	19	0.17
(1,460)	1:97:A:LEU:HD13	1:98:A:PHE:H	19	0.17
(1,457)	1:29:A:LYS:H	1:97:A:LEU:HB2	8	0.17
(1,457)	1:29:A:LYS:H	1:97:A:LEU:HB2	10	0.17
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB1	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB2	7	0.17
(1,455)	1:30:A:VAL:HB	1:96:A:ALA:HB3	7	0.17
(1,428)	1:38:A:THR:HG21	1:92:A:LEU:HD11	15	0.17
(1,428)	1:38:A:THR:HG21	1:92:A:LEU:HD12	15	0.17
(1,428)	1:38:A:THR:HG21	1:92:A:LEU:HD13	15	0.17
(1,428)	1:38:A:THR:HG22	1:92:A:LEU:HD11	15	0.17
(1,428)	1:38:A:THR:HG22	1:92:A:LEU:HD12	15	0.17
(1,428)	1:38:A:THR:HG22	1:92:A:LEU:HD13	15	0.17
(1,428)	1:38:A:THR:HG23	1:92:A:LEU:HD11	15	0.17
(1,428)	1:38:A:THR:HG23	1:92:A:LEU:HD12	15	0.17
(1,428)	1:38:A:THR:HG23	1:92:A:LEU:HD13	15	0.17
(1,410)	1:90:A:MET:HE1	1:96:A:ALA:H	4	0.17
(1,410)	1:90:A:MET:HE2	1:96:A:ALA:H	4	0.17
(1,410)	1:90:A:MET:HE3	1:96:A:ALA:H	4	0.17
(1,394)	1:74:A:LEU:HD11	1:88:A:ALA:HA	14	0.17
(1,394)	1:74:A:LEU:HD12	1:88:A:ALA:HA	14	0.17
(1,394)	1:74:A:LEU:HD13	1:88:A:ALA:HA	14	0.17
(1,388)	1:86:A:GLY:HA2	1:98:A:PHE:HD2	13	0.17
(1,383)	1:66:A:ARG:HG2	1:68:A:LYS:H	8	0.17
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG21	6	0.17
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG22	6	0.17
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG23	6	0.17
(1,316)	1:80:A:ILE:HB	1:104:A:LEU:HB3	14	0.17
(1,316)	1:80:A:ILE:HB	1:104:A:LEU:HB3	18	0.17
(1,315)	1:80:A:ILE:HD11	1:100:A:ILE:HG21	13	0.17
(1,315)	1:80:A:ILE:HD11	1:100:A:ILE:HG22	13	0.17
(1,315)	1:80:A:ILE:HD11	1:100:A:ILE:HG23	13	0.17
(1,315)	1:80:A:ILE:HD12	1:100:A:ILE:HG21	13	0.17
(1,315)	1:80:A:ILE:HD12	1:100:A:ILE:HG22	13	0.17
(1,315)	1:80:A:ILE:HD12	1:100:A:ILE:HG23	13	0.17
(1,315)	1:80:A:ILE:HD13	1:100:A:ILE:HG21	13	0.17
(1,315)	1:80:A:ILE:HD13	1:100:A:ILE:HG22	13	0.17
(1,315)	1:80:A:ILE:HD13	1:100:A:ILE:HG23	13	0.17
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD11	6	0.17
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD12	6	0.17
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD13	6	0.17
(1,242)	1:68:A:LYS:H	1:69:A:PRO:HD2	14	0.17
(1,240)	1:47:A:THR:HG21	1:69:A:PRO:HG3	12	0.17
(1,240)	1:47:A:THR:HG22	1:69:A:PRO:HG3	12	0.17
(1,240)	1:47:A:THR:HG23	1:69:A:PRO:HG3	12	0.17
(1,209)	1:64:A:ARG:HA	1:68:A:LYS:H	9	0.17
(1,208)	1:63:A:SER:H	1:64:A:ARG:HA	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,208)	1:63:A:SER:H	1:64:A:ARG:HA	11	0.17
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	11	0.17
(1,162)	1:53:A:ARG:HG2	1:59:A:GLN:H	16	0.17
(1,123)	1:46:A:VAL:HG11	1:130:A:VAL:HB	17	0.17
(1,123)	1:46:A:VAL:HG12	1:130:A:VAL:HB	17	0.17
(1,123)	1:46:A:VAL:HG13	1:130:A:VAL:HB	17	0.17
(1,98)	1:45:A:LYS:HB3	1:46:A:VAL:H	16	0.17
(1,89)	1:42:A:ALA:HB1	1:74:A:LEU:HA	19	0.17
(1,89)	1:42:A:ALA:HB2	1:74:A:LEU:HA	19	0.17
(1,89)	1:42:A:ALA:HB3	1:74:A:LEU:HA	19	0.17
(1,72)	1:40:A:PRO:HB3	1:41:A:GLN:H	10	0.17
(1,65)	1:38:A:THR:HG21	1:130:A:VAL:H	18	0.17
(1,65)	1:38:A:THR:HG22	1:130:A:VAL:H	18	0.17
(1,65)	1:38:A:THR:HG23	1:130:A:VAL:H	18	0.17
(1,42)	1:33:A:PRO:HA	1:94:A:GLU:HG2	2	0.17
(1,29)	1:27:A:GLU:H	1:27:A:GLU:HG2	17	0.17
(1,29)	1:27:A:GLU:H	1:27:A:GLU:HG2	20	0.17
(1,2)	1:28:A:LYS:HB2	1:30:A:VAL:H	18	0.17
(1,1648)	1:121:A:LEU:HD11	1:123:A:PHE:HD1	8	0.16
(1,1648)	1:121:A:LEU:HD12	1:123:A:PHE:HD1	8	0.16
(1,1648)	1:121:A:LEU:HD13	1:123:A:PHE:HD1	8	0.16
(1,1648)	1:121:A:LEU:HD21	1:123:A:PHE:HD1	8	0.16
(1,1648)	1:121:A:LEU:HD22	1:123:A:PHE:HD1	8	0.16
(1,1648)	1:121:A:LEU:HD23	1:123:A:PHE:HD1	8	0.16
(1,1584)	1:95:A:LYS:HG2	1:124:A:GLU:HB3	8	0.16
(1,1584)	1:95:A:LYS:HG3	1:124:A:GLU:HB3	8	0.16
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD11	3	0.16
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD12	3	0.16
(1,1546)	1:85:A:GLN:HE21	1:104:A:LEU:HD13	3	0.16
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD11	3	0.16
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD12	3	0.16
(1,1546)	1:85:A:GLN:HE22	1:104:A:LEU:HD13	3	0.16
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG11	2	0.16
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG12	2	0.16
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG13	2	0.16
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG21	2	0.16
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG22	2	0.16
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG23	2	0.16
(1,1511)	1:70:A:PHE:HB2	1:71:A:GLN:H	4	0.16
(1,1511)	1:70:A:PHE:HB3	1:71:A:GLN:H	4	0.16
(1,1505)	1:66:A:ARG:HG2	1:68:A:LYS:H	1	0.16
(1,1505)	1:66:A:ARG:HG3	1:68:A:LYS:H	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1460)	1:55:A:PRO:HG3	1:122:A:VAL:HG11	15	0.16
(1,1460)	1:55:A:PRO:HG3	1:122:A:VAL:HG12	15	0.16
(1,1460)	1:55:A:PRO:HG3	1:122:A:VAL:HG13	15	0.16
(1,1460)	1:55:A:PRO:HG3	1:122:A:VAL:HG21	15	0.16
(1,1460)	1:55:A:PRO:HG3	1:122:A:VAL:HG22	15	0.16
(1,1460)	1:55:A:PRO:HG3	1:122:A:VAL:HG23	15	0.16
(1,1384)	1:41:A:GLN:H	1:41:A:GLN:HB2	14	0.16
(1,1384)	1:41:A:GLN:H	1:41:A:GLN:HB3	14	0.16
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	9	0.16
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	17	0.16
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	17	0.16
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	17	0.16
(1,1301)	1:71:A:GLN:HA	1:71:A:GLN:HE21	5	0.16
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD21	17	0.16
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD22	17	0.16
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD23	17	0.16
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD21	20	0.16
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD22	20	0.16
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD23	20	0.16
(1,1218)	1:111:A:TYR:H	1:111:A:TYR:HB3	13	0.16
(1,1214)	1:111:A:TYR:H	1:115:A:ILE:H	12	0.16
(1,1197)	1:100:A:ILE:HG21	1:105:A:ALA:H	19	0.16
(1,1197)	1:100:A:ILE:HG22	1:105:A:ALA:H	19	0.16
(1,1197)	1:100:A:ILE:HG23	1:105:A:ALA:H	19	0.16
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB1	11	0.16
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB2	11	0.16
(1,1175)	1:102:A:TYR:H	1:105:A:ALA:HB3	11	0.16
(1,1147)	1:98:A:PHE:H	1:99:A:THR:H	20	0.16
(1,1116)	1:92:A:LEU:HD11	1:93:A:GLY:H	1	0.16
(1,1116)	1:92:A:LEU:HD12	1:93:A:GLY:H	1	0.16
(1,1116)	1:92:A:LEU:HD13	1:93:A:GLY:H	1	0.16
(1,1113)	1:91:A:THR:HG21	1:92:A:LEU:H	16	0.16
(1,1113)	1:91:A:THR:HG22	1:92:A:LEU:H	16	0.16
(1,1113)	1:91:A:THR:HG23	1:92:A:LEU:H	16	0.16
(1,1050)	1:80:A:ILE:HG12	1:84:A:ASP:H	11	0.16
(1,1041)	1:80:A:ILE:HG21	1:83:A:TRP:H	14	0.16
(1,1041)	1:80:A:ILE:HG22	1:83:A:TRP:H	14	0.16
(1,1041)	1:80:A:ILE:HG23	1:83:A:TRP:H	14	0.16
(1,952)	1:67:A:GLY:H	1:68:A:LYS:HB2	20	0.16
(1,858)	1:50:A:TYR:HD1	1:51:A:ASP:H	10	0.16
(1,836)	1:47:A:THR:H	1:128:A:LEU:H	3	0.16
(1,830)	1:46:A:VAL:H	1:72:A:PHE:HA	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	3	0.16
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	4	0.16
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	7	0.16
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	20	0.16
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG11	8	0.16
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG12	8	0.16
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG13	8	0.16
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	4	0.16
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	4	0.16
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	4	0.16
(1,775)	1:34:A:GLY:H	1:94:A:GLU:HB3	15	0.16
(1,695)	1:83:A:TRP:HZ2	1:123:A:PHE:HD1	1	0.16
(1,684)	1:48:A:VAL:HG21	1:50:A:TYR:HE1	4	0.16
(1,684)	1:48:A:VAL:HG22	1:50:A:TYR:HE1	4	0.16
(1,684)	1:48:A:VAL:HG23	1:50:A:TYR:HE1	4	0.16
(1,682)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	4	0.16
(1,661)	1:72:A:PHE:HB3	1:79:A:VAL:HG11	9	0.16
(1,661)	1:72:A:PHE:HB3	1:79:A:VAL:HG12	9	0.16
(1,661)	1:72:A:PHE:HB3	1:79:A:VAL:HG13	9	0.16
(1,653)	1:38:A:THR:HB	1:130:A:VAL:HB	5	0.16
(1,630)	1:127:A:LEU:HG	1:129:A:ALA:HA	8	0.16
(1,624)	1:49:A:HIS:HB3	1:126:A:GLU:HB3	18	0.16
(1,603)	1:123:A:PHE:H	1:124:A:GLU:HA	10	0.16
(1,601)	1:100:A:ILE:HD11	1:123:A:PHE:HB2	13	0.16
(1,601)	1:100:A:ILE:HD12	1:123:A:PHE:HB2	13	0.16
(1,601)	1:100:A:ILE:HD13	1:123:A:PHE:HB2	13	0.16
(1,563)	1:114:A:VAL:H	1:114:A:VAL:HB	7	0.16
(1,563)	1:114:A:VAL:H	1:114:A:VAL:HB	9	0.16
(1,563)	1:114:A:VAL:H	1:114:A:VAL:HB	13	0.16
(1,554)	1:106:A:TYR:HB2	1:110:A:GLY:HA2	14	0.16
(1,518)	1:80:A:ILE:HA	1:105:A:ALA:HA	15	0.16
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB1	2	0.16
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB2	2	0.16
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB3	2	0.16
(1,482)	1:100:A:ILE:HG21	1:104:A:LEU:HB2	6	0.16
(1,482)	1:100:A:ILE:HG22	1:104:A:LEU:HB2	6	0.16
(1,482)	1:100:A:ILE:HG23	1:104:A:LEU:HB2	6	0.16
(1,413)	1:90:A:MET:HE1	1:91:A:THR:H	10	0.16
(1,413)	1:90:A:MET:HE2	1:91:A:THR:H	10	0.16
(1,413)	1:90:A:MET:HE3	1:91:A:THR:H	10	0.16
(1,413)	1:90:A:MET:HE1	1:91:A:THR:H	13	0.16
(1,413)	1:90:A:MET:HE2	1:91:A:THR:H	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:90:A:MET:HE3	1:91:A:THR:H	13	0.16
(1,375)	1:74:A:LEU:HD11	1:84:A:ASP:HB3	1	0.16
(1,375)	1:74:A:LEU:HD12	1:84:A:ASP:HB3	1	0.16
(1,375)	1:74:A:LEU:HD13	1:84:A:ASP:HB3	1	0.16
(1,370)	1:81:A:LYS:HA	1:84:A:ASP:HB2	14	0.16
(1,364)	1:80:A:ILE:HD11	1:83:A:TRP:HA	14	0.16
(1,364)	1:80:A:ILE:HD12	1:83:A:TRP:HA	14	0.16
(1,364)	1:80:A:ILE:HD13	1:83:A:TRP:HA	14	0.16
(1,343)	1:66:A:ARG:HG3	1:68:A:LYS:H	18	0.16
(1,333)	1:81:A:LYS:HA	1:81:A:LYS:HD3	19	0.16
(1,289)	1:76:A:ALA:HB1	1:78:A:GLU:HB2	17	0.16
(1,289)	1:76:A:ALA:HB2	1:78:A:GLU:HB2	17	0.16
(1,289)	1:76:A:ALA:HB3	1:78:A:GLU:HB2	17	0.16
(1,283)	1:73:A:THR:HG21	1:76:A:ALA:HA	6	0.16
(1,283)	1:73:A:THR:HG22	1:76:A:ALA:HA	6	0.16
(1,283)	1:73:A:THR:HG23	1:76:A:ALA:HA	6	0.16
(1,216)	1:64:A:ARG:HA	1:64:A:ARG:HD3	14	0.16
(1,160)	1:53:A:ARG:HB2	1:59:A:GLN:HA	19	0.16
(1,158)	1:52:A:GLY:HA2	1:123:A:PHE:HD1	19	0.16
(1,156)	1:51:A:ASP:HA	1:124:A:GLU:H	14	0.16
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG11	14	0.16
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG12	14	0.16
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG13	14	0.16
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	11	0.16
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	11	0.16
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	11	0.16
(1,127)	1:47:A:THR:HB	1:48:A:VAL:HA	12	0.16
(1,103)	1:45:A:LYS:HG2	1:46:A:VAL:H	4	0.16
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG21	5	0.16
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG22	5	0.16
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG23	5	0.16
(1,64)	1:38:A:THR:HG21	1:39:A:LYS:H	18	0.16
(1,64)	1:38:A:THR:HG22	1:39:A:LYS:H	18	0.16
(1,64)	1:38:A:THR:HG23	1:39:A:LYS:H	18	0.16
(1,42)	1:33:A:PRO:HA	1:94:A:GLU:HG2	9	0.16
(1,1631)	1:109:A:ARG:HB2	1:110:A:GLY:H	15	0.15
(1,1631)	1:109:A:ARG:HB3	1:110:A:GLY:H	15	0.15
(1,1627)	1:109:A:ARG:HA	1:109:A:ARG:HG2	15	0.15
(1,1627)	1:109:A:ARG:HA	1:109:A:ARG:HG3	15	0.15
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD11	17	0.15
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD12	17	0.15
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD13	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD21	17	0.15
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD22	17	0.15
(1,1620)	1:106:A:TYR:HE2	1:121:A:LEU:HD23	17	0.15
(1,1599)	1:97:A:LEU:HD11	1:124:A:GLU:HB3	16	0.15
(1,1599)	1:97:A:LEU:HD12	1:124:A:GLU:HB3	16	0.15
(1,1599)	1:97:A:LEU:HD13	1:124:A:GLU:HB3	16	0.15
(1,1599)	1:97:A:LEU:HD21	1:124:A:GLU:HB3	16	0.15
(1,1599)	1:97:A:LEU:HD22	1:124:A:GLU:HB3	16	0.15
(1,1599)	1:97:A:LEU:HD23	1:124:A:GLU:HB3	16	0.15
(1,1594)	1:97:A:LEU:HD11	1:123:A:PHE:H	2	0.15
(1,1594)	1:97:A:LEU:HD12	1:123:A:PHE:H	2	0.15
(1,1594)	1:97:A:LEU:HD13	1:123:A:PHE:H	2	0.15
(1,1594)	1:97:A:LEU:HD21	1:123:A:PHE:H	2	0.15
(1,1594)	1:97:A:LEU:HD22	1:123:A:PHE:H	2	0.15
(1,1594)	1:97:A:LEU:HD23	1:123:A:PHE:H	2	0.15
(1,1493)	1:64:A:ARG:HG2	1:65:A:SER:HA	16	0.15
(1,1493)	1:64:A:ARG:HG3	1:65:A:SER:HA	16	0.15
(1,1491)	1:64:A:ARG:HA	1:64:A:ARG:HD2	17	0.15
(1,1491)	1:64:A:ARG:HA	1:64:A:ARG:HD3	17	0.15
(1,1441)	1:53:A:ARG:HD2	1:57:A:GLY:HA2	3	0.15
(1,1441)	1:53:A:ARG:HD3	1:57:A:GLY:HA2	3	0.15
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG2	18	0.15
(1,1439)	1:53:A:ARG:HG3	1:59:A:GLN:HG3	18	0.15
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB2	12	0.15
(1,1336)	1:25:A:GLN:H	1:26:A:LEU:HB3	12	0.15
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG2	9	0.15
(1,1331)	1:24:A:ALA:HA	1:25:A:GLN:HG3	9	0.15
(1,1308)	1:81:A:LYS:HD2	1:85:A:GLN:HE21	3	0.15
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	15	0.15
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB1	17	0.15
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB2	17	0.15
(1,1304)	1:71:A:GLN:HE22	1:129:A:ALA:HB3	17	0.15
(1,1301)	1:71:A:GLN:HA	1:71:A:GLN:HE21	8	0.15
(1,1301)	1:71:A:GLN:HA	1:71:A:GLN:HE21	16	0.15
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	14	0.15
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	14	0.15
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	14	0.15
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD21	6	0.15
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD22	6	0.15
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD23	6	0.15
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD21	19	0.15
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD22	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD23	19	0.15
(1,1276)	1:96:A:ALA:H	1:127:A:LEU:H	20	0.15
(1,1259)	1:124:A:GLU:H	1:125:A:VAL:HG11	6	0.15
(1,1259)	1:124:A:GLU:H	1:125:A:VAL:HG12	6	0.15
(1,1259)	1:124:A:GLU:H	1:125:A:VAL:HG13	6	0.15
(1,1218)	1:111:A:TYR:H	1:111:A:TYR:HB3	5	0.15
(1,1218)	1:111:A:TYR:H	1:111:A:TYR:HB3	15	0.15
(1,1218)	1:111:A:TYR:H	1:111:A:TYR:HB3	17	0.15
(1,1187)	1:104:A:LEU:H	1:107:A:GLY:H	7	0.15
(1,1184)	1:103:A:GLN:H	1:104:A:LEU:HB2	8	0.15
(1,1172)	1:102:A:TYR:H	1:105:A:ALA:H	6	0.15
(1,1147)	1:98:A:PHE:H	1:99:A:THR:H	18	0.15
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	10	0.15
(1,1116)	1:92:A:LEU:HD11	1:93:A:GLY:H	2	0.15
(1,1116)	1:92:A:LEU:HD12	1:93:A:GLY:H	2	0.15
(1,1116)	1:92:A:LEU:HD13	1:93:A:GLY:H	2	0.15
(1,1116)	1:92:A:LEU:HD11	1:93:A:GLY:H	17	0.15
(1,1116)	1:92:A:LEU:HD12	1:93:A:GLY:H	17	0.15
(1,1116)	1:92:A:LEU:HD13	1:93:A:GLY:H	17	0.15
(1,1050)	1:80:A:ILE:HG12	1:84:A:ASP:H	12	0.15
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD11	9	0.15
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD12	9	0.15
(1,1038)	1:83:A:TRP:H	1:104:A:LEU:HD13	9	0.15
(1,1037)	1:80:A:ILE:HG12	1:83:A:TRP:H	6	0.15
(1,1017)	1:76:A:ALA:HB1	1:79:A:VAL:H	16	0.15
(1,1017)	1:76:A:ALA:HB2	1:79:A:VAL:H	16	0.15
(1,1017)	1:76:A:ALA:HB3	1:79:A:VAL:H	16	0.15
(1,1006)	1:77:A:GLY:H	1:78:A:GLU:HB2	19	0.15
(1,1005)	1:77:A:GLY:H	1:78:A:GLU:H	18	0.15
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB1	12	0.15
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB2	12	0.15
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB3	12	0.15
(1,966)	1:69:A:PRO:HB3	1:70:A:PHE:H	9	0.15
(1,863)	1:50:A:TYR:HB2	1:51:A:ASP:H	4	0.15
(1,824)	1:44:A:LYS:HB3	1:45:A:LYS:H	15	0.15
(1,820)	1:44:A:LYS:H	1:44:A:LYS:HG3	10	0.15
(1,812)	1:43:A:GLY:H	1:44:A:LYS:HB2	3	0.15
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	10	0.15
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	19	0.15
(1,797)	1:41:A:GLN:H	1:41:A:GLN:HG2	10	0.15
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG11	10	0.15
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG12	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,794)	1:39:A:LYS:H	1:130:A:VAL:HG13	10	0.15
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	14	0.15
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	14	0.15
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	14	0.15
(1,781)	1:37:A:VAL:H	1:91:A:THR:HB	16	0.15
(1,775)	1:34:A:GLY:H	1:94:A:GLU:HB3	2	0.15
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG21	3	0.15
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG22	3	0.15
(1,693)	1:83:A:TRP:HD1	1:100:A:ILE:HG23	3	0.15
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG21	18	0.15
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG22	18	0.15
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG23	18	0.15
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB1	8	0.15
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB2	8	0.15
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB3	8	0.15
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB1	19	0.15
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB2	19	0.15
(1,648)	1:47:A:THR:H	1:129:A:ALA:HB3	19	0.15
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	2	0.15
(1,579)	1:102:A:TYR:HB2	1:119:A:ALA:HB1	17	0.15
(1,579)	1:102:A:TYR:HB2	1:119:A:ALA:HB2	17	0.15
(1,579)	1:102:A:TYR:HB2	1:119:A:ALA:HB3	17	0.15
(1,563)	1:114:A:VAL:H	1:114:A:VAL:HB	11	0.15
(1,563)	1:114:A:VAL:H	1:114:A:VAL:HB	18	0.15
(1,555)	1:106:A:TYR:HB3	1:110:A:GLY:HA2	19	0.15
(1,536)	1:102:A:TYR:HE2	1:108:A:GLU:HB2	13	0.15
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG21	16	0.15
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG22	16	0.15
(1,532)	1:106:A:TYR:HB2	1:115:A:ILE:HG23	16	0.15
(1,481)	1:100:A:ILE:HG21	1:104:A:LEU:HA	19	0.15
(1,481)	1:100:A:ILE:HG22	1:104:A:LEU:HA	19	0.15
(1,481)	1:100:A:ILE:HG23	1:104:A:LEU:HA	19	0.15
(1,460)	1:97:A:LEU:HD11	1:98:A:PHE:H	2	0.15
(1,460)	1:97:A:LEU:HD12	1:98:A:PHE:H	2	0.15
(1,460)	1:97:A:LEU:HD13	1:98:A:PHE:H	2	0.15
(1,457)	1:29:A:LYS:H	1:97:A:LEU:HB2	13	0.15
(1,415)	1:90:A:MET:HE1	1:94:A:GLU:HA	13	0.15
(1,415)	1:90:A:MET:HE2	1:94:A:GLU:HA	13	0.15
(1,415)	1:90:A:MET:HE3	1:94:A:GLU:HA	13	0.15
(1,413)	1:90:A:MET:HE1	1:91:A:THR:H	15	0.15
(1,413)	1:90:A:MET:HE2	1:91:A:THR:H	15	0.15
(1,413)	1:90:A:MET:HE3	1:91:A:THR:H	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,395)	1:40:A:PRO:HG2	1:88:A:ALA:HA	6	0.15
(1,376)	1:81:A:LYS:HG2	1:84:A:ASP:HB3	6	0.15
(1,369)	1:83:A:TRP:H	1:84:A:ASP:HB2	2	0.15
(1,369)	1:83:A:TRP:H	1:84:A:ASP:HB2	7	0.15
(1,355)	1:81:A:LYS:HB3	1:82:A:GLY:HA2	6	0.15
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG21	17	0.15
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG22	17	0.15
(1,353)	1:82:A:GLY:HA2	1:100:A:ILE:HG23	17	0.15
(1,349)	1:82:A:GLY:HA3	1:100:A:ILE:HG21	13	0.15
(1,349)	1:82:A:GLY:HA3	1:100:A:ILE:HG22	13	0.15
(1,349)	1:82:A:GLY:HA3	1:100:A:ILE:HG23	13	0.15
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD11	8	0.15
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD12	8	0.15
(1,334)	1:81:A:LYS:HA	1:104:A:LEU:HD13	8	0.15
(1,328)	1:80:A:ILE:HG13	1:83:A:TRP:H	11	0.15
(1,316)	1:80:A:ILE:HB	1:104:A:LEU:HB3	6	0.15
(1,242)	1:68:A:LYS:H	1:69:A:PRO:HD2	7	0.15
(1,228)	1:47:A:THR:HG21	1:69:A:PRO:HA	15	0.15
(1,228)	1:47:A:THR:HG22	1:69:A:PRO:HA	15	0.15
(1,228)	1:47:A:THR:HG23	1:69:A:PRO:HA	15	0.15
(1,224)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	19	0.15
(1,208)	1:63:A:SER:H	1:64:A:ARG:HA	8	0.15
(1,192)	1:59:A:GLN:HA	1:61:A:ASP:H	2	0.15
(1,160)	1:53:A:ARG:HB2	1:59:A:GLN:HA	12	0.15
(1,153)	1:51:A:ASP:HB2	1:124:A:GLU:HB3	16	0.15
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG11	4	0.15
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG12	4	0.15
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG13	4	0.15
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG11	18	0.15
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG12	18	0.15
(1,151)	1:50:A:TYR:HB2	1:125:A:VAL:HG13	18	0.15
(1,100)	1:45:A:LYS:HB3	1:46:A:VAL:HA	16	0.15
(1,98)	1:45:A:LYS:HB3	1:46:A:VAL:H	9	0.15
(1,85)	1:42:A:ALA:HA	1:74:A:LEU:HD21	14	0.15
(1,85)	1:42:A:ALA:HA	1:74:A:LEU:HD22	14	0.15
(1,85)	1:42:A:ALA:HA	1:74:A:LEU:HD23	14	0.15
(1,1619)	1:103:A:GLN:HG2	1:104:A:LEU:H	8	0.14
(1,1619)	1:103:A:GLN:HG3	1:104:A:LEU:H	8	0.14
(1,1606)	1:98:A:PHE:HB2	1:100:A:ILE:HD11	13	0.14
(1,1606)	1:98:A:PHE:HB2	1:100:A:ILE:HD12	13	0.14
(1,1606)	1:98:A:PHE:HB2	1:100:A:ILE:HD13	13	0.14
(1,1606)	1:98:A:PHE:HB3	1:100:A:ILE:HD11	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1606)	1:98:A:PHE:HB3	1:100:A:ILE:HD12	13	0.14
(1,1606)	1:98:A:PHE:HB3	1:100:A:ILE:HD13	13	0.14
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	19	0.14
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	19	0.14
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	19	0.14
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	19	0.14
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	19	0.14
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	19	0.14
(1,1594)	1:97:A:LEU:HD11	1:123:A:PHE:H	6	0.14
(1,1594)	1:97:A:LEU:HD12	1:123:A:PHE:H	6	0.14
(1,1594)	1:97:A:LEU:HD13	1:123:A:PHE:H	6	0.14
(1,1594)	1:97:A:LEU:HD21	1:123:A:PHE:H	6	0.14
(1,1594)	1:97:A:LEU:HD22	1:123:A:PHE:H	6	0.14
(1,1594)	1:97:A:LEU:HD23	1:123:A:PHE:H	6	0.14
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG11	7	0.14
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG12	7	0.14
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG13	7	0.14
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG21	7	0.14
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG22	7	0.14
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG23	7	0.14
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG11	10	0.14
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG12	10	0.14
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG13	10	0.14
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG21	10	0.14
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG22	10	0.14
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG23	10	0.14
(1,1506)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	13	0.14
(1,1506)	1:67:A:GLY:HA3	1:68:A:LYS:HB2	13	0.14
(1,1501)	1:66:A:ARG:HA	1:66:A:ARG:HG2	6	0.14
(1,1501)	1:66:A:ARG:HA	1:66:A:ARG:HG3	6	0.14
(1,1446)	1:54:A:PHE:H	1:58:A:LYS:HB2	17	0.14
(1,1446)	1:54:A:PHE:H	1:58:A:LYS:HB3	17	0.14
(1,1441)	1:53:A:ARG:HD2	1:57:A:GLY:HA2	4	0.14
(1,1441)	1:53:A:ARG:HD3	1:57:A:GLY:HA2	4	0.14
(1,1327)	1:19:A:PRO:HG2	1:56:A:ASP:H	11	0.14
(1,1327)	1:19:A:PRO:HG3	1:56:A:ASP:H	11	0.14
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	6	0.14
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	12	0.14
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB1	19	0.14
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB2	19	0.14
(1,1302)	1:71:A:GLN:HE21	1:129:A:ALA:HB3	19	0.14
(1,1300)	1:92:A:LEU:HD21	1:130:A:VAL:H	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1300)	1:92:A:LEU:HD22	1:130:A:VAL:H	9	0.14
(1,1300)	1:92:A:LEU:HD23	1:130:A:VAL:H	9	0.14
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD21	8	0.14
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD22	8	0.14
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD23	8	0.14
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD21	15	0.14
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD22	15	0.14
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD23	15	0.14
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD21	18	0.14
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD22	18	0.14
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD23	18	0.14
(1,1281)	1:95:A:LYS:HB2	1:127:A:LEU:H	2	0.14
(1,1276)	1:96:A:ALA:H	1:127:A:LEU:H	17	0.14
(1,1201)	1:106:A:TYR:H	1:106:A:TYR:HD2	12	0.14
(1,1184)	1:103:A:GLN:H	1:104:A:LEU:HB2	1	0.14
(1,1184)	1:103:A:GLN:H	1:104:A:LEU:HB2	3	0.14
(1,1184)	1:103:A:GLN:H	1:104:A:LEU:HB2	20	0.14
(1,1147)	1:98:A:PHE:H	1:99:A:THR:H	4	0.14
(1,1147)	1:98:A:PHE:H	1:99:A:THR:H	11	0.14
(1,1147)	1:98:A:PHE:H	1:99:A:THR:H	19	0.14
(1,1121)	1:34:A:GLY:HA3	1:94:A:GLU:H	2	0.14
(1,1120)	1:34:A:GLY:HA2	1:94:A:GLU:H	16	0.14
(1,1118)	1:34:A:GLY:H	1:94:A:GLU:H	18	0.14
(1,1113)	1:91:A:THR:HG21	1:92:A:LEU:H	11	0.14
(1,1113)	1:91:A:THR:HG22	1:92:A:LEU:H	11	0.14
(1,1113)	1:91:A:THR:HG23	1:92:A:LEU:H	11	0.14
(1,1113)	1:91:A:THR:HG21	1:92:A:LEU:H	14	0.14
(1,1113)	1:91:A:THR:HG22	1:92:A:LEU:H	14	0.14
(1,1113)	1:91:A:THR:HG23	1:92:A:LEU:H	14	0.14
(1,1104)	1:91:A:THR:H	1:127:A:LEU:HG	2	0.14
(1,1053)	1:80:A:ILE:HG21	1:84:A:ASP:H	2	0.14
(1,1053)	1:80:A:ILE:HG22	1:84:A:ASP:H	2	0.14
(1,1053)	1:80:A:ILE:HG23	1:84:A:ASP:H	2	0.14
(1,1036)	1:79:A:VAL:HB	1:83:A:TRP:H	16	0.14
(1,977)	1:47:A:THR:HG21	1:71:A:GLN:H	6	0.14
(1,977)	1:47:A:THR:HG22	1:71:A:GLN:H	6	0.14
(1,977)	1:47:A:THR:HG23	1:71:A:GLN:H	6	0.14
(1,965)	1:69:A:PRO:HG3	1:70:A:PHE:H	19	0.14
(1,887)	1:53:A:ARG:HB3	1:54:A:PHE:H	15	0.14
(1,828)	1:46:A:VAL:H	1:71:A:GLN:HA	9	0.14
(1,786)	1:38:A:THR:H	1:91:A:THR:HA	17	0.14
(1,744)	1:26:A:LEU:H	1:27:A:GLU:HG3	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:83:A:TRP:HD1	1:123:A:PHE:HD2	8	0.14
(1,684)	1:48:A:VAL:HG21	1:50:A:TYR:HE1	6	0.14
(1,684)	1:48:A:VAL:HG22	1:50:A:TYR:HE1	6	0.14
(1,684)	1:48:A:VAL:HG23	1:50:A:TYR:HE1	6	0.14
(1,681)	1:50:A:TYR:H	1:50:A:TYR:HD2	16	0.14
(1,680)	1:50:A:TYR:HB3	1:50:A:TYR:HD1	17	0.14
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG21	16	0.14
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG22	16	0.14
(1,666)	1:111:A:TYR:HD2	1:115:A:ILE:HG23	16	0.14
(1,616)	1:50:A:TYR:HA	1:125:A:VAL:HG11	2	0.14
(1,616)	1:50:A:TYR:HA	1:125:A:VAL:HG12	2	0.14
(1,616)	1:50:A:TYR:HA	1:125:A:VAL:HG13	2	0.14
(1,602)	1:100:A:ILE:HD11	1:123:A:PHE:HB3	7	0.14
(1,602)	1:100:A:ILE:HD12	1:123:A:PHE:HB3	7	0.14
(1,602)	1:100:A:ILE:HD13	1:123:A:PHE:HB3	7	0.14
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	8	0.14
(1,563)	1:114:A:VAL:H	1:114:A:VAL:HB	14	0.14
(1,563)	1:114:A:VAL:H	1:114:A:VAL:HB	20	0.14
(1,554)	1:106:A:TYR:HB2	1:110:A:GLY:HA2	17	0.14
(1,528)	1:80:A:ILE:HG21	1:106:A:TYR:HA	11	0.14
(1,528)	1:80:A:ILE:HG22	1:106:A:TYR:HA	11	0.14
(1,528)	1:80:A:ILE:HG23	1:106:A:TYR:HA	11	0.14
(1,470)	1:100:A:ILE:HB	1:121:A:LEU:HB2	18	0.14
(1,460)	1:97:A:LEU:HD11	1:98:A:PHE:H	9	0.14
(1,460)	1:97:A:LEU:HD12	1:98:A:PHE:H	9	0.14
(1,460)	1:97:A:LEU:HD13	1:98:A:PHE:H	9	0.14
(1,459)	1:97:A:LEU:HG	1:99:A:THR:H	19	0.14
(1,428)	1:38:A:THR:HG21	1:92:A:LEU:HD11	4	0.14
(1,428)	1:38:A:THR:HG21	1:92:A:LEU:HD12	4	0.14
(1,428)	1:38:A:THR:HG21	1:92:A:LEU:HD13	4	0.14
(1,428)	1:38:A:THR:HG22	1:92:A:LEU:HD11	4	0.14
(1,428)	1:38:A:THR:HG22	1:92:A:LEU:HD12	4	0.14
(1,428)	1:38:A:THR:HG22	1:92:A:LEU:HD13	4	0.14
(1,428)	1:38:A:THR:HG23	1:92:A:LEU:HD11	4	0.14
(1,428)	1:38:A:THR:HG23	1:92:A:LEU:HD12	4	0.14
(1,428)	1:38:A:THR:HG23	1:92:A:LEU:HD13	4	0.14
(1,422)	1:38:A:THR:HG21	1:91:A:THR:HA	11	0.14
(1,422)	1:38:A:THR:HG22	1:91:A:THR:HA	11	0.14
(1,422)	1:38:A:THR:HG23	1:91:A:THR:HA	11	0.14
(1,413)	1:90:A:MET:HE1	1:91:A:THR:H	16	0.14
(1,413)	1:90:A:MET:HE2	1:91:A:THR:H	16	0.14
(1,413)	1:90:A:MET:HE3	1:91:A:THR:H	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:90:A:MET:HE1	1:91:A:THR:H	20	0.14
(1,413)	1:90:A:MET:HE2	1:91:A:THR:H	20	0.14
(1,413)	1:90:A:MET:HE3	1:91:A:THR:H	20	0.14
(1,412)	1:90:A:MET:H	1:90:A:MET:HE1	2	0.14
(1,412)	1:90:A:MET:H	1:90:A:MET:HE2	2	0.14
(1,412)	1:90:A:MET:H	1:90:A:MET:HE3	2	0.14
(1,411)	1:90:A:MET:HE1	1:127:A:LEU:H	18	0.14
(1,411)	1:90:A:MET:HE2	1:127:A:LEU:H	18	0.14
(1,411)	1:90:A:MET:HE3	1:127:A:LEU:H	18	0.14
(1,377)	1:81:A:LYS:HD3	1:84:A:ASP:HB3	19	0.14
(1,364)	1:80:A:ILE:HD11	1:83:A:TRP:HA	4	0.14
(1,364)	1:80:A:ILE:HD12	1:83:A:TRP:HA	4	0.14
(1,364)	1:80:A:ILE:HD13	1:83:A:TRP:HA	4	0.14
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG21	17	0.14
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG22	17	0.14
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG23	17	0.14
(1,303)	1:50:A:TYR:HE1	1:79:A:VAL:HB	14	0.14
(1,265)	1:42:A:ALA:H	1:74:A:LEU:HB3	8	0.14
(1,258)	1:44:A:LYS:H	1:73:A:THR:HG21	6	0.14
(1,258)	1:44:A:LYS:H	1:73:A:THR:HG22	6	0.14
(1,258)	1:44:A:LYS:H	1:73:A:THR:HG23	6	0.14
(1,235)	1:69:A:PRO:HB2	1:128:A:LEU:HG	5	0.14
(1,231)	1:68:A:LYS:H	1:69:A:PRO:HA	6	0.14
(1,231)	1:68:A:LYS:H	1:69:A:PRO:HA	8	0.14
(1,231)	1:68:A:LYS:H	1:69:A:PRO:HA	18	0.14
(1,229)	1:69:A:PRO:HA	1:128:A:LEU:HG	16	0.14
(1,194)	1:53:A:ARG:HG2	1:59:A:GLN:HA	15	0.14
(1,185)	1:53:A:ARG:HB3	1:57:A:GLY:HA2	18	0.14
(1,177)	1:19:A:PRO:HG3	1:55:A:PRO:HG3	17	0.14
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG21	15	0.14
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG22	15	0.14
(1,174)	1:55:A:PRO:HB3	1:120:A:THR:HG23	15	0.14
(1,160)	1:53:A:ARG:HB2	1:59:A:GLN:HA	8	0.14
(1,157)	1:52:A:GLY:HA2	1:124:A:GLU:H	19	0.14
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	3	0.14
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	3	0.14
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	3	0.14
(1,121)	1:46:A:VAL:HG11	1:130:A:VAL:H	2	0.14
(1,121)	1:46:A:VAL:HG12	1:130:A:VAL:H	2	0.14
(1,121)	1:46:A:VAL:HG13	1:130:A:VAL:H	2	0.14
(1,119)	1:46:A:VAL:HG21	1:74:A:LEU:HD11	2	0.14
(1,119)	1:46:A:VAL:HG21	1:74:A:LEU:HD12	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:46:A:VAL:HG21	1:74:A:LEU:HD13	2	0.14
(1,119)	1:46:A:VAL:HG22	1:74:A:LEU:HD11	2	0.14
(1,119)	1:46:A:VAL:HG22	1:74:A:LEU:HD12	2	0.14
(1,119)	1:46:A:VAL:HG22	1:74:A:LEU:HD13	2	0.14
(1,119)	1:46:A:VAL:HG23	1:74:A:LEU:HD11	2	0.14
(1,119)	1:46:A:VAL:HG23	1:74:A:LEU:HD12	2	0.14
(1,119)	1:46:A:VAL:HG23	1:74:A:LEU:HD13	2	0.14
(1,114)	1:46:A:VAL:HG21	1:47:A:THR:H	3	0.14
(1,114)	1:46:A:VAL:HG22	1:47:A:THR:H	3	0.14
(1,114)	1:46:A:VAL:HG23	1:47:A:THR:H	3	0.14
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB1	18	0.14
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB2	18	0.14
(1,110)	1:46:A:VAL:HB	1:129:A:ALA:HB3	18	0.14
(1,98)	1:45:A:LYS:HB3	1:46:A:VAL:H	14	0.14
(1,95)	1:41:A:GLN:HG3	1:44:A:LYS:HG3	19	0.14
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG21	5	0.14
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG22	5	0.14
(1,84)	1:42:A:ALA:HA	1:73:A:THR:HG23	5	0.14
(1,29)	1:27:A:GLU:H	1:27:A:GLU:HG2	2	0.14
(1,26)	1:27:A:GLU:HG3	1:99:A:THR:H	3	0.14
(1,22)	1:27:A:GLU:HB3	1:99:A:THR:HB	7	0.14
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB1	16	0.14
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB2	16	0.14
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB3	16	0.14
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG11	20	0.13
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG12	20	0.13
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG13	20	0.13
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG21	20	0.13
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG22	20	0.13
(1,1537)	1:85:A:GLN:H	1:87:A:VAL:HG23	20	0.13
(1,1506)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	9	0.13
(1,1506)	1:67:A:GLY:HA3	1:68:A:LYS:HB2	9	0.13
(1,1491)	1:64:A:ARG:HA	1:64:A:ARG:HD2	19	0.13
(1,1491)	1:64:A:ARG:HA	1:64:A:ARG:HD3	19	0.13
(1,1490)	1:64:A:ARG:H	1:64:A:ARG:HD2	4	0.13
(1,1490)	1:64:A:ARG:H	1:64:A:ARG:HD3	4	0.13
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	5	0.13
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	5	0.13
(1,1474)	1:59:A:GLN:HG2	1:60:A:PHE:H	1	0.13
(1,1474)	1:59:A:GLN:HG3	1:60:A:PHE:H	1	0.13
(1,1440)	1:53:A:ARG:HD2	1:57:A:GLY:H	20	0.13
(1,1440)	1:53:A:ARG:HD3	1:57:A:GLY:H	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD11	18	0.13
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD12	18	0.13
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD13	18	0.13
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD21	18	0.13
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD22	18	0.13
(1,1437)	1:53:A:ARG:HB3	1:97:A:LEU:HD23	18	0.13
(1,1414)	1:45:A:LYS:HG2	1:73:A:THR:HA	6	0.13
(1,1414)	1:45:A:LYS:HG3	1:73:A:THR:HA	6	0.13
(1,1384)	1:41:A:GLN:H	1:41:A:GLN:HB2	4	0.13
(1,1384)	1:41:A:GLN:H	1:41:A:GLN:HB3	4	0.13
(1,1380)	1:40:A:PRO:HB2	1:41:A:GLN:H	9	0.13
(1,1380)	1:40:A:PRO:HB3	1:41:A:GLN:H	9	0.13
(1,1328)	1:19:A:PRO:HG2	1:56:A:ASP:HA	18	0.13
(1,1328)	1:19:A:PRO:HG3	1:56:A:ASP:HA	18	0.13
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	6	0.13
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	6	0.13
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	6	0.13
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	20	0.13
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	20	0.13
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	20	0.13
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD21	3	0.13
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD22	3	0.13
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD23	3	0.13
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD21	16	0.13
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD22	16	0.13
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD23	16	0.13
(1,1219)	1:111:A:TYR:H	1:115:A:ILE:HB	14	0.13
(1,1204)	1:100:A:ILE:HG21	1:106:A:TYR:H	17	0.13
(1,1204)	1:100:A:ILE:HG22	1:106:A:TYR:H	17	0.13
(1,1204)	1:100:A:ILE:HG23	1:106:A:TYR:H	17	0.13
(1,1199)	1:80:A:ILE:HG21	1:105:A:ALA:H	5	0.13
(1,1199)	1:80:A:ILE:HG22	1:105:A:ALA:H	5	0.13
(1,1199)	1:80:A:ILE:HG23	1:105:A:ALA:H	5	0.13
(1,1195)	1:80:A:ILE:HB	1:105:A:ALA:H	20	0.13
(1,1152)	1:98:A:PHE:H	1:123:A:PHE:HB3	9	0.13
(1,1152)	1:98:A:PHE:H	1:123:A:PHE:HB3	12	0.13
(1,1120)	1:34:A:GLY:HA2	1:94:A:GLU:H	6	0.13
(1,1116)	1:92:A:LEU:HD11	1:93:A:GLY:H	11	0.13
(1,1116)	1:92:A:LEU:HD12	1:93:A:GLY:H	11	0.13
(1,1116)	1:92:A:LEU:HD13	1:93:A:GLY:H	11	0.13
(1,1116)	1:92:A:LEU:HD11	1:93:A:GLY:H	19	0.13
(1,1116)	1:92:A:LEU:HD12	1:93:A:GLY:H	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1116)	1:92:A:LEU:HD13	1:93:A:GLY:H	19	0.13
(1,1113)	1:91:A:THR:HG21	1:92:A:LEU:H	7	0.13
(1,1113)	1:91:A:THR:HG22	1:92:A:LEU:H	7	0.13
(1,1113)	1:91:A:THR:HG23	1:92:A:LEU:H	7	0.13
(1,1084)	1:89:A:THR:H	1:90:A:MET:HG3	8	0.13
(1,1065)	1:79:A:VAL:HG21	1:85:A:GLN:H	4	0.13
(1,1065)	1:79:A:VAL:HG22	1:85:A:GLN:H	4	0.13
(1,1065)	1:79:A:VAL:HG23	1:85:A:GLN:H	4	0.13
(1,923)	1:71:A:GLN:HE21	1:72:A:PHE:H	12	0.13
(1,910)	1:55:A:PRO:HA	1:57:A:GLY:H	19	0.13
(1,909)	1:56:A:ASP:HA	1:57:A:GLY:H	14	0.13
(1,868)	1:51:A:ASP:H	1:125:A:VAL:HG11	6	0.13
(1,868)	1:51:A:ASP:H	1:125:A:VAL:HG12	6	0.13
(1,868)	1:51:A:ASP:H	1:125:A:VAL:HG13	6	0.13
(1,862)	1:50:A:TYR:HB3	1:51:A:ASP:H	10	0.13
(1,836)	1:47:A:THR:H	1:128:A:LEU:H	16	0.13
(1,813)	1:43:A:GLY:H	1:74:A:LEU:HG	17	0.13
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD21	15	0.13
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD22	15	0.13
(1,805)	1:42:A:ALA:H	1:74:A:LEU:HD23	15	0.13
(1,802)	1:41:A:GLN:H	1:74:A:LEU:HB3	7	0.13
(1,799)	1:40:A:PRO:HB2	1:41:A:GLN:H	13	0.13
(1,787)	1:37:A:VAL:HB	1:38:A:THR:H	9	0.13
(1,682)	1:50:A:TYR:HE2	1:70:A:PHE:HB2	18	0.13
(1,679)	1:50:A:TYR:HB2	1:50:A:TYR:HD2	5	0.13
(1,670)	1:115:A:ILE:HG21	1:119:A:ALA:HB1	9	0.13
(1,670)	1:115:A:ILE:HG21	1:119:A:ALA:HB2	9	0.13
(1,670)	1:115:A:ILE:HG21	1:119:A:ALA:HB3	9	0.13
(1,670)	1:115:A:ILE:HG22	1:119:A:ALA:HB1	9	0.13
(1,670)	1:115:A:ILE:HG22	1:119:A:ALA:HB2	9	0.13
(1,670)	1:115:A:ILE:HG22	1:119:A:ALA:HB3	9	0.13
(1,670)	1:115:A:ILE:HG23	1:119:A:ALA:HB1	9	0.13
(1,670)	1:115:A:ILE:HG23	1:119:A:ALA:HB2	9	0.13
(1,670)	1:115:A:ILE:HG23	1:119:A:ALA:HB3	9	0.13
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	17	0.13
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	17	0.13
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	17	0.13
(1,629)	1:92:A:LEU:HA	1:127:A:LEU:HG	14	0.13
(1,598)	1:123:A:PHE:HB3	1:124:A:GLU:HA	7	0.13
(1,581)	1:55:A:PRO:HG3	1:120:A:THR:HB	10	0.13
(1,579)	1:102:A:TYR:HB2	1:119:A:ALA:HB1	15	0.13
(1,579)	1:102:A:TYR:HB2	1:119:A:ALA:HB2	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:102:A:TYR:HB2	1:119:A:ALA:HB3	15	0.13
(1,548)	1:102:A:TYR:HE2	1:108:A:GLU:HG3	19	0.13
(1,542)	1:108:A:GLU:HA	1:118:A:LYS:HG3	12	0.13
(1,500)	1:81:A:LYS:HB2	1:104:A:LEU:HA	6	0.13
(1,498)	1:103:A:GLN:HA	1:104:A:LEU:HG	16	0.13
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD11	2	0.13
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD12	2	0.13
(1,483)	1:100:A:ILE:HG21	1:104:A:LEU:HD13	2	0.13
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD11	2	0.13
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD12	2	0.13
(1,483)	1:100:A:ILE:HG22	1:104:A:LEU:HD13	2	0.13
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD11	2	0.13
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD12	2	0.13
(1,483)	1:100:A:ILE:HG23	1:104:A:LEU:HD13	2	0.13
(1,460)	1:97:A:LEU:HD11	1:98:A:PHE:H	18	0.13
(1,460)	1:97:A:LEU:HD12	1:98:A:PHE:H	18	0.13
(1,460)	1:97:A:LEU:HD13	1:98:A:PHE:H	18	0.13
(1,457)	1:29:A:LYS:H	1:97:A:LEU:HB2	18	0.13
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB1	16	0.13
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB2	16	0.13
(1,454)	1:94:A:GLU:HG2	1:96:A:ALA:HB3	16	0.13
(1,411)	1:90:A:MET:HE1	1:127:A:LEU:H	16	0.13
(1,411)	1:90:A:MET:HE2	1:127:A:LEU:H	16	0.13
(1,411)	1:90:A:MET:HE3	1:127:A:LEU:H	16	0.13
(1,378)	1:81:A:LYS:HA	1:84:A:ASP:HB3	9	0.13
(1,369)	1:83:A:TRP:H	1:84:A:ASP:HB2	12	0.13
(1,365)	1:79:A:VAL:HG21	1:83:A:TRP:HA	15	0.13
(1,365)	1:79:A:VAL:HG22	1:83:A:TRP:HA	15	0.13
(1,365)	1:79:A:VAL:HG23	1:83:A:TRP:HA	15	0.13
(1,343)	1:66:A:ARG:HG3	1:68:A:LYS:H	20	0.13
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD21	5	0.13
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD22	5	0.13
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD23	5	0.13
(1,333)	1:81:A:LYS:HA	1:81:A:LYS:HD3	3	0.13
(1,328)	1:80:A:ILE:HG13	1:83:A:TRP:H	13	0.13
(1,326)	1:80:A:ILE:HG13	1:104:A:LEU:HB3	1	0.13
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG21	10	0.13
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG22	10	0.13
(1,320)	1:80:A:ILE:HG21	1:100:A:ILE:HG23	10	0.13
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG21	10	0.13
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG22	10	0.13
(1,320)	1:80:A:ILE:HG22	1:100:A:ILE:HG23	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG21	10	0.13
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG22	10	0.13
(1,320)	1:80:A:ILE:HG23	1:100:A:ILE:HG23	10	0.13
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD11	3	0.13
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD12	3	0.13
(1,299)	1:79:A:VAL:HA	1:80:A:ILE:HD13	3	0.13
(1,280)	1:74:A:LEU:HG	1:75:A:GLY:HA3	14	0.13
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD21	3	0.13
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD22	3	0.13
(1,267)	1:43:A:GLY:H	1:74:A:LEU:HD23	3	0.13
(1,229)	1:69:A:PRO:HA	1:128:A:LEU:HG	18	0.13
(1,224)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	17	0.13
(1,208)	1:63:A:SER:H	1:64:A:ARG:HA	14	0.13
(1,179)	1:54:A:PHE:HB2	1:55:A:PRO:HD3	15	0.13
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	20	0.13
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	20	0.13
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	20	0.13
(1,127)	1:47:A:THR:HB	1:48:A:VAL:HA	1	0.13
(1,127)	1:47:A:THR:HB	1:48:A:VAL:HA	7	0.13
(1,119)	1:46:A:VAL:HG21	1:74:A:LEU:HD11	15	0.13
(1,119)	1:46:A:VAL:HG21	1:74:A:LEU:HD12	15	0.13
(1,119)	1:46:A:VAL:HG21	1:74:A:LEU:HD13	15	0.13
(1,119)	1:46:A:VAL:HG22	1:74:A:LEU:HD11	15	0.13
(1,119)	1:46:A:VAL:HG22	1:74:A:LEU:HD12	15	0.13
(1,119)	1:46:A:VAL:HG22	1:74:A:LEU:HD13	15	0.13
(1,119)	1:46:A:VAL:HG23	1:74:A:LEU:HD11	15	0.13
(1,119)	1:46:A:VAL:HG23	1:74:A:LEU:HD12	15	0.13
(1,119)	1:46:A:VAL:HG23	1:74:A:LEU:HD13	15	0.13
(1,98)	1:45:A:LYS:HB3	1:46:A:VAL:H	5	0.13
(1,93)	1:41:A:GLN:HG3	1:44:A:LYS:HG2	13	0.13
(1,89)	1:42:A:ALA:HB1	1:74:A:LEU:HA	2	0.13
(1,89)	1:42:A:ALA:HB2	1:74:A:LEU:HA	2	0.13
(1,89)	1:42:A:ALA:HB3	1:74:A:LEU:HA	2	0.13
(1,89)	1:42:A:ALA:HB1	1:74:A:LEU:HA	3	0.13
(1,89)	1:42:A:ALA:HB2	1:74:A:LEU:HA	3	0.13
(1,89)	1:42:A:ALA:HB3	1:74:A:LEU:HA	3	0.13
(1,72)	1:40:A:PRO:HB3	1:41:A:GLN:H	13	0.13
(1,70)	1:38:A:THR:HG21	1:92:A:LEU:HG	14	0.13
(1,70)	1:38:A:THR:HG22	1:92:A:LEU:HG	14	0.13
(1,70)	1:38:A:THR:HG23	1:92:A:LEU:HG	14	0.13
(1,16)	1:41:A:GLN:H	1:41:A:GLN:HB2	4	0.13
(1,16)	1:41:A:GLN:H	1:41:A:GLN:HB2	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1647)	1:121:A:LEU:HD11	1:122:A:VAL:H	2	0.12
(1,1647)	1:121:A:LEU:HD12	1:122:A:VAL:H	2	0.12
(1,1647)	1:121:A:LEU:HD13	1:122:A:VAL:H	2	0.12
(1,1647)	1:121:A:LEU:HD21	1:122:A:VAL:H	2	0.12
(1,1647)	1:121:A:LEU:HD22	1:122:A:VAL:H	2	0.12
(1,1647)	1:121:A:LEU:HD23	1:122:A:VAL:H	2	0.12
(1,1647)	1:121:A:LEU:HD11	1:122:A:VAL:H	6	0.12
(1,1647)	1:121:A:LEU:HD12	1:122:A:VAL:H	6	0.12
(1,1647)	1:121:A:LEU:HD13	1:122:A:VAL:H	6	0.12
(1,1647)	1:121:A:LEU:HD21	1:122:A:VAL:H	6	0.12
(1,1647)	1:121:A:LEU:HD22	1:122:A:VAL:H	6	0.12
(1,1647)	1:121:A:LEU:HD23	1:122:A:VAL:H	6	0.12
(1,1647)	1:121:A:LEU:HD11	1:122:A:VAL:H	12	0.12
(1,1647)	1:121:A:LEU:HD12	1:122:A:VAL:H	12	0.12
(1,1647)	1:121:A:LEU:HD13	1:122:A:VAL:H	12	0.12
(1,1647)	1:121:A:LEU:HD21	1:122:A:VAL:H	12	0.12
(1,1647)	1:121:A:LEU:HD22	1:122:A:VAL:H	12	0.12
(1,1647)	1:121:A:LEU:HD23	1:122:A:VAL:H	12	0.12
(1,1622)	1:108:A:GLU:HA	1:118:A:LYS:HB2	13	0.12
(1,1622)	1:108:A:GLU:HA	1:118:A:LYS:HB3	13	0.12
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB2	7	0.12
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB3	7	0.12
(1,1525)	1:78:A:GLU:HG2	1:79:A:VAL:HG11	16	0.12
(1,1525)	1:78:A:GLU:HG2	1:79:A:VAL:HG12	16	0.12
(1,1525)	1:78:A:GLU:HG2	1:79:A:VAL:HG13	16	0.12
(1,1525)	1:78:A:GLU:HG3	1:79:A:VAL:HG11	16	0.12
(1,1525)	1:78:A:GLU:HG3	1:79:A:VAL:HG12	16	0.12
(1,1525)	1:78:A:GLU:HG3	1:79:A:VAL:HG13	16	0.12
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	8	0.12
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	8	0.12
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	8	0.12
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	8	0.12
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	8	0.12
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	8	0.12
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	9	0.12
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	9	0.12
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG11	20	0.12
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG12	20	0.12
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG13	20	0.12
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG21	20	0.12
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG22	20	0.12
(1,1478)	1:60:A:PHE:HB2	1:114:A:VAL:HG23	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG11	20	0.12
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG12	20	0.12
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG13	20	0.12
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG21	20	0.12
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG22	20	0.12
(1,1478)	1:60:A:PHE:HB3	1:114:A:VAL:HG23	20	0.12
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA2	4	0.12
(1,1427)	1:49:A:HIS:HE1	1:67:A:GLY:HA3	4	0.12
(1,1284)	1:127:A:LEU:H	1:127:A:LEU:HG	1	0.12
(1,1284)	1:127:A:LEU:H	1:127:A:LEU:HG	4	0.12
(1,1276)	1:96:A:ALA:H	1:127:A:LEU:H	12	0.12
(1,1250)	1:123:A:PHE:H	1:123:A:PHE:HB3	10	0.12
(1,1236)	1:119:A:ALA:HB1	1:120:A:THR:H	18	0.12
(1,1236)	1:119:A:ALA:HB2	1:120:A:THR:H	18	0.12
(1,1236)	1:119:A:ALA:HB3	1:120:A:THR:H	18	0.12
(1,1219)	1:111:A:TYR:H	1:115:A:ILE:HB	2	0.12
(1,1218)	1:111:A:TYR:H	1:111:A:TYR:HB3	1	0.12
(1,1216)	1:110:A:GLY:HA2	1:111:A:TYR:H	5	0.12
(1,1204)	1:100:A:ILE:HG21	1:106:A:TYR:H	12	0.12
(1,1204)	1:100:A:ILE:HG22	1:106:A:TYR:H	12	0.12
(1,1204)	1:100:A:ILE:HG23	1:106:A:TYR:H	12	0.12
(1,1193)	1:105:A:ALA:H	1:107:A:GLY:H	6	0.12
(1,1184)	1:103:A:GLN:H	1:104:A:LEU:HB2	12	0.12
(1,1172)	1:102:A:TYR:H	1:105:A:ALA:H	19	0.12
(1,1152)	1:98:A:PHE:H	1:123:A:PHE:HB3	8	0.12
(1,1152)	1:98:A:PHE:H	1:123:A:PHE:HB3	13	0.12
(1,1147)	1:98:A:PHE:H	1:99:A:THR:H	13	0.12
(1,1113)	1:91:A:THR:HG21	1:92:A:LEU:H	6	0.12
(1,1113)	1:91:A:THR:HG22	1:92:A:LEU:H	6	0.12
(1,1113)	1:91:A:THR:HG23	1:92:A:LEU:H	6	0.12
(1,1113)	1:91:A:THR:HG21	1:92:A:LEU:H	12	0.12
(1,1113)	1:91:A:THR:HG22	1:92:A:LEU:H	12	0.12
(1,1113)	1:91:A:THR:HG23	1:92:A:LEU:H	12	0.12
(1,1113)	1:91:A:THR:HG21	1:92:A:LEU:H	17	0.12
(1,1113)	1:91:A:THR:HG22	1:92:A:LEU:H	17	0.12
(1,1113)	1:91:A:THR:HG23	1:92:A:LEU:H	17	0.12
(1,1106)	1:37:A:VAL:H	1:92:A:LEU:H	10	0.12
(1,1097)	1:34:A:GLY:HA3	1:91:A:THR:H	15	0.12
(1,1092)	1:90:A:MET:H	1:90:A:MET:HG3	6	0.12
(1,1065)	1:79:A:VAL:HG21	1:85:A:GLN:H	18	0.12
(1,1065)	1:79:A:VAL:HG22	1:85:A:GLN:H	18	0.12
(1,1065)	1:79:A:VAL:HG23	1:85:A:GLN:H	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1055)	1:83:A:TRP:H	1:85:A:GLN:H	2	0.12
(1,1037)	1:80:A:ILE:HG12	1:83:A:TRP:H	3	0.12
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG21	7	0.12
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG22	7	0.12
(1,1030)	1:82:A:GLY:H	1:100:A:ILE:HG23	7	0.12
(1,1001)	1:73:A:THR:HB	1:76:A:ALA:H	7	0.12
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB1	18	0.12
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB2	18	0.12
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB3	18	0.12
(1,966)	1:69:A:PRO:HB3	1:70:A:PHE:H	12	0.12
(1,952)	1:67:A:GLY:H	1:68:A:LYS:HB2	6	0.12
(1,919)	1:60:A:PHE:HD1	1:61:A:ASP:H	20	0.12
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	7	0.12
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	14	0.12
(1,909)	1:56:A:ASP:HA	1:57:A:GLY:H	17	0.12
(1,897)	1:59:A:GLN:HE21	1:62:A:SER:HB3	17	0.12
(1,866)	1:51:A:ASP:H	1:124:A:GLU:HB3	5	0.12
(1,863)	1:50:A:TYR:HB2	1:51:A:ASP:H	1	0.12
(1,863)	1:50:A:TYR:HB2	1:51:A:ASP:H	6	0.12
(1,830)	1:46:A:VAL:H	1:72:A:PHE:HA	11	0.12
(1,813)	1:43:A:GLY:H	1:74:A:LEU:HG	19	0.12
(1,806)	1:42:A:ALA:H	1:74:A:LEU:HG	14	0.12
(1,806)	1:42:A:ALA:H	1:74:A:LEU:HG	19	0.12
(1,797)	1:41:A:GLN:H	1:41:A:GLN:HG2	12	0.12
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG21	12	0.12
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG22	12	0.12
(1,795)	1:39:A:LYS:H	1:130:A:VAL:HG23	12	0.12
(1,789)	1:38:A:THR:H	1:91:A:THR:HG21	1	0.12
(1,789)	1:38:A:THR:H	1:91:A:THR:HG22	1	0.12
(1,789)	1:38:A:THR:H	1:91:A:THR:HG23	1	0.12
(1,787)	1:37:A:VAL:HB	1:38:A:THR:H	10	0.12
(1,787)	1:37:A:VAL:HB	1:38:A:THR:H	12	0.12
(1,781)	1:37:A:VAL:H	1:91:A:THR:HB	9	0.12
(1,751)	1:27:A:GLU:HG2	1:28:A:LYS:H	10	0.12
(1,748)	1:27:A:GLU:H	1:99:A:THR:HB	1	0.12
(1,748)	1:27:A:GLU:H	1:99:A:THR:HB	15	0.12
(1,697)	1:79:A:VAL:HG11	1:83:A:TRP:HZ3	9	0.12
(1,697)	1:79:A:VAL:HG12	1:83:A:TRP:HZ3	9	0.12
(1,697)	1:79:A:VAL:HG13	1:83:A:TRP:HZ3	9	0.12
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG21	16	0.12
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG22	16	0.12
(1,665)	1:110:A:GLY:H	1:115:A:ILE:HG23	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD11	10	0.12
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD12	10	0.12
(1,637)	1:46:A:VAL:HB	1:127:A:LEU:HD13	10	0.12
(1,578)	1:119:A:ALA:HB1	1:120:A:THR:HB	1	0.12
(1,578)	1:119:A:ALA:HB2	1:120:A:THR:HB	1	0.12
(1,578)	1:119:A:ALA:HB3	1:120:A:THR:HB	1	0.12
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG21	13	0.12
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG22	13	0.12
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG23	13	0.12
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG21	18	0.12
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG22	18	0.12
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG23	18	0.12
(1,546)	1:108:A:GLU:HG3	1:118:A:LYS:HG2	3	0.12
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB1	14	0.12
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB2	14	0.12
(1,495)	1:102:A:TYR:HB2	1:105:A:ALA:HB3	14	0.12
(1,481)	1:100:A:ILE:HG21	1:104:A:LEU:HA	10	0.12
(1,481)	1:100:A:ILE:HG22	1:104:A:LEU:HA	10	0.12
(1,481)	1:100:A:ILE:HG23	1:104:A:LEU:HA	10	0.12
(1,470)	1:100:A:ILE:HB	1:121:A:LEU:HB2	16	0.12
(1,460)	1:97:A:LEU:HD11	1:98:A:PHE:H	16	0.12
(1,460)	1:97:A:LEU:HD12	1:98:A:PHE:H	16	0.12
(1,460)	1:97:A:LEU:HD13	1:98:A:PHE:H	16	0.12
(1,459)	1:97:A:LEU:HG	1:99:A:THR:H	11	0.12
(1,444)	1:31:A:LEU:HG	1:95:A:LYS:HB3	6	0.12
(1,422)	1:38:A:THR:HG21	1:91:A:THR:HA	6	0.12
(1,422)	1:38:A:THR:HG22	1:91:A:THR:HA	6	0.12
(1,422)	1:38:A:THR:HG23	1:91:A:THR:HA	6	0.12
(1,419)	1:34:A:GLY:HA3	1:91:A:THR:HA	1	0.12
(1,405)	1:85:A:GLN:HA	1:89:A:THR:HG21	6	0.12
(1,405)	1:85:A:GLN:HA	1:89:A:THR:HG22	6	0.12
(1,405)	1:85:A:GLN:HA	1:89:A:THR:HG23	6	0.12
(1,345)	1:82:A:GLY:HA3	1:85:A:GLN:H	6	0.12
(1,328)	1:80:A:ILE:HG13	1:83:A:TRP:H	20	0.12
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG21	11	0.12
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG22	11	0.12
(1,317)	1:80:A:ILE:HB	1:100:A:ILE:HG23	11	0.12
(1,316)	1:80:A:ILE:HB	1:104:A:LEU:HB3	2	0.12
(1,309)	1:80:A:ILE:HA	1:81:A:LYS:HB2	4	0.12
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG21	3	0.12
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG22	3	0.12
(1,306)	1:79:A:VAL:HB	1:80:A:ILE:HG23	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,289)	1:76:A:ALA:HB1	1:78:A:GLU:HB2	13	0.12
(1,289)	1:76:A:ALA:HB2	1:78:A:GLU:HB2	13	0.12
(1,289)	1:76:A:ALA:HB3	1:78:A:GLU:HB2	13	0.12
(1,227)	1:67:A:GLY:HA3	1:68:A:LYS:HB2	6	0.12
(1,224)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	6	0.12
(1,224)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	12	0.12
(1,220)	1:66:A:ARG:HA	1:66:A:ARG:HD2	4	0.12
(1,192)	1:59:A:GLN:HA	1:61:A:ASP:H	17	0.12
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG21	4	0.12
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG22	4	0.12
(1,175)	1:55:A:PRO:HG2	1:120:A:THR:HG23	4	0.12
(1,149)	1:50:A:TYR:HB2	1:123:A:PHE:HD2	15	0.12
(1,130)	1:48:A:VAL:HG11	1:50:A:TYR:HD1	9	0.12
(1,130)	1:48:A:VAL:HG12	1:50:A:TYR:HD1	9	0.12
(1,130)	1:48:A:VAL:HG13	1:50:A:TYR:HD1	9	0.12
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	10	0.12
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	10	0.12
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	10	0.12
(1,127)	1:47:A:THR:HB	1:48:A:VAL:HA	11	0.12
(1,109)	1:46:A:VAL:HB	1:129:A:ALA:H	10	0.12
(1,75)	1:38:A:THR:HB	1:40:A:PRO:HG3	6	0.12
(1,49)	1:35:A:ASP:HA	1:37:A:VAL:HG21	15	0.12
(1,49)	1:35:A:ASP:HA	1:37:A:VAL:HG22	15	0.12
(1,49)	1:35:A:ASP:HA	1:37:A:VAL:HG23	15	0.12
(1,26)	1:27:A:GLU:HG3	1:99:A:THR:H	9	0.12
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB1	17	0.12
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB2	17	0.12
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB3	17	0.12
(1,16)	1:41:A:GLN:H	1:41:A:GLN:HB2	7	0.12
(1,1647)	1:121:A:LEU:HD11	1:122:A:VAL:H	13	0.11
(1,1647)	1:121:A:LEU:HD12	1:122:A:VAL:H	13	0.11
(1,1647)	1:121:A:LEU:HD13	1:122:A:VAL:H	13	0.11
(1,1647)	1:121:A:LEU:HD21	1:122:A:VAL:H	13	0.11
(1,1647)	1:121:A:LEU:HD22	1:122:A:VAL:H	13	0.11
(1,1647)	1:121:A:LEU:HD23	1:122:A:VAL:H	13	0.11
(1,1625)	1:108:A:GLU:HG2	1:118:A:LYS:HG3	2	0.11
(1,1625)	1:108:A:GLU:HG3	1:118:A:LYS:HG3	2	0.11
(1,1576)	1:92:A:LEU:HD11	1:130:A:VAL:HB	17	0.11
(1,1576)	1:92:A:LEU:HD12	1:130:A:VAL:HB	17	0.11
(1,1576)	1:92:A:LEU:HD13	1:130:A:VAL:HB	17	0.11
(1,1576)	1:92:A:LEU:HD21	1:130:A:VAL:HB	17	0.11
(1,1576)	1:92:A:LEU:HD22	1:130:A:VAL:HB	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1576)	1:92:A:LEU:HD23	1:130:A:VAL:HB	17	0.11
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB2	5	0.11
(1,1528)	1:82:A:GLY:HA3	1:85:A:GLN:HB3	5	0.11
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE21	20	0.11
(1,1526)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	20	0.11
(1,1523)	1:78:A:GLU:HA	1:78:A:GLU:HG2	10	0.11
(1,1523)	1:78:A:GLU:HA	1:78:A:GLU:HG3	10	0.11
(1,1506)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	1	0.11
(1,1506)	1:67:A:GLY:HA3	1:68:A:LYS:HB2	1	0.11
(1,1506)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	14	0.11
(1,1506)	1:67:A:GLY:HA3	1:68:A:LYS:HB2	14	0.11
(1,1490)	1:64:A:ARG:H	1:64:A:ARG:HD2	5	0.11
(1,1490)	1:64:A:ARG:H	1:64:A:ARG:HD3	5	0.11
(1,1483)	1:62:A:SER:HB2	1:63:A:SER:H	15	0.11
(1,1483)	1:62:A:SER:HB3	1:63:A:SER:H	15	0.11
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE21	5	0.11
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE22	5	0.11
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE21	9	0.11
(1,1471)	1:59:A:GLN:H	1:59:A:GLN:HE22	9	0.11
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG11	5	0.11
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG12	5	0.11
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG13	5	0.11
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG21	5	0.11
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG22	5	0.11
(1,1454)	1:54:A:PHE:HE1	1:114:A:VAL:HG23	5	0.11
(1,1398)	1:43:A:GLY:HA2	1:73:A:THR:HG21	4	0.11
(1,1398)	1:43:A:GLY:HA2	1:73:A:THR:HG22	4	0.11
(1,1398)	1:43:A:GLY:HA2	1:73:A:THR:HG23	4	0.11
(1,1398)	1:43:A:GLY:HA3	1:73:A:THR:HG21	4	0.11
(1,1398)	1:43:A:GLY:HA3	1:73:A:THR:HG22	4	0.11
(1,1398)	1:43:A:GLY:HA3	1:73:A:THR:HG23	4	0.11
(1,1367)	1:35:A:ASP:HB2	1:37:A:VAL:HG21	8	0.11
(1,1367)	1:35:A:ASP:HB2	1:37:A:VAL:HG22	8	0.11
(1,1367)	1:35:A:ASP:HB2	1:37:A:VAL:HG23	8	0.11
(1,1367)	1:35:A:ASP:HB3	1:37:A:VAL:HG21	8	0.11
(1,1367)	1:35:A:ASP:HB3	1:37:A:VAL:HG22	8	0.11
(1,1367)	1:35:A:ASP:HB3	1:37:A:VAL:HG23	8	0.11
(1,1324)	1:19:A:PRO:HG2	1:55:A:PRO:HG2	1	0.11
(1,1324)	1:19:A:PRO:HG3	1:55:A:PRO:HG2	1	0.11
(1,1317)	1:13:A:GLU:HB2	1:14:A:ALA:H	15	0.11
(1,1317)	1:13:A:GLU:HB3	1:14:A:ALA:H	15	0.11
(1,1309)	1:81:A:LYS:HD2	1:85:A:GLN:HE22	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1308)	1:81:A:LYS:HD2	1:85:A:GLN:HE21	20	0.11
(1,1305)	1:71:A:GLN:HA	1:71:A:GLN:HE22	20	0.11
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	5	0.11
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	5	0.11
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	5	0.11
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB1	17	0.11
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB2	17	0.11
(1,1287)	1:128:A:LEU:H	1:129:A:ALA:HB3	17	0.11
(1,1284)	1:127:A:LEU:H	1:127:A:LEU:HG	7	0.11
(1,1284)	1:127:A:LEU:H	1:127:A:LEU:HG	17	0.11
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD21	14	0.11
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD22	14	0.11
(1,1283)	1:127:A:LEU:H	1:127:A:LEU:HD23	14	0.11
(1,1276)	1:96:A:ALA:H	1:127:A:LEU:H	16	0.11
(1,1259)	1:124:A:GLU:H	1:125:A:VAL:HG11	11	0.11
(1,1259)	1:124:A:GLU:H	1:125:A:VAL:HG12	11	0.11
(1,1259)	1:124:A:GLU:H	1:125:A:VAL:HG13	11	0.11
(1,1236)	1:119:A:ALA:HB1	1:120:A:THR:H	10	0.11
(1,1236)	1:119:A:ALA:HB2	1:120:A:THR:H	10	0.11
(1,1236)	1:119:A:ALA:HB3	1:120:A:THR:H	10	0.11
(1,1236)	1:119:A:ALA:HB1	1:120:A:THR:H	12	0.11
(1,1236)	1:119:A:ALA:HB2	1:120:A:THR:H	12	0.11
(1,1236)	1:119:A:ALA:HB3	1:120:A:THR:H	12	0.11
(1,1236)	1:119:A:ALA:HB1	1:120:A:THR:H	16	0.11
(1,1236)	1:119:A:ALA:HB2	1:120:A:THR:H	16	0.11
(1,1236)	1:119:A:ALA:HB3	1:120:A:THR:H	16	0.11
(1,1193)	1:105:A:ALA:H	1:107:A:GLY:H	3	0.11
(1,1193)	1:105:A:ALA:H	1:107:A:GLY:H	14	0.11
(1,1193)	1:105:A:ALA:H	1:107:A:GLY:H	17	0.11
(1,1184)	1:103:A:GLN:H	1:104:A:LEU:HB2	15	0.11
(1,1147)	1:98:A:PHE:H	1:99:A:THR:H	5	0.11
(1,1147)	1:98:A:PHE:H	1:99:A:THR:H	6	0.11
(1,1113)	1:91:A:THR:HG21	1:92:A:LEU:H	10	0.11
(1,1113)	1:91:A:THR:HG22	1:92:A:LEU:H	10	0.11
(1,1113)	1:91:A:THR:HG23	1:92:A:LEU:H	10	0.11
(1,1106)	1:37:A:VAL:H	1:92:A:LEU:H	19	0.11
(1,1105)	1:38:A:THR:H	1:92:A:LEU:H	8	0.11
(1,1104)	1:91:A:THR:H	1:127:A:LEU:HG	14	0.11
(1,1065)	1:79:A:VAL:HG21	1:85:A:GLN:H	20	0.11
(1,1065)	1:79:A:VAL:HG22	1:85:A:GLN:H	20	0.11
(1,1065)	1:79:A:VAL:HG23	1:85:A:GLN:H	20	0.11
(1,1009)	1:76:A:ALA:H	1:78:A:GLU:H	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG21	12	0.11
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG22	12	0.11
(1,1008)	1:77:A:GLY:H	1:79:A:VAL:HG23	12	0.11
(1,1003)	1:74:A:LEU:HB3	1:76:A:ALA:H	20	0.11
(1,977)	1:47:A:THR:HG21	1:71:A:GLN:H	3	0.11
(1,977)	1:47:A:THR:HG22	1:71:A:GLN:H	3	0.11
(1,977)	1:47:A:THR:HG23	1:71:A:GLN:H	3	0.11
(1,910)	1:55:A:PRO:HA	1:57:A:GLY:H	20	0.11
(1,887)	1:53:A:ARG:HB3	1:54:A:PHE:H	2	0.11
(1,868)	1:51:A:ASP:H	1:125:A:VAL:HG11	2	0.11
(1,868)	1:51:A:ASP:H	1:125:A:VAL:HG12	2	0.11
(1,868)	1:51:A:ASP:H	1:125:A:VAL:HG13	2	0.11
(1,863)	1:50:A:TYR:HB2	1:51:A:ASP:H	19	0.11
(1,837)	1:47:A:THR:H	1:71:A:GLN:HA	15	0.11
(1,836)	1:47:A:THR:H	1:128:A:LEU:H	2	0.11
(1,828)	1:46:A:VAL:H	1:71:A:GLN:HA	1	0.11
(1,787)	1:37:A:VAL:HB	1:38:A:THR:H	16	0.11
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG21	10	0.11
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG22	10	0.11
(1,783)	1:37:A:VAL:H	1:91:A:THR:HG23	10	0.11
(1,744)	1:26:A:LEU:H	1:27:A:GLU:HG3	7	0.11
(1,684)	1:48:A:VAL:HG21	1:50:A:TYR:HE1	10	0.11
(1,684)	1:48:A:VAL:HG22	1:50:A:TYR:HE1	10	0.11
(1,684)	1:48:A:VAL:HG23	1:50:A:TYR:HE1	10	0.11
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG21	6	0.11
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG22	6	0.11
(1,657)	1:38:A:THR:HB	1:130:A:VAL:HG23	6	0.11
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG11	11	0.11
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG12	11	0.11
(1,656)	1:38:A:THR:HB	1:130:A:VAL:HG13	11	0.11
(1,581)	1:55:A:PRO:HG3	1:120:A:THR:HB	2	0.11
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG21	7	0.11
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG22	7	0.11
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG23	7	0.11
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG21	9	0.11
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG22	9	0.11
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG23	9	0.11
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG21	11	0.11
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG22	11	0.11
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG23	11	0.11
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG21	14	0.11
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG22	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG23	14	0.11
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG21	20	0.11
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG22	20	0.11
(1,562)	1:114:A:VAL:HA	1:114:A:VAL:HG23	20	0.11
(1,536)	1:102:A:TYR:HE2	1:108:A:GLU:HB2	19	0.11
(1,498)	1:103:A:GLN:HA	1:104:A:LEU:HG	1	0.11
(1,498)	1:103:A:GLN:HA	1:104:A:LEU:HG	2	0.11
(1,487)	1:102:A:TYR:HA	1:105:A:ALA:HB1	14	0.11
(1,487)	1:102:A:TYR:HA	1:105:A:ALA:HB2	14	0.11
(1,487)	1:102:A:TYR:HA	1:105:A:ALA:HB3	14	0.11
(1,425)	1:92:A:LEU:HG	1:93:A:GLY:H	14	0.11
(1,413)	1:90:A:MET:HE1	1:91:A:THR:H	5	0.11
(1,413)	1:90:A:MET:HE2	1:91:A:THR:H	5	0.11
(1,413)	1:90:A:MET:HE3	1:91:A:THR:H	5	0.11
(1,378)	1:81:A:LYS:HA	1:84:A:ASP:HB3	16	0.11
(1,355)	1:81:A:LYS:HB3	1:82:A:GLY:HA2	17	0.11
(1,347)	1:82:A:GLY:HA3	1:104:A:LEU:HB2	4	0.11
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD21	18	0.11
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD22	18	0.11
(1,341)	1:81:A:LYS:HG3	1:104:A:LEU:HD23	18	0.11
(1,328)	1:80:A:ILE:HG13	1:83:A:TRP:H	12	0.11
(1,294)	1:78:A:GLU:H	1:78:A:GLU:HG2	15	0.11
(1,276)	1:74:A:LEU:HD11	1:88:A:ALA:H	14	0.11
(1,276)	1:74:A:LEU:HD12	1:88:A:ALA:H	14	0.11
(1,276)	1:74:A:LEU:HD13	1:88:A:ALA:H	14	0.11
(1,274)	1:74:A:LEU:HD11	1:87:A:VAL:H	19	0.11
(1,274)	1:74:A:LEU:HD12	1:87:A:VAL:H	19	0.11
(1,274)	1:74:A:LEU:HD13	1:87:A:VAL:H	19	0.11
(1,266)	1:74:A:LEU:HD21	1:75:A:GLY:H	11	0.11
(1,266)	1:74:A:LEU:HD22	1:75:A:GLY:H	11	0.11
(1,266)	1:74:A:LEU:HD23	1:75:A:GLY:H	11	0.11
(1,224)	1:67:A:GLY:HA2	1:68:A:LYS:HB2	4	0.11
(1,220)	1:66:A:ARG:HA	1:66:A:ARG:HD2	8	0.11
(1,208)	1:63:A:SER:H	1:64:A:ARG:HA	17	0.11
(1,198)	1:59:A:GLN:HG2	1:61:A:ASP:H	10	0.11
(1,169)	1:53:A:ARG:HD2	1:59:A:GLN:H	16	0.11
(1,161)	1:53:A:ARG:HA	1:60:A:PHE:H	8	0.11
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	2	0.11
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	2	0.11
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	2	0.11
(1,129)	1:48:A:VAL:HG11	1:128:A:LEU:H	15	0.11
(1,129)	1:48:A:VAL:HG12	1:128:A:LEU:H	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,129)	1:48:A:VAL:HG13	1:128:A:LEU:H	15	0.11
(1,127)	1:47:A:THR:HB	1:48:A:VAL:HA	15	0.11
(1,123)	1:46:A:VAL:HG11	1:130:A:VAL:HB	8	0.11
(1,123)	1:46:A:VAL:HG12	1:130:A:VAL:HB	8	0.11
(1,123)	1:46:A:VAL:HG13	1:130:A:VAL:HB	8	0.11
(1,114)	1:46:A:VAL:HG21	1:47:A:THR:H	8	0.11
(1,114)	1:46:A:VAL:HG22	1:47:A:THR:H	8	0.11
(1,114)	1:46:A:VAL:HG23	1:47:A:THR:H	8	0.11
(1,109)	1:46:A:VAL:HB	1:129:A:ALA:H	9	0.11
(1,100)	1:45:A:LYS:HB3	1:46:A:VAL:HA	14	0.11
(1,98)	1:45:A:LYS:HB3	1:46:A:VAL:H	11	0.11
(1,98)	1:45:A:LYS:HB3	1:46:A:VAL:H	12	0.11
(1,98)	1:45:A:LYS:HB3	1:46:A:VAL:H	15	0.11
(1,78)	1:40:A:PRO:HD3	1:91:A:THR:HG21	2	0.11
(1,78)	1:40:A:PRO:HD3	1:91:A:THR:HG22	2	0.11
(1,78)	1:40:A:PRO:HD3	1:91:A:THR:HG23	2	0.11
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG21	16	0.11
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG22	16	0.11
(1,73)	1:40:A:PRO:HB3	1:46:A:VAL:HG23	16	0.11
(1,68)	1:38:A:THR:HG21	1:92:A:LEU:HA	20	0.11
(1,68)	1:38:A:THR:HG22	1:92:A:LEU:HA	20	0.11
(1,68)	1:38:A:THR:HG23	1:92:A:LEU:HA	20	0.11
(1,45)	1:34:A:GLY:HA3	1:94:A:GLU:HB2	12	0.11
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB1	5	0.11
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB2	5	0.11
(1,17)	1:41:A:GLN:HA	1:42:A:ALA:HB3	5	0.11
(1,1647)	1:121:A:LEU:HD11	1:122:A:VAL:H	7	0.1
(1,1647)	1:121:A:LEU:HD12	1:122:A:VAL:H	7	0.1
(1,1647)	1:121:A:LEU:HD13	1:122:A:VAL:H	7	0.1
(1,1647)	1:121:A:LEU:HD21	1:122:A:VAL:H	7	0.1
(1,1647)	1:121:A:LEU:HD22	1:122:A:VAL:H	7	0.1
(1,1647)	1:121:A:LEU:HD23	1:122:A:VAL:H	7	0.1
(1,1596)	1:97:A:LEU:HD11	1:124:A:GLU:H	10	0.1
(1,1596)	1:97:A:LEU:HD12	1:124:A:GLU:H	10	0.1
(1,1596)	1:97:A:LEU:HD13	1:124:A:GLU:H	10	0.1
(1,1596)	1:97:A:LEU:HD21	1:124:A:GLU:H	10	0.1
(1,1596)	1:97:A:LEU:HD22	1:124:A:GLU:H	10	0.1
(1,1596)	1:97:A:LEU:HD23	1:124:A:GLU:H	10	0.1
(1,1594)	1:97:A:LEU:HD11	1:123:A:PHE:H	20	0.1
(1,1594)	1:97:A:LEU:HD12	1:123:A:PHE:H	20	0.1
(1,1594)	1:97:A:LEU:HD13	1:123:A:PHE:H	20	0.1
(1,1594)	1:97:A:LEU:HD21	1:123:A:PHE:H	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1594)	1:97:A:LEU:HD22	1:123:A:PHE:H	20	0.1
(1,1594)	1:97:A:LEU:HD23	1:123:A:PHE:H	20	0.1
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB2	13	0.1
(1,1532)	1:84:A:ASP:HB2	1:85:A:GLN:HB3	13	0.1
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB1	4	0.1
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB2	4	0.1
(1,1519)	1:71:A:GLN:HG2	1:129:A:ALA:HB3	4	0.1
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB1	4	0.1
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB2	4	0.1
(1,1519)	1:71:A:GLN:HG3	1:129:A:ALA:HB3	4	0.1
(1,1491)	1:64:A:ARG:HA	1:64:A:ARG:HD2	3	0.1
(1,1491)	1:64:A:ARG:HA	1:64:A:ARG:HD3	3	0.1
(1,1490)	1:64:A:ARG:H	1:64:A:ARG:HD2	20	0.1
(1,1490)	1:64:A:ARG:H	1:64:A:ARG:HD3	20	0.1
(1,1433)	1:51:A:ASP:HB2	1:124:A:GLU:HB3	12	0.1
(1,1433)	1:51:A:ASP:HB3	1:124:A:GLU:HB3	12	0.1
(1,1346)	1:28:A:LYS:HG2	1:30:A:VAL:H	9	0.1
(1,1346)	1:28:A:LYS:HG3	1:30:A:VAL:H	9	0.1
(1,1193)	1:105:A:ALA:H	1:107:A:GLY:H	12	0.1
(1,1126)	1:94:A:GLU:H	1:127:A:LEU:HG	13	0.1
(1,1106)	1:37:A:VAL:H	1:92:A:LEU:H	12	0.1
(1,1106)	1:37:A:VAL:H	1:92:A:LEU:H	14	0.1
(1,1105)	1:38:A:THR:H	1:92:A:LEU:H	12	0.1
(1,1065)	1:79:A:VAL:HG21	1:85:A:GLN:H	9	0.1
(1,1065)	1:79:A:VAL:HG22	1:85:A:GLN:H	9	0.1
(1,1065)	1:79:A:VAL:HG23	1:85:A:GLN:H	9	0.1
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB1	7	0.1
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB2	7	0.1
(1,984)	1:73:A:THR:H	1:76:A:ALA:HB3	7	0.1
(1,938)	1:64:A:ARG:H	1:64:A:ARG:HG3	14	0.1
(1,930)	1:63:A:SER:H	1:64:A:ARG:HB3	16	0.1
(1,913)	1:53:A:ARG:HB3	1:57:A:GLY:H	15	0.1
(1,901)	1:59:A:GLN:HG2	1:59:A:GLN:HE22	19	0.1
(1,866)	1:51:A:ASP:H	1:124:A:GLU:HB3	17	0.1
(1,836)	1:47:A:THR:H	1:128:A:LEU:H	1	0.1
(1,812)	1:43:A:GLY:H	1:44:A:LYS:HB2	20	0.1
(1,807)	1:42:A:ALA:H	1:43:A:GLY:H	17	0.1
(1,806)	1:42:A:ALA:H	1:74:A:LEU:HG	16	0.1
(1,781)	1:37:A:VAL:H	1:91:A:THR:HB	11	0.1
(1,776)	1:33:A:PRO:HB2	1:34:A:GLY:H	17	0.1
(1,686)	1:102:A:TYR:HE2	1:118:A:LYS:HA	14	0.1
(1,638)	1:127:A:LEU:HD11	1:129:A:ALA:HB1	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:127:A:LEU:HD11	1:129:A:ALA:HB2	15	0.1
(1,638)	1:127:A:LEU:HD11	1:129:A:ALA:HB3	15	0.1
(1,638)	1:127:A:LEU:HD12	1:129:A:ALA:HB1	15	0.1
(1,638)	1:127:A:LEU:HD12	1:129:A:ALA:HB2	15	0.1
(1,638)	1:127:A:LEU:HD12	1:129:A:ALA:HB3	15	0.1
(1,638)	1:127:A:LEU:HD13	1:129:A:ALA:HB1	15	0.1
(1,638)	1:127:A:LEU:HD13	1:129:A:ALA:HB2	15	0.1
(1,638)	1:127:A:LEU:HD13	1:129:A:ALA:HB3	15	0.1
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD11	6	0.1
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD12	6	0.1
(1,634)	1:47:A:THR:H	1:127:A:LEU:HD13	6	0.1
(1,603)	1:123:A:PHE:H	1:124:A:GLU:HA	4	0.1
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG21	4	0.1
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG22	4	0.1
(1,584)	1:55:A:PRO:HG3	1:120:A:THR:HG23	4	0.1
(1,578)	1:119:A:ALA:HB1	1:120:A:THR:HB	4	0.1
(1,578)	1:119:A:ALA:HB2	1:120:A:THR:HB	4	0.1
(1,578)	1:119:A:ALA:HB3	1:120:A:THR:HB	4	0.1
(1,578)	1:119:A:ALA:HB1	1:120:A:THR:HB	20	0.1
(1,578)	1:119:A:ALA:HB2	1:120:A:THR:HB	20	0.1
(1,578)	1:119:A:ALA:HB3	1:120:A:THR:HB	20	0.1
(1,543)	1:108:A:GLU:HA	1:118:A:LYS:HG2	2	0.1
(1,521)	1:80:A:ILE:HD11	1:105:A:ALA:HA	8	0.1
(1,521)	1:80:A:ILE:HD12	1:105:A:ALA:HA	8	0.1
(1,521)	1:80:A:ILE:HD13	1:105:A:ALA:HA	8	0.1
(1,520)	1:100:A:ILE:HG21	1:105:A:ALA:HA	2	0.1
(1,520)	1:100:A:ILE:HG22	1:105:A:ALA:HA	2	0.1
(1,520)	1:100:A:ILE:HG23	1:105:A:ALA:HA	2	0.1
(1,518)	1:80:A:ILE:HA	1:105:A:ALA:HA	19	0.1
(1,350)	1:82:A:GLY:HA3	1:104:A:LEU:HD11	18	0.1
(1,350)	1:82:A:GLY:HA3	1:104:A:LEU:HD12	18	0.1
(1,350)	1:82:A:GLY:HA3	1:104:A:LEU:HD13	18	0.1
(1,330)	1:79:A:VAL:HG21	1:83:A:TRP:HE3	9	0.1
(1,330)	1:79:A:VAL:HG22	1:83:A:TRP:HE3	9	0.1
(1,330)	1:79:A:VAL:HG23	1:83:A:TRP:HE3	9	0.1
(1,278)	1:74:A:LEU:HD11	1:87:A:VAL:HB	14	0.1
(1,278)	1:74:A:LEU:HD12	1:87:A:VAL:HB	14	0.1
(1,278)	1:74:A:LEU:HD13	1:87:A:VAL:HB	14	0.1
(1,208)	1:63:A:SER:H	1:64:A:ARG:HA	3	0.1
(1,191)	1:54:A:PHE:HD1	1:58:A:LYS:HD3	14	0.1
(1,127)	1:47:A:THR:HB	1:48:A:VAL:HA	8	0.1
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG21	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG22	19	0.1
(1,90)	1:43:A:GLY:HA3	1:73:A:THR:HG23	19	0.1
(1,64)	1:38:A:THR:HG21	1:39:A:LYS:H	13	0.1
(1,64)	1:38:A:THR:HG22	1:39:A:LYS:H	13	0.1
(1,64)	1:38:A:THR:HG23	1:39:A:LYS:H	13	0.1
(1,48)	1:34:A:GLY:HA2	1:94:A:GLU:HB3	15	0.1
(1,45)	1:34:A:GLY:HA3	1:94:A:GLU:HB2	18	0.1
(1,16)	1:41:A:GLN:H	1:41:A:GLN:HB2	11	0.1

10 Dihedral-angle violation analysis

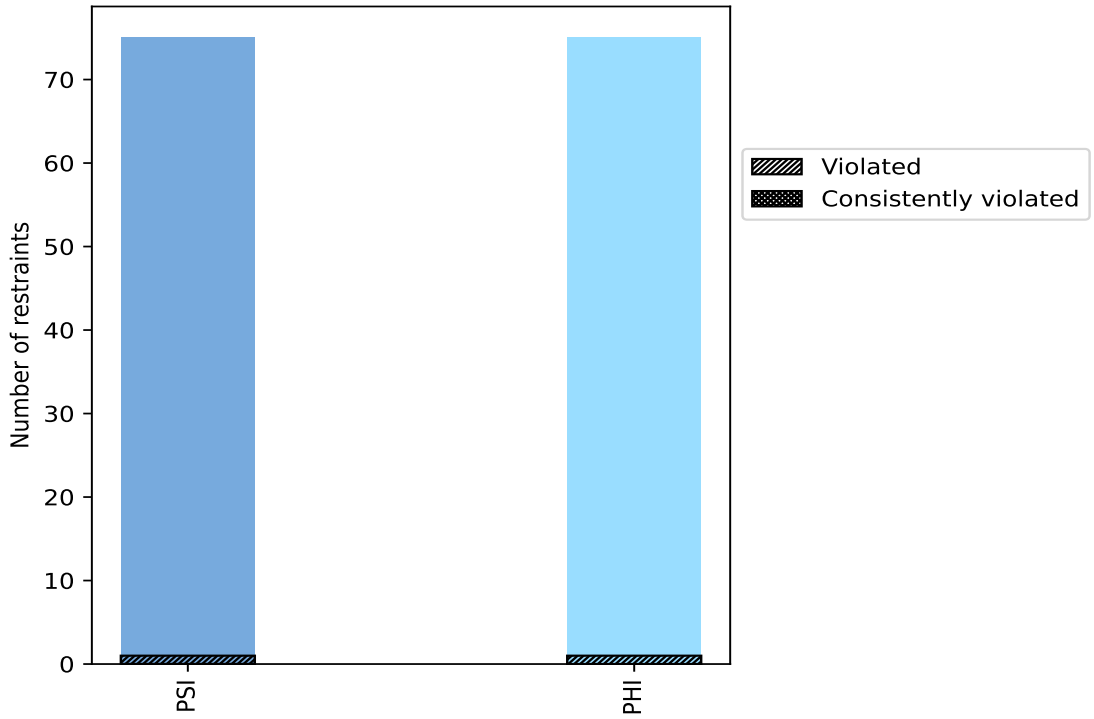
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	75	50.0	1	1.3	0.7	0	0.0	0.0
PHI	75	50.0	1	1.3	0.7	0	0.0	0.0
Total	150	100.0	2	1.3	1.3	0	0.0	0.0

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



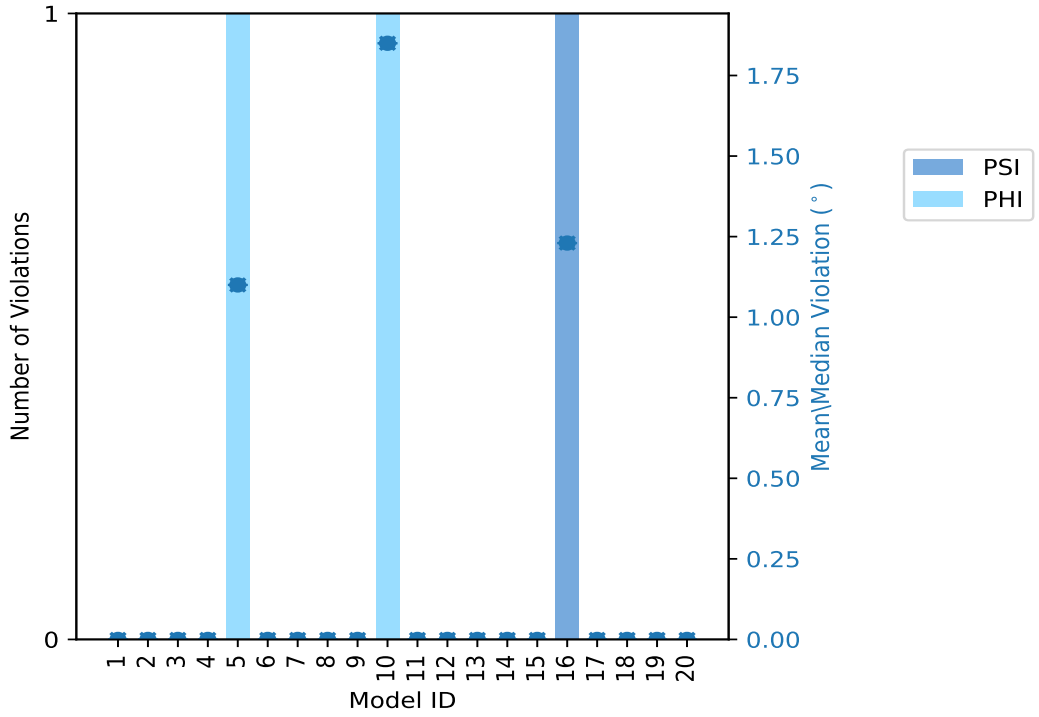
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0.0	0.0	0.0	0.0
5	0	1	1	1.1	1.1	0.0	1.1
6	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0.0	0.0	0.0	0.0
10	0	1	1	1.85	1.85	0.0	1.85
11	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0.0	0.0	0.0	0.0
16	1	0	1	1.23	1.23	0.0	1.23
17	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
1	0	1	1	5.0
0	1	1	2	10.0
0	0	0	3	15.0
0	0	0	4	20.0
0	0	0	5	25.0
0	0	0	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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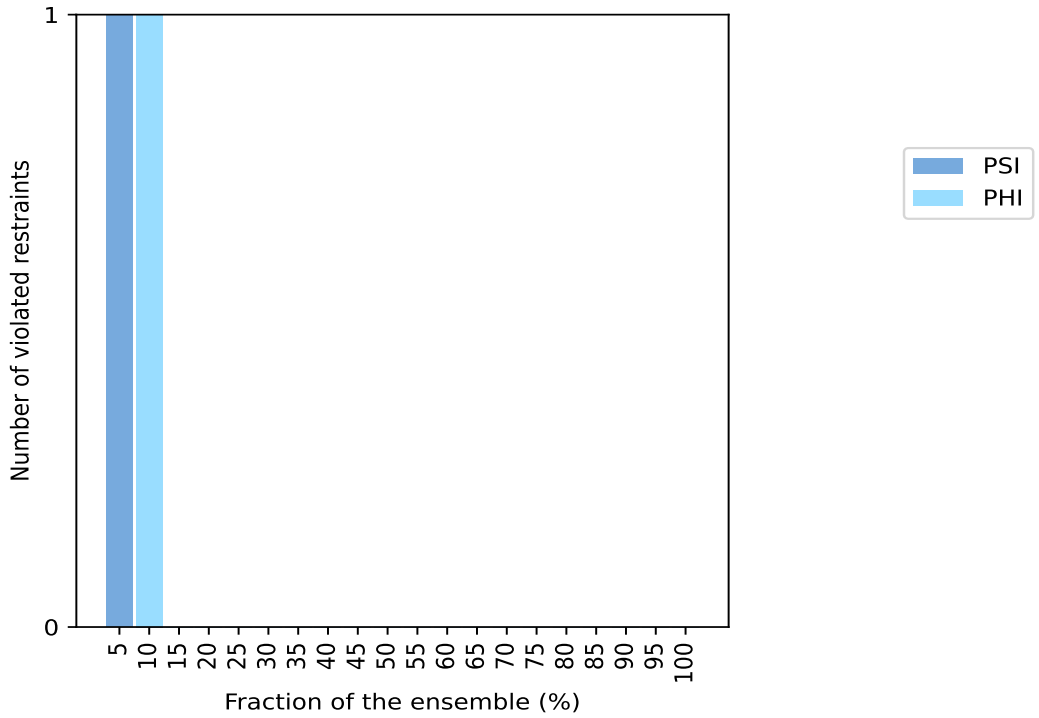
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

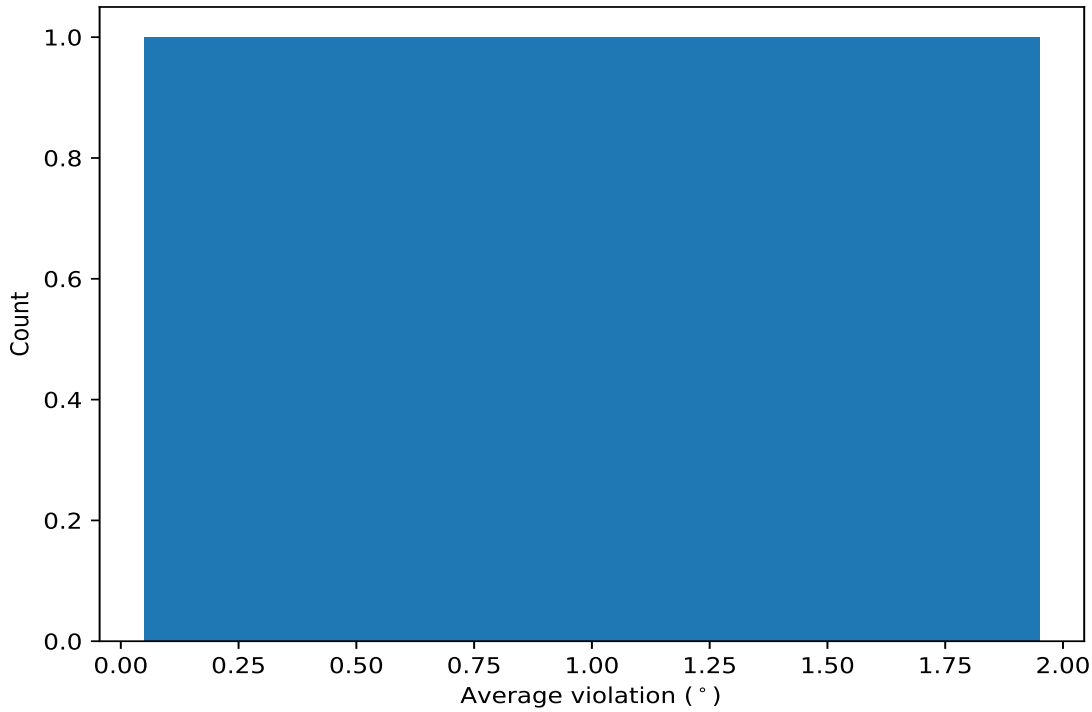


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,39)	1:50:A:TYR:C	1:51:A:ASP:N	1:51:A:ASP:CA	1:51:A:ASP:C	2	1.48	0.38	1.48

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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

10.5.2 Table: All violated dihedral-angle restraints

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 (°)
(1,39)	1:50:A:TYR:C	1:51:A:ASP:N	1:51:A:ASP:CA	1:51:A:ASP:C	10	1.85
(1,54)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:SER:N	16	1.23
(1,39)	1:50:A:TYR:C	1:51:A:ASP:N	1:51:A:ASP:CA	1:51:A:ASP:C	5	1.1