



Full wwPDB NMR Structure Validation Report ⓘ

Mar 4, 2026 – 11:45 PM UTC

PDB ID : 2L7J / pdb_00002l7j
BMRB ID : 17358
Title : Solution structure of the third Immunoglobulin-like domain of nectin-1
Authors : Clausen, O.; Poulsen, F.M.
Deposited on : 2010-12-13

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

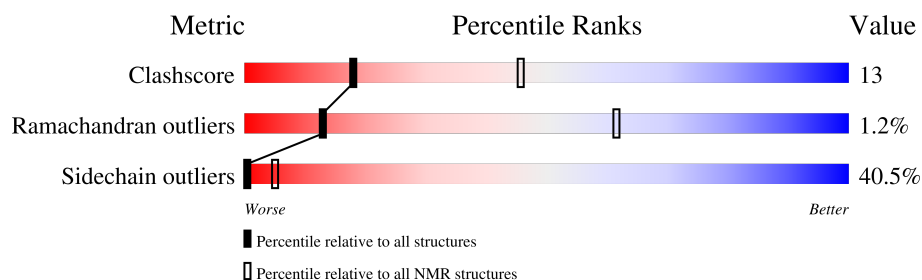
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 51%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	95	41% 44% 7% 7%

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:244-A:254, A:258-A:334 (88)	0.57	1

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1466 atoms, of which 718 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Poliovirus receptor-related 1.

Mol	Chain	Residues	Atoms						Trace
1	A	95	Total	C	H	N	O	S	0
			1466	472	718	127	147	2	

There is a discrepancy between the modelled and reference sequences:

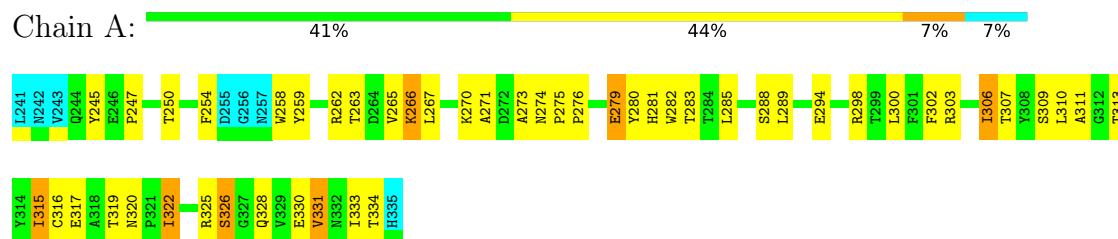
Chain	Residue	Modelled	Actual	Comment	Reference
A	335	HIS	-	expression tag	UNP Q6P9M9

4 Residue-property plots

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: Poliovirus receptor-related 1

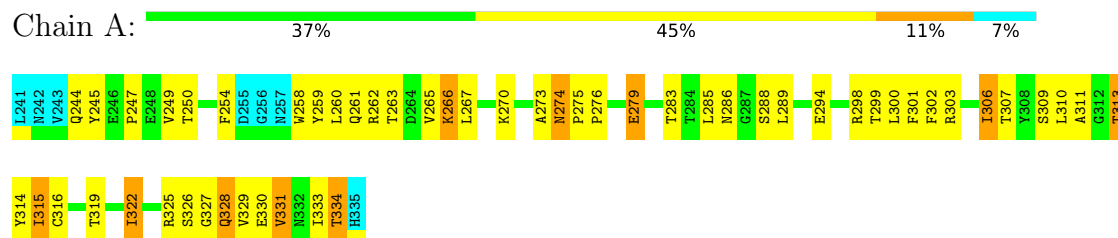


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

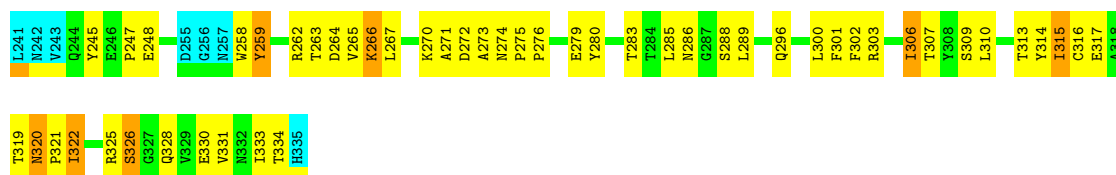
- Molecule 1: Poliovirus receptor-related 1



4.2.2 Score per residue for model 2

- Molecule 1: Poliovirus receptor-related 1

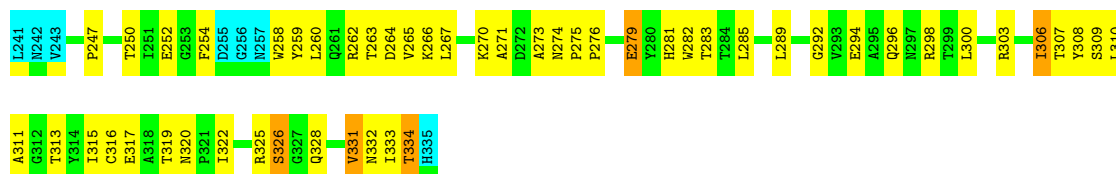




4.2.3 Score per residue for model 3

- Molecule 1: Poliovirus receptor-related 1

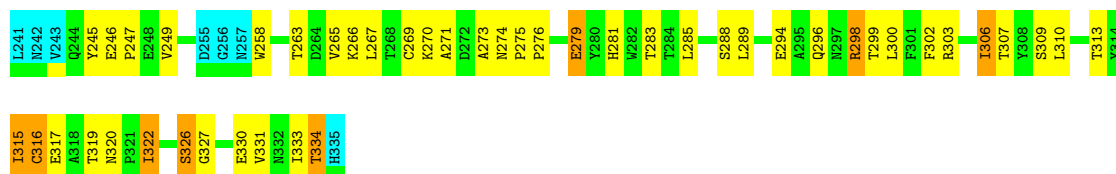
Chain A: 39% 48% 5% 7%



4.2.4 Score per residue for model 4

- Molecule 1: Poliovirus receptor-related 1

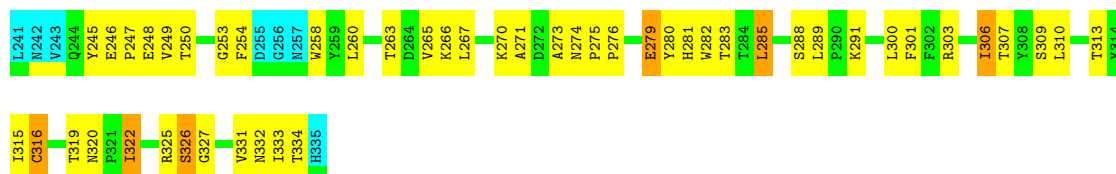
Chain A: 44% 40% 8% 7%



4.2.5 Score per residue for model 5

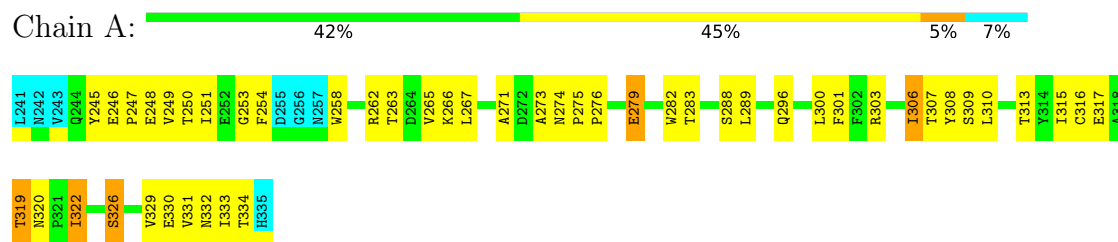
- Molecule 1: Poliovirus receptor-related 1

Chain A: 41% 45% 6% 7%



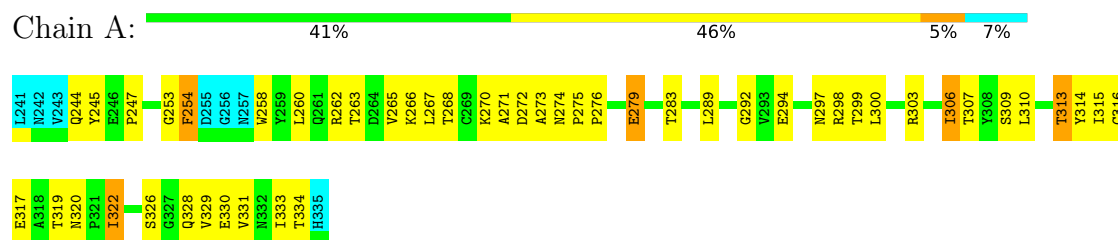
4.2.6 Score per residue for model 6

- Molecule 1: Poliovirus receptor-related 1



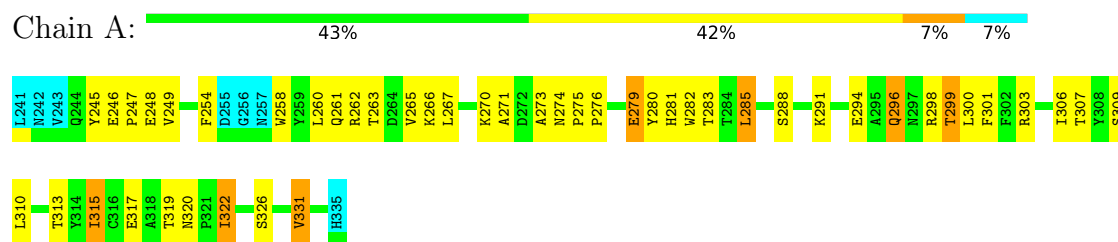
4.2.7 Score per residue for model 7

- Molecule 1: Poliovirus receptor-related 1



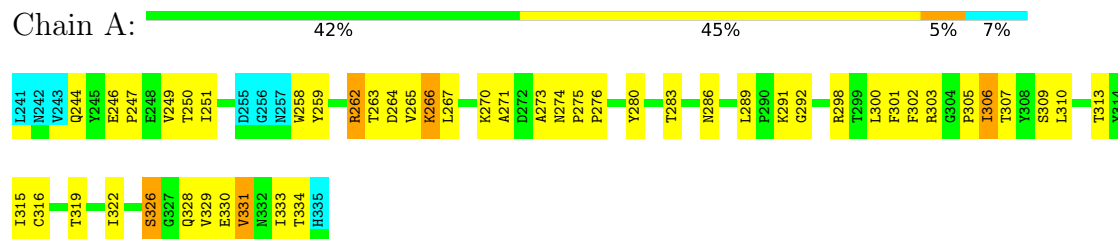
4.2.8 Score per residue for model 8

- Molecule 1: Poliovirus receptor-related 1



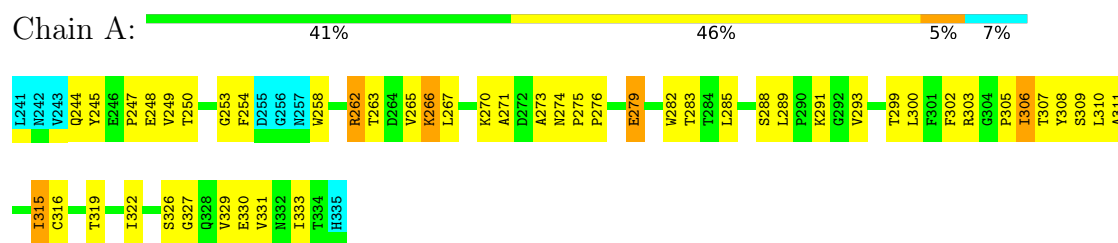
4.2.9 Score per residue for model 9

- Molecule 1: Poliovirus receptor-related 1



4.2.10 Score per residue for model 10

- Molecule 1: Poliovirus receptor-related 1



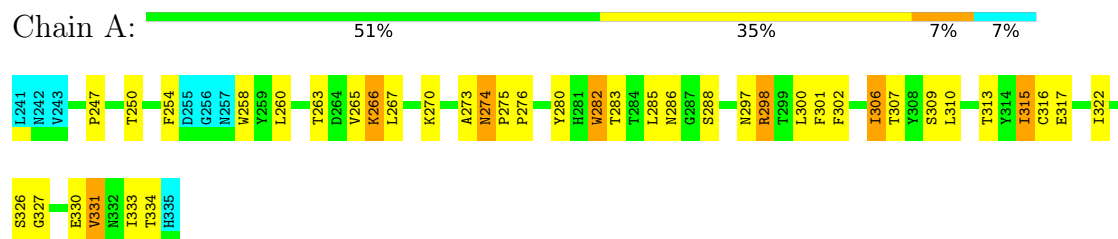
4.2.11 Score per residue for model 11

- Molecule 1: Poliovirus receptor-related 1



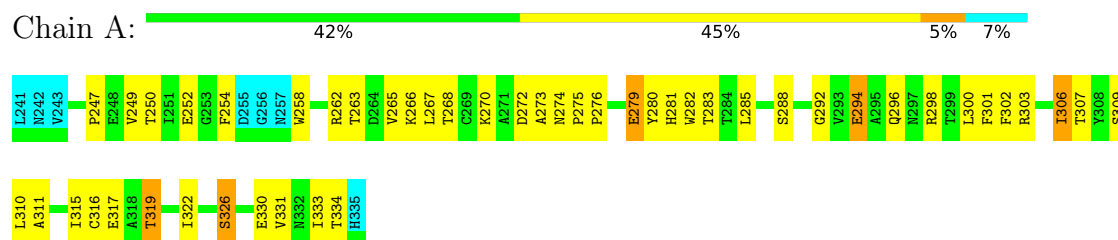
4.2.12 Score per residue for model 12

- Molecule 1: Poliovirus receptor-related 1



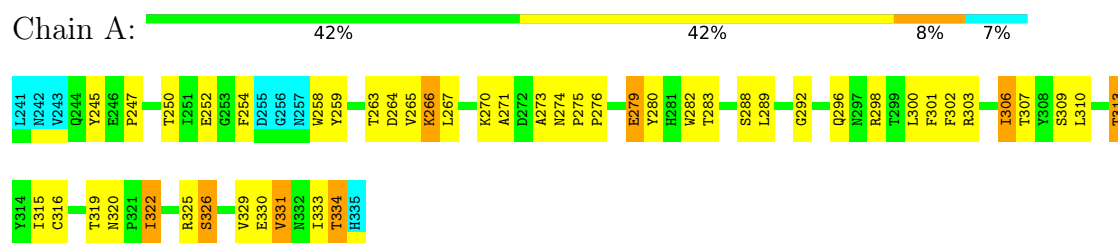
4.2.13 Score per residue for model 13

- Molecule 1: Poliovirus receptor-related 1



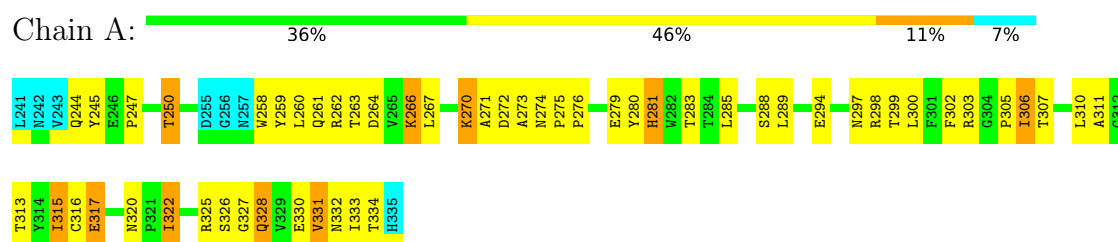
4.2.14 Score per residue for model 14

- Molecule 1: Poliovirus receptor-related 1



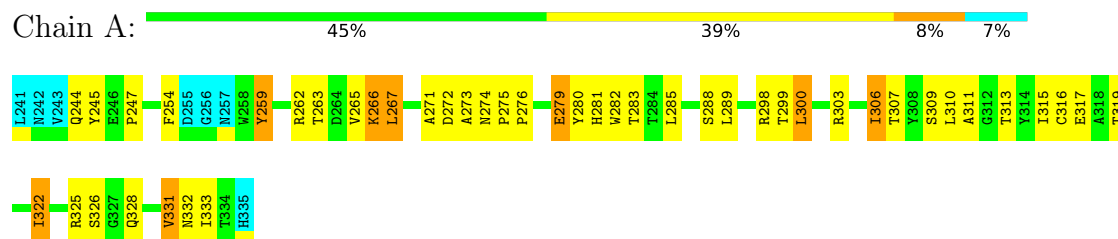
4.2.15 Score per residue for model 15

- Molecule 1: Poliovirus receptor-related 1



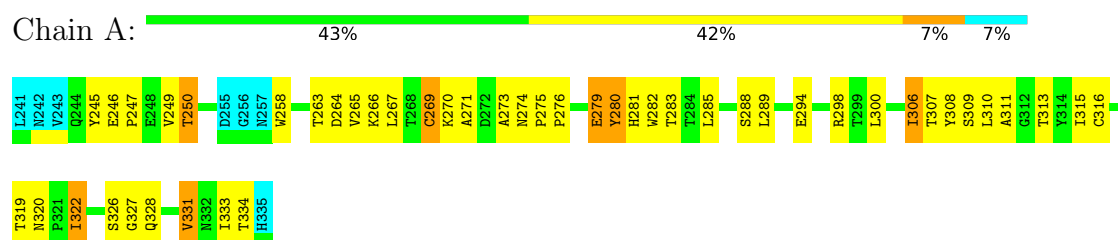
4.2.16 Score per residue for model 16

- Molecule 1: Poliovirus receptor-related 1



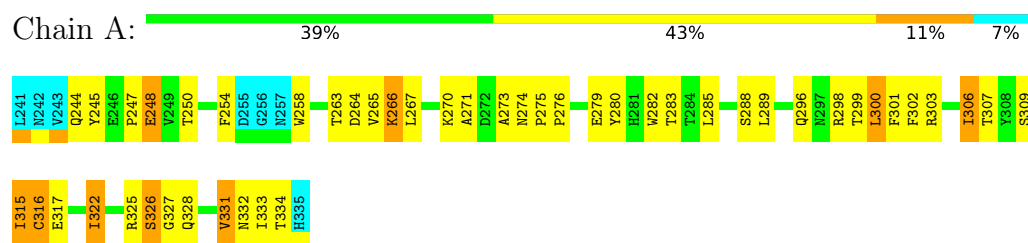
4.2.17 Score per residue for model 17

- Molecule 1: Poliovirus receptor-related 1



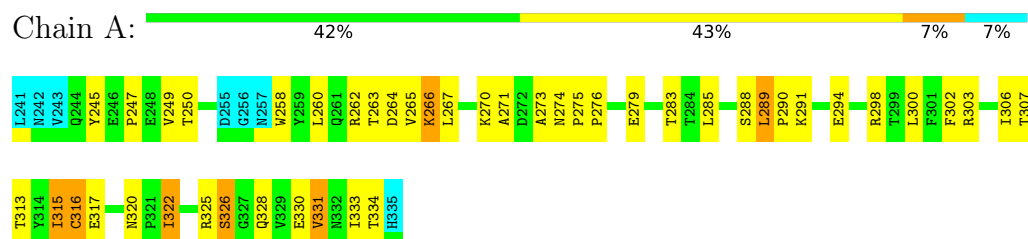
4.2.18 Score per residue for model 18

- Molecule 1: Poliovirus receptor-related 1



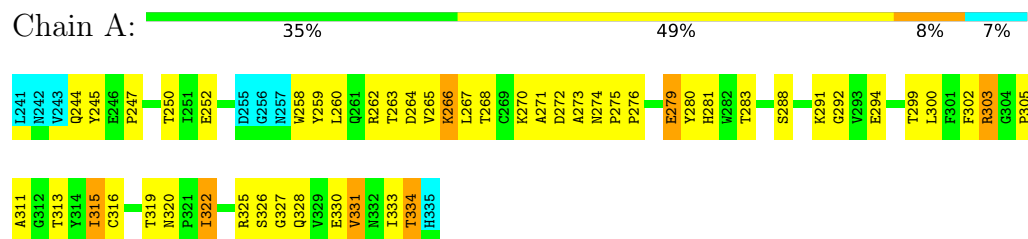
4.2.19 Score per residue for model 19

- Molecule 1: Poliovirus receptor-related 1



4.2.20 Score per residue for model 20

- Molecule 1: Poliovirus receptor-related 1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	refinement	
CYANA	structure solution	
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	630
Number of shifts mapped to atoms	630
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	51%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.46±0.01	0±0/713 (0.0± 0.0%)	0.68±0.01	0±0/977 (0.0± 0.0%)
All	All	0.46	0/14260 (0.0%)	0.68	1/19540 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	297	ASN	CB-CA-C	-5.01	110.82	116.63	7	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	694	669	668	18±3
All	All	13880	13380	13360	361

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:253:GLY:HA3	1:A:267:LEU:HD23	0.78	1.55	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:274:ASN:HB3	1:A:275:PRO:HD3	0.73	1.59	9	19
1:A:311:ALA:HA	1:A:331:VAL:HG22	0.70	1.64	19	6
1:A:258:TRP:HZ2	1:A:267:LEU:HD21	0.68	1.46	18	16
1:A:254:PHE:HB3	1:A:258:TRP:NE1	0.67	2.05	5	5
1:A:313:THR:HG23	1:A:330:GLU:HG2	0.66	1.67	1	2
1:A:306:ILE:HG23	1:A:333:ILE:HD12	0.66	1.67	13	18
1:A:311:ALA:HB2	1:A:333:ILE:HG12	0.65	1.68	10	5
1:A:265:VAL:HB	1:A:306:ILE:HD12	0.62	1.70	6	6
1:A:247:PRO:HB2	1:A:271:ALA:HB1	0.62	1.70	9	13
1:A:313:THR:HG23	1:A:330:GLU:HG3	0.62	1.70	19	3
1:A:265:VAL:HG11	1:A:306:ILE:HB	0.62	1.71	7	17
1:A:258:TRP:CZ2	1:A:267:LEU:HD21	0.61	2.30	18	19
1:A:259:TYR:HD1	1:A:262:ARG:HD2	0.60	1.56	9	1
1:A:247:PRO:HA	1:A:273:ALA:HB2	0.60	1.73	10	20
1:A:254:PHE:HB3	1:A:258:TRP:CD1	0.59	2.32	5	2
1:A:254:PHE:HB3	1:A:267:LEU:HD23	0.59	1.74	16	1
1:A:258:TRP:CZ3	1:A:331:VAL:HA	0.59	2.33	19	10
1:A:280:TYR:HE2	1:A:298:ARG:HB3	0.59	1.56	17	1
1:A:252:GLU:HB2	1:A:268:THR:HB	0.58	1.75	13	1
1:A:320:ASN:HB3	1:A:322:ILE:HD12	0.55	1.77	19	10
1:A:248:GLU:O	1:A:271:ALA:HA	0.55	2.02	5	7
1:A:275:PRO:HG2	1:A:322:ILE:HD11	0.54	1.80	15	4
1:A:258:TRP:CE3	1:A:331:VAL:HA	0.54	2.38	19	6
1:A:258:TRP:HD1	1:A:265:VAL:HG12	0.54	1.63	7	4
1:A:280:TYR:CE2	1:A:298:ARG:HB3	0.54	2.37	17	1
1:A:266:LYS:HA	1:A:302:PHE:CD1	0.53	2.39	20	11
1:A:244:GLN:HG2	1:A:274:ASN:HD22	0.53	1.62	7	1
1:A:292:GLY:O	1:A:303:ARG:HB2	0.52	2.05	7	6
1:A:279:GLU:CB	1:A:319:THR:HB	0.52	2.35	8	10
1:A:315:ILE:HG23	1:A:328:GLN:HB3	0.52	1.81	2	9
1:A:245:TYR:CE1	1:A:273:ALA:HA	0.52	2.40	18	2
1:A:245:TYR:O	1:A:322:ILE:HD13	0.51	2.06	7	16
1:A:262:ARG:HB3	1:A:265:VAL:HG13	0.51	1.81	10	1
1:A:269:CYS:O	1:A:298:ARG:HD3	0.51	2.06	4	1
1:A:247:PRO:HD3	1:A:320:ASN:HB2	0.51	1.81	2	6
1:A:294:GLU:HB2	1:A:303:ARG:HG2	0.50	1.83	13	1
1:A:316:CYS:O	1:A:326:SER:HA	0.50	2.06	9	10
1:A:296:GLN:HG2	1:A:296:GLN:O	0.50	2.04	8	1
1:A:260:LEU:O	1:A:305:PRO:HB2	0.50	2.07	20	2
1:A:254:PHE:HB2	1:A:265:VAL:HA	0.49	1.82	5	1
1:A:260:LEU:HD23	1:A:306:ILE:O	0.49	2.07	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:314:TYR:O	1:A:328:GLN:HA	0.49	2.08	2	5
1:A:267:LEU:HD13	1:A:329:VAL:HG11	0.48	1.85	10	2
1:A:285:LEU:HD12	1:A:315:ILE:HD11	0.48	1.86	8	1
1:A:262:ARG:O	1:A:305:PRO:HA	0.48	2.09	9	3
1:A:282:TRP:HE1	1:A:300:LEU:HD21	0.47	1.70	11	1
1:A:315:ILE:HA	1:A:327:GLY:O	0.47	2.10	12	10
1:A:259:TYR:CD1	1:A:262:ARG:HD2	0.46	2.44	9	1
1:A:259:TYR:HA	1:A:334:THR:OG1	0.46	2.10	3	4
1:A:297:ASN:OD1	1:A:298:ARG:HD2	0.46	2.10	12	1
1:A:248:GLU:OE1	1:A:248:GLU:HA	0.45	2.11	11	1
1:A:281:HIS:HB3	1:A:317:GLU:OE2	0.45	2.12	15	1
1:A:280:TYR:HB3	1:A:282:TRP:CZ3	0.45	2.47	12	1
1:A:274:ASN:CB	1:A:275:PRO:HD3	0.44	2.39	5	6
1:A:250:THR:HB	1:A:270:LYS:HG3	0.44	1.89	17	1
1:A:279:GLU:HB2	1:A:319:THR:HB	0.44	1.89	13	5
1:A:260:LEU:HG	1:A:333:ILE:HG22	0.44	1.89	15	1
1:A:252:GLU:O	1:A:267:LEU:HA	0.44	2.12	3	1
1:A:259:TYR:HA	1:A:334:THR:HB	0.44	1.90	2	1
1:A:320:ASN:OD1	1:A:321:PRO:HD2	0.43	2.13	2	1
1:A:269:CYS:O	1:A:298:ARG:HB2	0.43	2.14	17	1
1:A:260:LEU:HG	1:A:333:ILE:CG2	0.43	2.43	5	1
1:A:306:ILE:CG2	1:A:333:ILE:HD12	0.42	2.44	16	3
1:A:279:GLU:HB3	1:A:319:THR:HB	0.42	1.91	8	1
1:A:266:LYS:HB2	1:A:300:LEU:O	0.42	2.13	18	2
1:A:260:LEU:HA	1:A:306:ILE:HG22	0.42	1.91	8	1
1:A:250:THR:HB	1:A:270:LYS:CG	0.42	2.44	17	1
1:A:302:PHE:CE2	1:A:306:ILE:HG13	0.42	2.49	9	3
1:A:265:VAL:HG23	1:A:302:PHE:CB	0.42	2.44	4	1
1:A:258:TRP:CD1	1:A:306:ILE:HD12	0.42	2.49	2	4
1:A:251:ILE:HG13	1:A:329:VAL:HB	0.41	1.92	6	2
1:A:310:LEU:HD12	1:A:310:LEU:HA	0.41	1.78	18	1
1:A:289:LEU:HG	1:A:290:PRO:HD2	0.41	1.92	19	1
1:A:285:LEU:HD23	1:A:285:LEU:HA	0.41	1.78	5	1
1:A:259:TYR:CD2	1:A:262:ARG:HG3	0.41	2.51	16	1
1:A:296:GLN:OE1	1:A:299:THR:HB	0.41	2.16	8	1
1:A:313:THR:HA	1:A:330:GLU:HA	0.41	1.93	14	1
1:A:252:GLU:O	1:A:268:THR:N	0.40	2.51	20	1
1:A:308:TYR:HA	1:A:333:ILE:HG13	0.40	1.92	3	4
1:A:320:ASN:HB3	1:A:321:PRO:HD2	0.40	1.93	11	1
1:A:250:THR:HB	1:A:270:LYS:HE3	0.40	1.94	15	1
1:A:259:TYR:HB2	1:A:262:ARG:HB2	0.40	1.94	15	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	88/95 (93%)	82±1 (93±1%)	5±1 (5±1%)	1±0 (1±0%)	13	61
All	All	1760/1900 (93%)	1644 (93%)	95 (5%)	21 (1%)	13	61

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	276	PRO	20
1	A	334	THR	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	75/81 (93%)	45±3 (60±4%)	30±3 (40±4%)	0	5
All	All	1500/1620 (93%)	893 (60%)	607 (40%)	0	5

All 59 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	263	THR	20
1	A	266	LYS	20
1	A	283	THR	20
1	A	300	LEU	20
1	A	307	THR	20
1	A	310	LEU	20
1	A	326	SER	20
1	A	322	ILE	19

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Mol	Chain	Res	Type	Models (Total)
1	A	331	VAL	19
1	A	306	ILE	18
1	A	309	SER	18
1	A	270	LYS	17
1	A	279	GLU	17
1	A	315	ILE	17
1	A	288	SER	16
1	A	289	LEU	16
1	A	334	THR	16
1	A	250	THR	15
1	A	285	LEU	15
1	A	313	THR	15
1	A	298	ARG	14
1	A	262	ARG	12
1	A	303	ARG	12
1	A	316	CYS	12
1	A	280	TYR	12
1	A	317	GLU	12
1	A	325	ARG	11
1	A	282	TRP	11
1	A	249	VAL	10
1	A	294	GLU	10
1	A	301	PHE	10
1	A	264	ASP	10
1	A	281	HIS	10
1	A	299	THR	9
1	A	296	GLN	9
1	A	244	GLN	8
1	A	330	GLU	8
1	A	254	PHE	7
1	A	291	LYS	7
1	A	272	ASP	6
1	A	332	ASN	6
1	A	246	GLU	6
1	A	260	LEU	4
1	A	286	ASN	4
1	A	328	GLN	4
1	A	261	GLN	3
1	A	274	ASN	3
1	A	259	TYR	3
1	A	319	THR	3
1	A	329	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	A	308	TYR	2
1	A	248	GLU	2
1	A	320	ASN	1
1	A	268	THR	1
1	A	293	VAL	1
1	A	252	GLU	1
1	A	297	ASN	1
1	A	267	LEU	1
1	A	269	CYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 51% for the well-defined parts and 50% 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 [i](#)

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

Total number of shifts	630
Number of shifts mapped to atoms	630
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	89	0.27 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	81	-0.11 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	84	-0.24 ± 0.48	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 51%, i.e. 596 atoms were assigned a chemical shift out of a possible 1176. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	319/435 (73%)	158/177 (89%)	83/176 (47%)	78/82 (95%)
Sidechain	277/634 (44%)	201/412 (49%)	76/198 (38%)	0/24 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/107 (0%)	0/51 (0%)	0/52 (0%)	0/4 (0%)
Overall	596/1176 (51%)	359/640 (56%)	159/426 (37%)	78/110 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 50%, i.e. 629 atoms were assigned a chemical shift out of a possible 1264. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	340/471 (72%)	167/192 (87%)	89/190 (47%)	84/89 (94%)
Sidechain	289/678 (43%)	208/440 (47%)	81/212 (38%)	0/26 (0%)
Aromatic	0/115 (0%)	0/55 (0%)	0/54 (0%)	0/6 (0%)
Overall	629/1264 (50%)	375/687 (55%)	170/456 (37%)	84/121 (69%)

7.1.4 Statistically unusual chemical shifts ⓘ

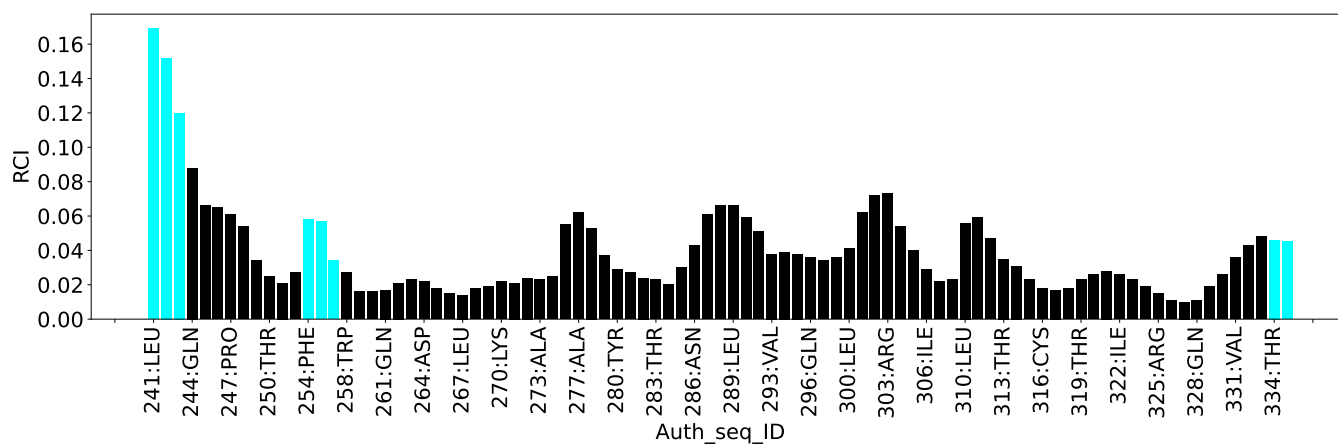
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	307	THR	HB	1.17	2.57 – 5.77	-9.4
1	A	300	LEU	HD11	-1.19	-0.61 – 2.12	-7.1
1	A	300	LEU	HD12	-1.19	-0.61 – 2.12	-7.1
1	A	300	LEU	HD13	-1.19	-0.61 – 2.12	-7.1
1	A	300	LEU	HD21	-1.19	-0.65 – 2.13	-6.9
1	A	300	LEU	HD22	-1.19	-0.65 – 2.13	-6.9
1	A	300	LEU	HD23	-1.19	-0.65 – 2.13	-6.9
1	A	265	VAL	HG21	-0.77	-0.58 – 2.19	-5.7
1	A	265	VAL	HG22	-0.77	-0.58 – 2.19	-5.7
1	A	265	VAL	HG23	-0.77	-0.58 – 2.19	-5.7

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1258
Intra-residue ($ i-j =0$)	262
Sequential ($ i-j =1$)	345
Medium range ($ i-j >1$ and $ i-j <5$)	100
Long range ($ i-j \geq 5$)	551
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	13.2
Number of long range restraints per residue ¹	5.8

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	31.8	0.2
0.2-0.5 (Medium)	52.5	0.5
>0.5 (Large)	91.3	5.61

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

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

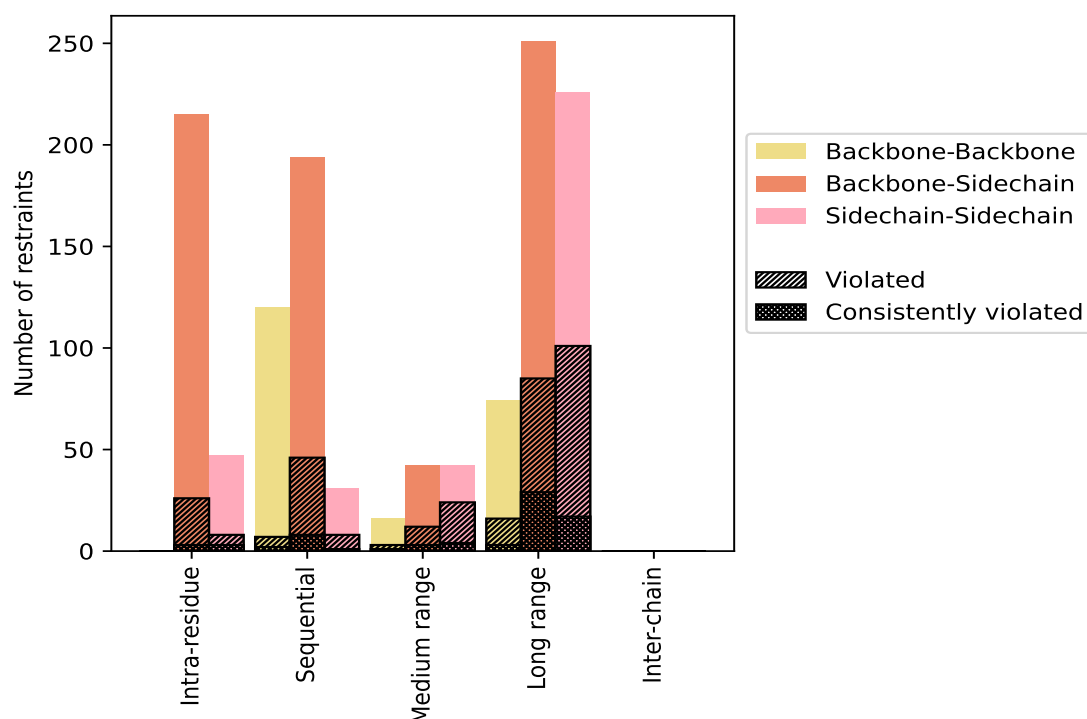
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	262	20.8	34	13.0	2.7	6	2.3	0.5
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	215	17.1	26	12.1	2.1	3	1.4	0.2
Sidechain-Sidechain	47	3.7	8	17.0	0.6	3	6.4	0.2
Sequential (i-j =1)	345	27.4	61	17.7	4.8	11	3.2	0.9
Backbone-Backbone	120	9.5	7	5.8	0.6	2	1.7	0.2
Backbone-Sidechain	194	15.4	46	23.7	3.7	8	4.1	0.6
Sidechain-Sidechain	31	2.5	8	25.8	0.6	1	3.2	0.1
Medium range (i-j >1 & i-j <5)	100	7.9	39	39.0	3.1	8	8.0	0.6
Backbone-Backbone	16	1.3	3	18.8	0.2	1	6.2	0.1
Backbone-Sidechain	42	3.3	12	28.6	1.0	3	7.1	0.2
Sidechain-Sidechain	42	3.3	24	57.1	1.9	4	9.5	0.3
Long range (i-j ≥5)	551	43.8	202	36.7	16.1	49	8.9	3.9
Backbone-Backbone	74	5.9	16	21.6	1.3	3	4.1	0.2
Backbone-Sidechain	251	20.0	85	33.9	6.8	29	11.6	2.3
Sidechain-Sidechain	226	18.0	101	44.7	8.0	17	7.5	1.4
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	0	0.0	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	1258	100.0	336	26.7	26.7	74	5.9	5.9
Backbone-Backbone	210	16.7	26	12.4	2.1	6	2.9	0.5
Backbone-Sidechain	702	55.8	169	24.1	13.4	43	6.1	3.4
Sidechain-Sidechain	346	27.5	141	40.8	11.2	25	7.2	2.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	19	32	19	107	0	177	0.94	5.31	1.02	0.54
2	15	33	25	111	0	184	0.88	4.8	0.93	0.53
3	15	30	25	109	0	179	0.82	4.71	0.99	0.46
4	17	32	21	116	0	186	0.87	5.53	0.95	0.52
5	13	31	20	106	0	170	0.9	4.67	0.99	0.49
6	20	33	25	106	0	184	0.89	4.6	0.94	0.5
7	16	29	26	104	0	175	0.98	4.67	1.05	0.59
8	17	29	20	107	0	173	0.87	5.02	0.98	0.49
9	14	29	26	103	0	172	0.89	4.51	0.94	0.55
10	16	26	19	111	0	172	0.92	5.04	0.98	0.56

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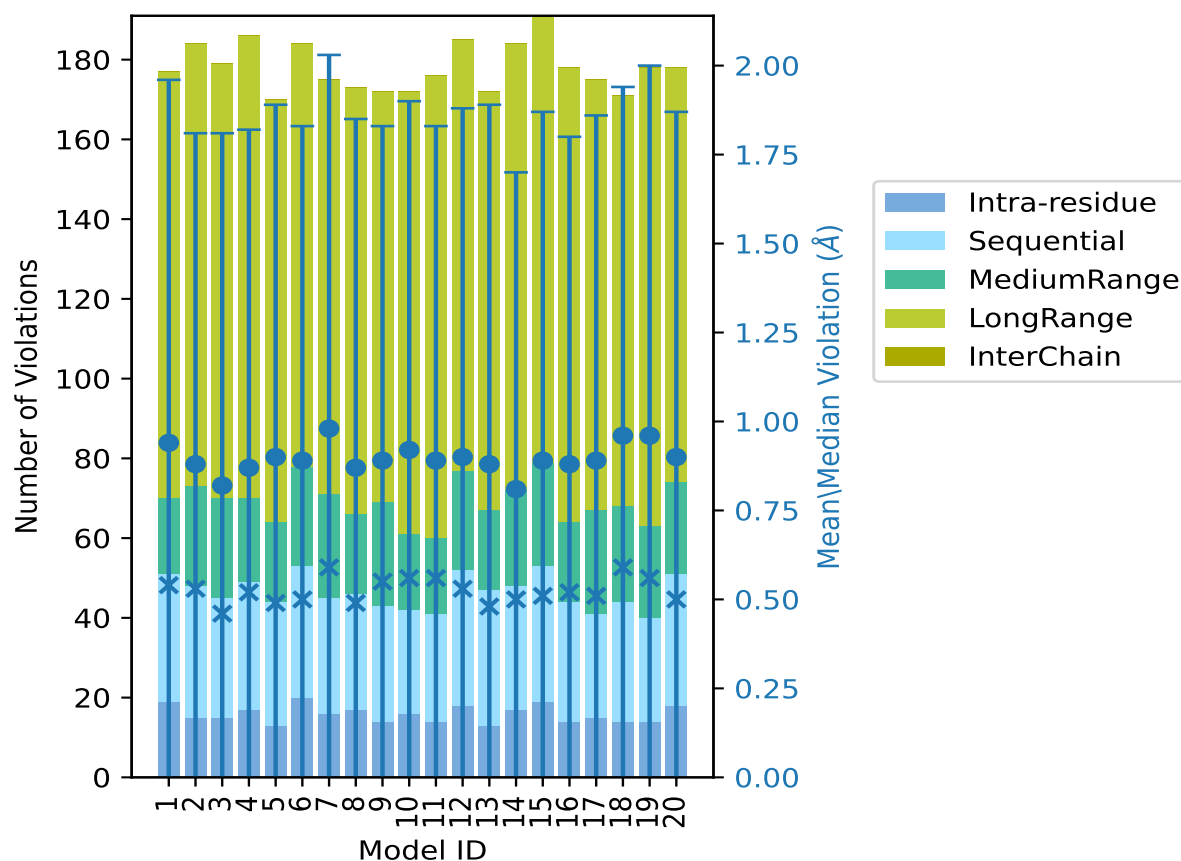
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	14	27	19	116	0	176	0.89	4.6	0.94	0.56
12	18	34	25	108	0	185	0.9	4.64	0.98	0.53
13	13	34	20	105	0	172	0.88	4.69	1.01	0.48
14	17	31	24	112	0	184	0.81	4.83	0.89	0.5
15	19	34	26	112	0	191	0.89	5.28	0.98	0.51
16	14	30	20	114	0	178	0.88	4.73	0.92	0.52
17	15	26	26	108	0	175	0.89	4.48	0.97	0.51
18	14	30	24	103	0	171	0.96	4.59	0.98	0.59
19	14	26	23	115	0	178	0.96	5.61	1.04	0.56
20	18	33	23	104	0	178	0.9	4.6	0.97	0.5

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

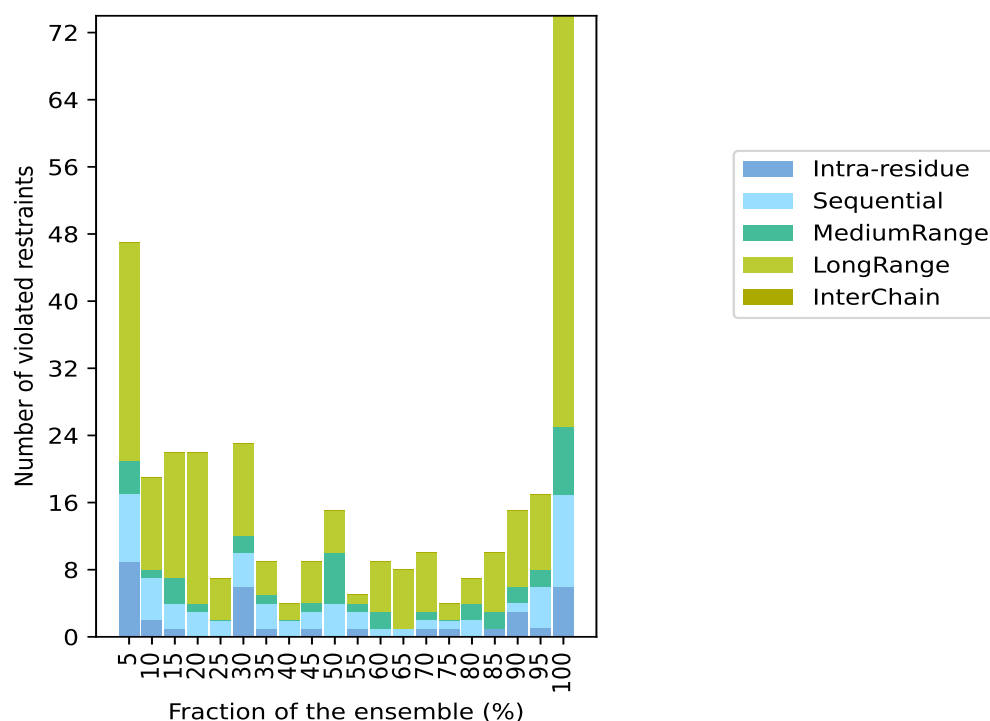
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 922(IR:228, SQ:284, MR:61, LR:349, IC:0) restraints are not 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	%
9	8	4	26	0	47	1	5.0
2	5	1	11	0	19	2	10.0
1	3	3	15	0	22	3	15.0
0	3	1	18	0	22	4	20.0
0	2	0	5	0	7	5	25.0
6	4	2	11	0	23	6	30.0
1	3	1	4	0	9	7	35.0
0	2	0	2	0	4	8	40.0
1	2	1	5	0	9	9	45.0
0	4	6	5	0	15	10	50.0
1	2	1	1	0	5	11	55.0
0	1	2	6	0	9	12	60.0
0	1	0	7	0	8	13	65.0
1	1	1	7	0	10	14	70.0
1	1	0	2	0	4	15	75.0
0	2	2	3	0	7	16	80.0
1	0	2	7	0	10	17	85.0
3	1	2	9	0	15	18	90.0
1	5	2	9	0	17	19	95.0
6	11	8	49	0	74	20	100.0

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

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

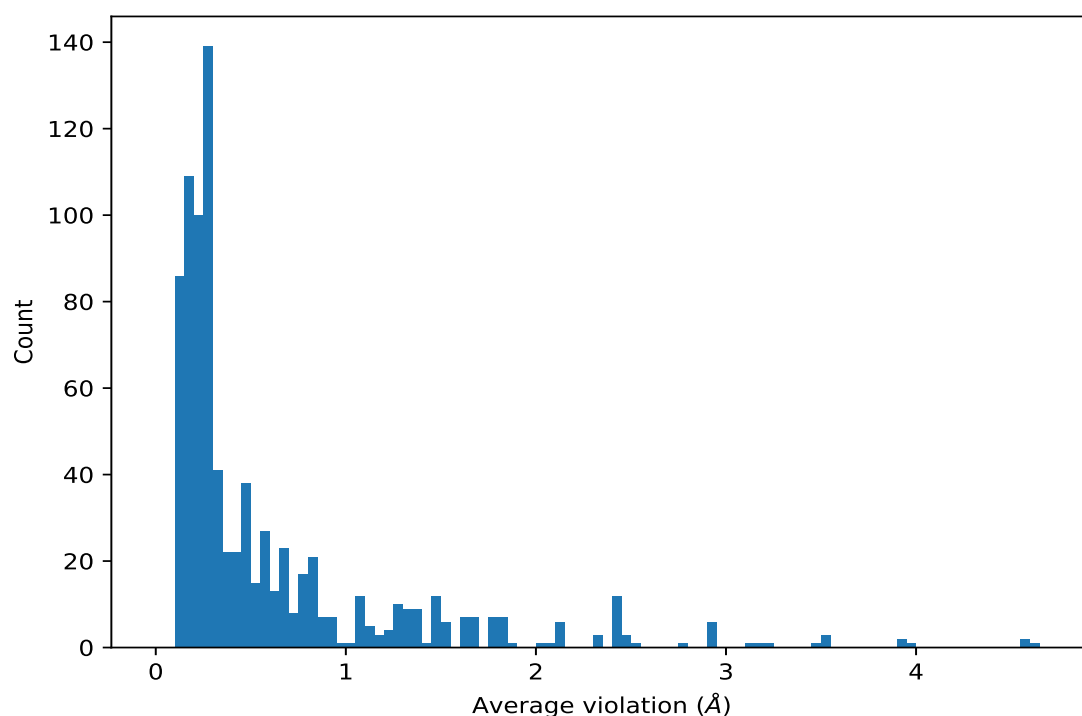
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	20	4.61	0.12	4.61
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	20	4.6	0.33	4.59
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	20	4.6	0.33	4.59
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	20	3.99	0.84	4.01
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	20	3.91	0.33	3.9
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	20	3.91	0.33	3.9
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	20	3.54	0.98	3.74
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	20	3.54	0.98	3.74
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	20	3.45	0.87	3.7
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	20	3.23	0.26	3.22
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	20	3.19	0.87	3.4
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	20	3.14	0.86	3.33
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	20	2.92	0.14	2.92
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	20	2.92	0.14	2.92
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	20	2.92	0.14	2.92
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	20	2.92	0.14	2.92

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	20	2.92	0.14	2.92
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	20	2.92	0.14	2.92
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	20	2.77	0.83	3.2
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	20	2.42	0.41	2.39
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	20	2.42	0.41	2.39
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	20	2.42	0.41	2.39
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	20	2.42	0.41	2.39
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	20	2.42	0.41	2.39
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	20	2.42	0.41	2.39
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	20	2.34	0.08	2.34
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	20	2.33	0.76	2.63
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	20	2.33	0.76	2.63
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	20	2.14	0.16	2.13
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	20	2.14	0.16	2.13
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	20	2.14	0.16	2.13
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	20	2.14	0.16	2.13
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	20	2.14	0.16	2.13
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	20	2.14	0.16	2.13
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	20	2.09	0.87	2.5
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	20	1.84	0.24	1.82
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	20	1.83	0.16	1.86
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	20	1.83	0.16	1.86
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	20	1.83	0.16	1.86
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	20	1.83	0.16	1.86
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	20	1.83	0.16	1.86
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	20	1.83	0.16	1.86
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	20	1.64	0.61	1.76
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	20	1.64	0.61	1.76
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	20	1.64	0.61	1.76
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	20	1.61	0.18	1.62
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	20	1.61	0.18	1.62
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	20	1.53	0.08	1.53
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	20	1.53	0.08	1.53
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	20	1.53	0.08	1.53
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	20	1.53	0.21	1.54
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	20	1.53	0.21	1.54
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	20	1.53	0.21	1.54
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	20	1.49	0.84	1.7
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	20	1.49	0.84	1.7
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	20	1.49	0.84	1.7
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	20	1.49	0.84	1.7
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	20	1.49	0.84	1.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	20	1.49	0.84	1.7
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	20	1.49	0.73	1.42
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	20	1.47	0.11	1.48
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	20	1.47	0.11	1.48
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	20	1.47	0.11	1.48
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	20	1.44	0.45	1.43
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	20	1.36	0.13	1.38
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	20	1.36	0.13	1.38
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	20	1.36	0.13	1.38
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	20	1.31	0.17	1.27
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	20	1.31	0.17	1.27
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	20	1.25	0.16	1.18
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	20	1.25	0.16	1.18
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	20	1.25	0.16	1.18
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	20	1.25	0.16	1.18
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	20	1.25	0.16	1.18
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	20	1.25	0.16	1.18
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	20	1.22	0.27	1.21
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	20	1.22	0.27	1.21
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	20	1.22	0.27	1.21
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	20	1.22	0.06	1.22
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	20	1.15	0.16	1.17
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	20	1.15	0.16	1.17
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	20	1.15	0.16	1.17
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	20	1.09	0.03	1.08
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	20	1.09	0.03	1.08
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	20	1.09	0.03	1.08
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	20	1.06	0.33	1.17
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	20	1.06	0.33	1.17
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	20	1.06	0.33	1.17
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	20	1.06	0.33	1.17
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	20	1.06	0.33	1.17
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	20	1.06	0.33	1.17
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	20	1.05	0.25	1.0
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	20	1.05	0.25	1.0
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	20	1.05	0.25	1.0
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	20	0.92	0.14	0.92
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	20	0.9	0.18	0.88
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	20	0.9	0.18	0.88
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	20	0.9	0.18	0.88
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	20	0.88	0.06	0.9
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	20	0.88	0.06	0.9

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	20	0.83	0.25	0.84
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	20	0.83	0.25	0.84
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	20	0.83	0.25	0.84
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	20	0.83	0.13	0.87
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	20	0.83	0.13	0.87
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	20	0.8	0.17	0.82
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	20	0.8	0.1	0.81
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	20	0.8	0.05	0.81
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	20	0.77	0.15	0.77
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	20	0.77	0.15	0.77
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	20	0.77	0.15	0.77
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	20	0.77	0.15	0.77
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	20	0.77	0.15	0.77
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	20	0.77	0.15	0.77
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	20	0.77	0.15	0.77
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	20	0.77	0.15	0.77
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	20	0.77	0.15	0.77
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	20	0.77	0.15	0.77
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	20	0.77	0.15	0.77
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	20	0.77	0.15	0.77
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	20	0.77	0.05	0.78
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	20	0.77	0.05	0.78
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	20	0.77	0.05	0.78
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	20	0.74	0.24	0.76
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	20	0.74	0.24	0.76
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	20	0.72	0.07	0.73
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	20	0.72	0.07	0.73
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	20	0.72	0.07	0.73
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	20	0.71	0.1	0.71
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	20	0.71	0.1	0.71
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	20	0.67	0.29	0.59
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	20	0.67	0.29	0.59
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	20	0.67	0.29	0.59
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	20	0.66	0.26	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	20	0.65	0.02	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	20	0.65	0.02	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	20	0.65	0.02	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	20	0.65	0.02	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	20	0.65	0.02	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	20	0.65	0.02	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	20	0.65	0.02	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	20	0.65	0.02	0.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	20	0.65	0.02	0.64
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	20	0.64	0.2	0.61
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	20	0.64	0.06	0.64
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	20	0.62	0.17	0.58
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	20	0.62	0.17	0.58
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	20	0.62	0.17	0.58
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	20	0.62	0.17	0.58
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	20	0.62	0.17	0.58
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	20	0.62	0.17	0.58
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	20	0.59	0.22	0.57
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	20	0.59	0.22	0.57
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	20	0.59	0.22	0.57
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	20	0.59	0.22	0.57
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	20	0.59	0.22	0.57
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	20	0.59	0.22	0.57
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	20	0.59	0.22	0.57
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	20	0.59	0.22	0.57
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	20	0.59	0.22	0.57
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	20	0.59	0.22	0.57
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	20	0.59	0.22	0.57
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	20	0.59	0.22	0.57
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	20	0.57	0.16	0.57
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	20	0.57	0.16	0.57
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	20	0.57	0.16	0.57
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	20	0.56	0.01	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	20	0.56	0.01	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	20	0.56	0.01	0.56
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	20	0.54	0.13	0.56
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	20	0.52	0.1	0.55
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	20	0.51	0.14	0.53
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	20	0.51	0.14	0.53
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	20	0.51	0.14	0.53
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	20	0.5	0.14	0.5
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	20	0.48	0.12	0.52
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	20	0.48	0.12	0.52
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	20	0.48	0.12	0.52
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	20	0.47	0.11	0.49
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	20	0.47	0.16	0.47
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	20	0.45	0.2	0.44
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	20	0.45	0.2	0.44
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	20	0.45	0.2	0.44
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	20	0.43	0.05	0.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	20	0.41	0.13	0.38
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	20	0.41	0.13	0.38
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	20	0.41	0.13	0.38
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	20	0.41	0.1	0.4
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	20	0.39	0.01	0.39
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	20	0.39	0.01	0.39
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	20	0.39	0.01	0.39
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	20	0.39	0.1	0.39
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	20	0.39	0.1	0.39
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	20	0.39	0.1	0.39
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	20	0.39	0.1	0.39
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	20	0.39	0.1	0.39
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	20	0.39	0.1	0.39
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	20	0.35	0.04	0.35
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	20	0.25	0.07	0.24
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	20	0.25	0.07	0.24
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	20	0.25	0.07	0.24
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	20	0.25	0.07	0.24
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	20	0.25	0.07	0.24
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	20	0.25	0.07	0.24
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	20	0.23	0.02	0.22
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	20	0.23	0.02	0.22
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	20	0.23	0.02	0.22
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	20	0.23	0.02	0.22
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	20	0.23	0.02	0.22
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	20	0.23	0.02	0.22
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	20	0.23	0.02	0.22
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	20	0.23	0.02	0.22
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	20	0.23	0.02	0.22
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	20	0.21	0.06	0.18
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	19	2.47	0.91	2.45
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	19	2.47	0.91	2.45
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	19	1.88	0.84	2.19
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	19	1.7	0.9	1.91
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	19	1.7	0.9	1.91
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	19	1.7	0.9	1.91
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	19	1.7	0.9	1.91
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	19	1.7	0.9	1.91
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	19	1.7	0.9	1.91
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	19	1.38	0.68	1.55
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	19	1.38	0.68	1.55
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	19	1.38	0.68	1.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	19	1.28	0.8	0.83
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	19	1.28	0.8	0.83
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	19	1.18	0.49	1.36
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	19	1.18	0.49	1.36
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	19	1.18	0.49	1.36
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	19	0.64	0.17	0.67
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	19	0.64	0.17	0.67
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	19	0.55	0.35	0.45
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	19	0.5	0.22	0.47
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	19	0.5	0.22	0.47
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	19	0.5	0.22	0.47
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	19	0.47	0.18	0.45
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	19	0.47	0.18	0.45
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	19	0.47	0.18	0.45
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	19	0.47	0.18	0.45
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	19	0.47	0.18	0.45
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	19	0.47	0.18	0.45
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	19	0.47	0.18	0.45
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	19	0.47	0.18	0.45
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	19	0.47	0.18	0.45
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	19	0.33	0.06	0.35
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	19	0.33	0.06	0.35
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	19	0.31	0.09	0.3
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	19	0.31	0.09	0.3
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	19	0.31	0.09	0.3
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	19	0.3	0.04	0.31
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	19	0.3	0.04	0.31
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	19	0.3	0.04	0.31
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	19	0.3	0.04	0.31
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	19	0.3	0.04	0.31
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	19	0.3	0.04	0.31
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	19	0.21	0.03	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	19	0.21	0.03	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	19	0.21	0.03	0.22
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	19	0.19	0.02	0.19
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	19	0.19	0.02	0.19
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	19	0.19	0.02	0.19
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	19	0.17	0.07	0.16
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	19	0.17	0.05	0.18
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	18	2.0	0.69	2.0
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	18	1.75	0.59	2.0
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	18	1.68	0.62	1.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	18	1.4	0.35	1.48
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	18	1.4	0.35	1.48
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	18	1.4	0.35	1.48
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	18	0.87	0.33	0.94
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	18	0.87	0.33	0.94
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	18	0.87	0.33	0.94
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	18	0.62	0.21	0.66
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	18	0.62	0.21	0.66
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	18	0.62	0.21	0.66
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	18	0.56	0.23	0.62
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	18	0.56	0.23	0.56
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	18	0.46	0.2	0.45
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	18	0.46	0.2	0.45
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	18	0.46	0.2	0.45
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	18	0.46	0.2	0.45
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	18	0.46	0.2	0.45
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	18	0.46	0.2	0.45
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	18	0.42	0.25	0.36
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	18	0.33	0.11	0.32
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	18	0.33	0.11	0.32
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	18	0.33	0.11	0.32
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	18	0.31	0.07	0.34
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	18	0.31	0.07	0.34
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	18	0.31	0.07	0.34
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	18	0.21	0.05	0.22
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	18	0.21	0.05	0.22
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	18	0.21	0.05	0.22
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	18	0.2	0.04	0.18
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	18	0.17	0.05	0.16
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	17	1.79	1.23	2.33
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	17	1.79	1.23	2.33
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	17	1.79	1.23	2.33
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	17	1.79	1.23	2.33
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	17	1.79	1.23	2.33
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	17	1.79	1.23	2.33
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	17	1.64	0.55	1.78
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	17	1.64	0.55	1.78
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	17	1.27	0.62	1.12
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	17	1.27	0.62	1.12
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	17	1.02	0.3	1.15
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	17	0.72	0.22	0.66
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	17	0.51	0.25	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	17	0.51	0.25	0.48
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	17	0.51	0.25	0.48
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	17	0.45	0.1	0.43
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	17	0.37	0.14	0.46
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	17	0.3	0.09	0.33
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	17	0.3	0.09	0.33
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	17	0.27	0.07	0.27
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	17	0.27	0.07	0.27
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	17	0.27	0.07	0.27
(1,816)	1:299:A:THR:HG21	1:301:A:PHE:HZ	16	1.33	0.85	1.06
(1,816)	1:299:A:THR:HG22	1:301:A:PHE:HZ	16	1.33	0.85	1.06
(1,816)	1:299:A:THR:HG23	1:301:A:PHE:HZ	16	1.33	0.85	1.06
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD11	16	0.4	0.17	0.38
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD12	16	0.4	0.17	0.38
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD13	16	0.4	0.17	0.38
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD11	16	0.4	0.17	0.38
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD12	16	0.4	0.17	0.38
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD13	16	0.4	0.17	0.38
(1,397)	1:318:A:ALA:H	1:326:A:SER:HB3	16	0.34	0.15	0.33
(1,645)	1:251:A:ILE:HD11	1:314:A:TYR:H	16	0.27	0.09	0.28
(1,645)	1:251:A:ILE:HD12	1:314:A:TYR:H	16	0.27	0.09	0.28
(1,645)	1:251:A:ILE:HD13	1:314:A:TYR:H	16	0.27	0.09	0.28
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD11	16	0.26	0.09	0.26
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD12	16	0.26	0.09	0.26
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD13	16	0.26	0.09	0.26
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD11	16	0.26	0.09	0.26
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD12	16	0.26	0.09	0.26
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD13	16	0.26	0.09	0.26
(1,608)	1:250:A:THR:HA	1:251:A:ILE:HG13	16	0.18	0.05	0.18
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD11	16	0.15	0.01	0.16
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD12	16	0.15	0.01	0.16
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD13	16	0.15	0.01	0.16
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD11	16	0.15	0.01	0.16
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD12	16	0.15	0.01	0.16
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD13	16	0.15	0.01	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD11	16	0.15	0.01	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD12	16	0.15	0.01	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD13	16	0.15	0.01	0.16
(1,641)	1:251:A:ILE:HD11	1:316:A:CYS:HA	15	0.3	0.12	0.31
(1,641)	1:251:A:ILE:HD12	1:316:A:CYS:HA	15	0.3	0.12	0.31
(1,641)	1:251:A:ILE:HD13	1:316:A:CYS:HA	15	0.3	0.12	0.31
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG2	15	0.28	0.13	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG3	15	0.28	0.13	0.27
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG2	15	0.28	0.13	0.27
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG3	15	0.28	0.13	0.27
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG2	15	0.28	0.13	0.27
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG3	15	0.28	0.13	0.27
(1,1173)	1:293:A:VAL:HG11	1:294:A:GLU:H	15	0.21	0.05	0.23
(1,1173)	1:293:A:VAL:HG12	1:294:A:GLU:H	15	0.21	0.05	0.23
(1,1173)	1:293:A:VAL:HG13	1:294:A:GLU:H	15	0.21	0.05	0.23
(1,1173)	1:293:A:VAL:HG21	1:294:A:GLU:H	15	0.21	0.05	0.23
(1,1173)	1:293:A:VAL:HG22	1:294:A:GLU:H	15	0.21	0.05	0.23
(1,1173)	1:293:A:VAL:HG23	1:294:A:GLU:H	15	0.21	0.05	0.23
(1,565)	1:243:A:VAL:HA	1:243:A:VAL:HB	15	0.15	0.02	0.15
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB2	14	1.3	0.52	1.31
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB3	14	1.3	0.52	1.31
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB2	14	1.3	0.52	1.31
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB3	14	1.3	0.52	1.31
(1,65)	1:251:A:ILE:HG21	1:254:A:PHE:H	14	0.95	0.44	1.04
(1,65)	1:251:A:ILE:HG22	1:254:A:PHE:H	14	0.95	0.44	1.04
(1,65)	1:251:A:ILE:HG23	1:254:A:PHE:H	14	0.95	0.44	1.04
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG21	14	0.82	0.49	0.86
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG22	14	0.82	0.49	0.86
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG23	14	0.82	0.49	0.86
(1,157)	1:268:A:THR:H	1:269:A:CYS:HB2	14	0.52	0.25	0.61
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	14	0.34	0.13	0.32
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	14	0.34	0.13	0.32
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	14	0.34	0.13	0.32
(1,644)	1:251:A:ILE:HD11	1:328:A:GLN:HA	14	0.29	0.07	0.29
(1,644)	1:251:A:ILE:HD12	1:328:A:GLN:HA	14	0.29	0.07	0.29
(1,644)	1:251:A:ILE:HD13	1:328:A:GLN:HA	14	0.29	0.07	0.29
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG21	14	0.27	0.13	0.32
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG22	14	0.27	0.13	0.32
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG23	14	0.27	0.13	0.32
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG21	14	0.27	0.13	0.32
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG22	14	0.27	0.13	0.32
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG23	14	0.27	0.13	0.32
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB2	14	0.27	0.08	0.28
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB3	14	0.27	0.08	0.28
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB2	14	0.27	0.08	0.28
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB3	14	0.27	0.08	0.28
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB2	14	0.27	0.08	0.28
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB3	14	0.27	0.08	0.28
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD11	14	0.19	0.03	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD12	14	0.19	0.03	0.18
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD13	14	0.19	0.03	0.18
(1,853)	1:313:A:THR:HG21	1:328:A:GLN:HA	14	0.17	0.03	0.17
(1,853)	1:313:A:THR:HG22	1:328:A:GLN:HA	14	0.17	0.03	0.17
(1,853)	1:313:A:THR:HG23	1:328:A:GLN:HA	14	0.17	0.03	0.17
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG21	13	0.82	0.36	0.93
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG22	13	0.82	0.36	0.93
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG23	13	0.82	0.36	0.93
(1,537)	1:251:A:ILE:HD11	1:316:A:CYS:HB2	13	0.55	0.11	0.52
(1,537)	1:251:A:ILE:HD12	1:316:A:CYS:HB2	13	0.55	0.11	0.52
(1,537)	1:251:A:ILE:HD13	1:316:A:CYS:HB2	13	0.55	0.11	0.52
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG21	13	0.25	0.09	0.22
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG22	13	0.25	0.09	0.22
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG23	13	0.25	0.09	0.22
(1,905)	1:247:A:PRO:HD2	1:322:A:ILE:HG12	13	0.25	0.09	0.26
(1,905)	1:247:A:PRO:HD3	1:322:A:ILE:HG12	13	0.25	0.09	0.26
(1,655)	1:301:A:PHE:HA	1:302:A:PHE:HE1	13	0.22	0.08	0.22
(1,612)	1:250:A:THR:HB	1:270:A:LYS:HB2	13	0.19	0.08	0.16
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG21	13	0.18	0.05	0.16
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG22	13	0.18	0.05	0.16
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG23	13	0.18	0.05	0.16
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	13	0.18	0.05	0.16
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	13	0.18	0.05	0.16
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	13	0.18	0.05	0.16
(1,627)	1:251:A:ILE:HG21	1:267:A:LEU:HG	13	0.18	0.05	0.18
(1,627)	1:251:A:ILE:HG22	1:267:A:LEU:HG	13	0.18	0.05	0.18
(1,627)	1:251:A:ILE:HG23	1:267:A:LEU:HG	13	0.18	0.05	0.18
(1,900)	1:244:A:GLN:HB3	1:322:A:ILE:HA	12	0.86	0.49	0.97
(1,1082)	1:260:A:LEU:HD11	1:308:A:TYR:HD1	12	0.82	0.33	0.8
(1,1082)	1:260:A:LEU:HD12	1:308:A:TYR:HD1	12	0.82	0.33	0.8
(1,1082)	1:260:A:LEU:HD13	1:308:A:TYR:HD1	12	0.82	0.33	0.8
(1,1082)	1:260:A:LEU:HD21	1:308:A:TYR:HD1	12	0.82	0.33	0.8
(1,1082)	1:260:A:LEU:HD22	1:308:A:TYR:HD1	12	0.82	0.33	0.8
(1,1082)	1:260:A:LEU:HD23	1:308:A:TYR:HD1	12	0.82	0.33	0.8
(1,539)	1:267:A:LEU:HB2	1:269:A:CYS:HB2	12	0.67	0.33	0.79
(1,539)	1:267:A:LEU:HB3	1:269:A:CYS:HB2	12	0.67	0.33	0.79
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG21	12	0.48	0.17	0.44
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG22	12	0.48	0.17	0.44
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG23	12	0.48	0.17	0.44
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD11	12	0.3	0.19	0.24
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD12	12	0.3	0.19	0.24
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD13	12	0.3	0.19	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD21	12	0.3	0.19	0.24
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD22	12	0.3	0.19	0.24
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD23	12	0.3	0.19	0.24
(1,1208)	1:310:A:LEU:HD11	1:314:A:TYR:HE1	12	0.28	0.13	0.24
(1,1208)	1:310:A:LEU:HD12	1:314:A:TYR:HE1	12	0.28	0.13	0.24
(1,1208)	1:310:A:LEU:HD13	1:314:A:TYR:HE1	12	0.28	0.13	0.24
(1,1208)	1:310:A:LEU:HD21	1:314:A:TYR:HE1	12	0.28	0.13	0.24
(1,1208)	1:310:A:LEU:HD22	1:314:A:TYR:HE1	12	0.28	0.13	0.24
(1,1208)	1:310:A:LEU:HD23	1:314:A:TYR:HE1	12	0.28	0.13	0.24
(1,732)	1:267:A:LEU:HB2	1:302:A:PHE:HD1	12	0.24	0.13	0.19
(1,732)	1:267:A:LEU:HB3	1:302:A:PHE:HD1	12	0.24	0.13	0.19
(1,630)	1:251:A:ILE:HG21	1:268:A:THR:HB	12	0.19	0.05	0.2
(1,630)	1:251:A:ILE:HG22	1:268:A:THR:HB	12	0.19	0.05	0.2
(1,630)	1:251:A:ILE:HG23	1:268:A:THR:HB	12	0.19	0.05	0.2
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB1	12	0.15	0.04	0.16
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB2	12	0.15	0.04	0.16
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB3	12	0.15	0.04	0.16
(1,67)	1:255:A:ASP:H	1:257:A:ASN:H	11	0.98	0.35	0.93
(1,495)	1:331:A:VAL:HB	1:332:A:ASN:H	11	0.37	0.1	0.4
(1,727)	1:266:A:LYS:HG3	1:267:A:LEU:H	11	0.22	0.08	0.22
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB1	11	0.18	0.05	0.2
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB2	11	0.18	0.05	0.2
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB3	11	0.18	0.05	0.2
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB1	11	0.18	0.05	0.2
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB2	11	0.18	0.05	0.2
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB3	11	0.18	0.05	0.2
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG21	11	0.11	0.01	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG22	11	0.11	0.01	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG23	11	0.11	0.01	0.1
(1,563)	1:243:A:VAL:HA	1:245:A:TYR:HD1	10	3.54	0.19	3.62
(1,567)	1:243:A:VAL:HB	1:245:A:TYR:HE1	10	2.54	0.37	2.6
(1,568)	1:243:A:VAL:HB	1:245:A:TYR:HD1	10	2.49	0.49	2.44
(1,1000)	1:243:A:VAL:HG11	1:245:A:TYR:HD1	10	2.44	0.39	2.54
(1,1000)	1:243:A:VAL:HG12	1:245:A:TYR:HD1	10	2.44	0.39	2.54
(1,1000)	1:243:A:VAL:HG13	1:245:A:TYR:HD1	10	2.44	0.39	2.54
(1,1000)	1:243:A:VAL:HG21	1:245:A:TYR:HD1	10	2.44	0.39	2.54
(1,1000)	1:243:A:VAL:HG22	1:245:A:TYR:HD1	10	2.44	0.39	2.54
(1,1000)	1:243:A:VAL:HG23	1:245:A:TYR:HD1	10	2.44	0.39	2.54
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB3	10	1.48	0.25	1.38
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB2	10	1.48	0.25	1.38
(1,574)	1:244:A:GLN:HA	1:245:A:TYR:HE1	10	0.87	0.26	0.76
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB3	10	0.79	0.23	0.79

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB2	10	0.79	0.23	0.79
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD11	10	0.49	0.26	0.4
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD12	10	0.49	0.26	0.4
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD13	10	0.49	0.26	0.4
(1,573)	1:244:A:GLN:HA	1:245:A:TYR:HD1	10	0.46	0.18	0.39
(1,731)	1:267:A:LEU:HB2	1:314:A:TYR:HE2	10	0.4	0.21	0.34
(1,731)	1:267:A:LEU:HB3	1:314:A:TYR:HE2	10	0.4	0.21	0.34
(1,810)	1:296:A:GLN:HG2	1:299:A:THR:HB	10	0.39	0.14	0.46
(1,810)	1:296:A:GLN:HG3	1:299:A:THR:HB	10	0.39	0.14	0.46
(1,1192)	1:303:A:ARG:HG2	1:304:A:GLY:H	10	0.23	0.07	0.25
(1,1192)	1:303:A:ARG:HG3	1:304:A:GLY:H	10	0.23	0.07	0.25
(1,420)	1:318:A:ALA:HB1	1:320:A:ASN:H	10	0.2	0.04	0.2
(1,420)	1:318:A:ALA:HB2	1:320:A:ASN:H	10	0.2	0.04	0.2
(1,420)	1:318:A:ALA:HB3	1:320:A:ASN:H	10	0.2	0.04	0.2
(1,876)	1:315:A:ILE:HD11	1:328:A:GLN:HA	10	0.18	0.05	0.18
(1,876)	1:315:A:ILE:HD12	1:328:A:GLN:HA	10	0.18	0.05	0.18
(1,876)	1:315:A:ILE:HD13	1:328:A:GLN:HA	10	0.18	0.05	0.18
(1,594)	1:246:A:GLU:HA	1:247:A:PRO:HB2	10	0.11	0.01	0.12
(1,739)	1:268:A:THR:HG21	1:269:A:CYS:HB3	9	0.66	0.05	0.65
(1,739)	1:268:A:THR:HG22	1:269:A:CYS:HB3	9	0.66	0.05	0.65
(1,739)	1:268:A:THR:HG23	1:269:A:CYS:HB3	9	0.66	0.05	0.65
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG21	9	0.59	0.46	0.46
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG22	9	0.59	0.46	0.46
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG23	9	0.59	0.46	0.46
(1,770)	1:274:A:ASN:HB2	1:322:A:ILE:HG13	9	0.35	0.2	0.28
(1,770)	1:274:A:ASN:HB3	1:322:A:ILE:HG13	9	0.35	0.2	0.28
(1,757)	1:245:A:TYR:HD1	1:273:A:ALA:HA	9	0.34	0.11	0.34
(1,776)	1:273:A:ALA:HB1	1:277:A:ALA:HA	9	0.33	0.14	0.28
(1,776)	1:273:A:ALA:HB2	1:277:A:ALA:HA	9	0.33	0.14	0.28
(1,776)	1:273:A:ALA:HB3	1:277:A:ALA:HA	9	0.33	0.14	0.28
(1,740)	1:268:A:THR:HA	1:269:A:CYS:HB3	9	0.32	0.02	0.32
(1,101)	1:261:A:GLN:H	1:305:A:PRO:HB2	9	0.31	0.17	0.25
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD2	9	0.17	0.03	0.18
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD3	9	0.17	0.03	0.18
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD2	9	0.17	0.03	0.18
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD3	9	0.17	0.03	0.18
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD2	9	0.17	0.03	0.18
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD3	9	0.17	0.03	0.18
(1,646)	1:259:A:TYR:HB3	1:259:A:TYR:HE1	9	0.13	0.01	0.14
(1,21)	1:244:A:GLN:HB3	1:245:A:TYR:H	8	0.53	0.2	0.6
(1,511)	1:259:A:TYR:HB3	1:334:A:THR:H	8	0.28	0.06	0.29
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB1	8	0.25	0.07	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB2	8	0.25	0.07	0.28
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB3	8	0.25	0.07	0.28
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB1	8	0.25	0.07	0.28
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB2	8	0.25	0.07	0.28
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB3	8	0.25	0.07	0.28
(1,1250)	1:330:A:GLU:HB2	1:331:A:VAL:H	8	0.22	0.08	0.24
(1,1250)	1:330:A:GLU:HB3	1:331:A:VAL:H	8	0.22	0.08	0.24
(1,723)	1:266:A:LYS:HD2	1:301:A:PHE:HZ	7	1.14	0.47	1.02
(1,723)	1:266:A:LYS:HD3	1:301:A:PHE:HZ	7	1.14	0.47	1.02
(1,1093)	1:262:A:ARG:HA	1:262:A:ARG:HD2	7	0.68	0.13	0.65
(1,1093)	1:262:A:ARG:HA	1:262:A:ARG:HD3	7	0.68	0.13	0.65
(1,939)	1:327:A:GLY:HA3	1:328:A:GLN:HG2	7	0.45	0.17	0.39
(1,939)	1:327:A:GLY:HA3	1:328:A:GLN:HG3	7	0.45	0.17	0.39
(1,270)	1:296:A:GLN:HG2	1:299:A:THR:H	7	0.33	0.14	0.32
(1,270)	1:296:A:GLN:HG3	1:299:A:THR:H	7	0.33	0.14	0.32
(1,1142)	1:280:A:TYR:H	1:281:A:HIS:HB2	7	0.25	0.09	0.28
(1,1142)	1:280:A:TYR:H	1:281:A:HIS:HB3	7	0.25	0.09	0.28
(1,639)	1:251:A:ILE:HD11	1:314:A:TYR:HB3	7	0.25	0.09	0.26
(1,639)	1:251:A:ILE:HD12	1:314:A:TYR:HB3	7	0.25	0.09	0.26
(1,639)	1:251:A:ILE:HD13	1:314:A:TYR:HB3	7	0.25	0.09	0.26
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB1	7	0.14	0.03	0.12
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB2	7	0.14	0.03	0.12
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB3	7	0.14	0.03	0.12
(1,546)	1:267:A:LEU:HB2	1:300:A:LEU:HA	7	0.13	0.03	0.12
(1,546)	1:267:A:LEU:HB3	1:300:A:LEU:HA	7	0.13	0.03	0.12
(1,828)	1:263:A:THR:HG21	1:305:A:PRO:HB3	7	0.13	0.01	0.12
(1,828)	1:263:A:THR:HG22	1:305:A:PRO:HB3	7	0.13	0.01	0.12
(1,828)	1:263:A:THR:HG23	1:305:A:PRO:HB3	7	0.13	0.01	0.12
(1,722)	1:266:A:LYS:HD2	1:301:A:PHE:HD1	6	0.85	0.23	0.77
(1,678)	1:262:A:ARG:HB2	1:264:A:ASP:HB3	6	0.7	0.31	0.57
(1,678)	1:262:A:ARG:HB3	1:264:A:ASP:HB3	6	0.7	0.31	0.57
(1,72)	1:258:A:TRP:H	1:334:A:THR:H	6	0.42	0.16	0.45
(1,726)	1:266:A:LYS:HG3	1:301:A:PHE:HD1	6	0.4	0.34	0.26
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD11	6	0.35	0.14	0.32
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD12	6	0.35	0.14	0.32
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD13	6	0.35	0.14	0.32
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD21	6	0.35	0.14	0.32
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD22	6	0.35	0.14	0.32
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD23	6	0.35	0.14	0.32
(1,1122)	1:270:A:LYS:HB2	1:270:A:LYS:HD2	6	0.32	0.16	0.28
(1,1122)	1:270:A:LYS:HB2	1:270:A:LYS:HD3	6	0.32	0.16	0.28
(1,544)	1:258:A:TRP:HA	1:259:A:TYR:HD1	6	0.32	0.08	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1168)	1:291:A:LYS:HA	1:291:A:LYS:HG2	6	0.32	0.09	0.36
(1,1168)	1:291:A:LYS:HA	1:291:A:LYS:HG3	6	0.32	0.09	0.36
(1,13)	1:244:A:GLN:H	1:244:A:GLN:HB2	6	0.3	0.07	0.31
(1,70)	1:257:A:ASN:H	1:258:A:TRP:HA	6	0.28	0.07	0.3
(1,1109)	1:267:A:LEU:HD11	1:268:A:THR:H	6	0.28	0.22	0.16
(1,1109)	1:267:A:LEU:HD12	1:268:A:THR:H	6	0.28	0.22	0.16
(1,1109)	1:267:A:LEU:HD13	1:268:A:THR:H	6	0.28	0.22	0.16
(1,1109)	1:267:A:LEU:HD21	1:268:A:THR:H	6	0.28	0.22	0.16
(1,1109)	1:267:A:LEU:HD22	1:268:A:THR:H	6	0.28	0.22	0.16
(1,1109)	1:267:A:LEU:HD23	1:268:A:THR:H	6	0.28	0.22	0.16
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG11	6	0.26	0.15	0.22
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG12	6	0.26	0.15	0.22
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG13	6	0.26	0.15	0.22
(1,1175)	1:293:A:VAL:HG11	1:302:A:PHE:H	6	0.25	0.08	0.26
(1,1175)	1:293:A:VAL:HG12	1:302:A:PHE:H	6	0.25	0.08	0.26
(1,1175)	1:293:A:VAL:HG13	1:302:A:PHE:H	6	0.25	0.08	0.26
(1,1175)	1:293:A:VAL:HG21	1:302:A:PHE:H	6	0.25	0.08	0.26
(1,1175)	1:293:A:VAL:HG22	1:302:A:PHE:H	6	0.25	0.08	0.26
(1,1175)	1:293:A:VAL:HG23	1:302:A:PHE:H	6	0.25	0.08	0.26
(1,718)	1:266:A:LYS:HB2	1:301:A:PHE:HZ	6	0.24	0.13	0.22
(1,718)	1:266:A:LYS:HB3	1:301:A:PHE:HZ	6	0.24	0.13	0.22
(1,259)	1:294:A:GLU:H	1:294:A:GLU:HG3	6	0.24	0.08	0.29
(1,259)	1:294:A:GLU:H	1:294:A:GLU:HG2	6	0.24	0.08	0.29
(1,683)	1:247:A:PRO:HB2	1:325:A:ARG:HB2	6	0.21	0.08	0.2
(1,290)	1:265:A:VAL:H	1:302:A:PHE:H	6	0.21	0.06	0.22
(1,535)	1:249:A:VAL:HG11	1:316:A:CYS:HB3	6	0.21	0.06	0.2
(1,535)	1:249:A:VAL:HG12	1:316:A:CYS:HB3	6	0.21	0.06	0.2
(1,535)	1:249:A:VAL:HG13	1:316:A:CYS:HB3	6	0.21	0.06	0.2
(1,123)	1:265:A:VAL:H	1:266:A:LYS:HG2	6	0.21	0.11	0.17
(1,682)	1:262:A:ARG:HA	1:262:A:ARG:HD2	6	0.2	0.1	0.16
(1,682)	1:262:A:ARG:HA	1:262:A:ARG:HD3	6	0.2	0.1	0.16
(1,613)	1:250:A:THR:HG21	1:252:A:GLU:HG2	6	0.15	0.02	0.16
(1,613)	1:250:A:THR:HG21	1:252:A:GLU:HG3	6	0.15	0.02	0.16
(1,613)	1:250:A:THR:HG22	1:252:A:GLU:HG2	6	0.15	0.02	0.16
(1,613)	1:250:A:THR:HG22	1:252:A:GLU:HG3	6	0.15	0.02	0.16
(1,613)	1:250:A:THR:HG23	1:252:A:GLU:HG2	6	0.15	0.02	0.16
(1,613)	1:250:A:THR:HG23	1:252:A:GLU:HG3	6	0.15	0.02	0.16
(1,1195)	1:306:A:ILE:H	1:306:A:ILE:HG12	6	0.11	0.01	0.11
(1,1195)	1:306:A:ILE:H	1:306:A:ILE:HG13	6	0.11	0.01	0.11
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD11	6	0.11	0.01	0.11
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD12	6	0.11	0.01	0.11
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD13	6	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,564)	1:243:A:VAL:HA	1:244:A:GLN:HG3	5	0.46	0.17	0.42
(1,940)	1:251:A:ILE:HD11	1:327:A:GLY:HA2	5	0.38	0.11	0.36
(1,940)	1:251:A:ILE:HD12	1:327:A:GLY:HA2	5	0.38	0.11	0.36
(1,940)	1:251:A:ILE:HD13	1:327:A:GLY:HA2	5	0.38	0.11	0.36
(1,1010)	1:246:A:GLU:HB2	1:325:A:ARG:HD2	5	0.28	0.06	0.28
(1,1010)	1:246:A:GLU:HB2	1:325:A:ARG:HD3	5	0.28	0.06	0.28
(1,1010)	1:246:A:GLU:HB3	1:325:A:ARG:HD2	5	0.28	0.06	0.28
(1,1010)	1:246:A:GLU:HB3	1:325:A:ARG:HD3	5	0.28	0.06	0.28
(1,827)	1:261:A:GLN:HA	1:305:A:PRO:HB2	5	0.25	0.13	0.2
(1,555)	1:300:A:LEU:HB2	1:314:A:TYR:HB2	5	0.21	0.08	0.2
(1,555)	1:300:A:LEU:HB3	1:314:A:TYR:HB2	5	0.21	0.08	0.2
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG21	5	0.19	0.04	0.2
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG22	5	0.19	0.04	0.2
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG23	5	0.19	0.04	0.2
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG21	5	0.19	0.04	0.2
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG22	5	0.19	0.04	0.2
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG23	5	0.19	0.04	0.2
(1,115)	1:263:A:THR:HG21	1:264:A:ASP:H	5	0.11	0.01	0.11
(1,115)	1:263:A:THR:HG22	1:264:A:ASP:H	5	0.11	0.01	0.11
(1,115)	1:263:A:THR:HG23	1:264:A:ASP:H	5	0.11	0.01	0.11
(1,658)	1:308:A:TYR:HD1	1:333:A:ILE:HB	4	0.69	0.31	0.71
(1,1004)	1:244:A:GLN:HG2	1:322:A:ILE:HG13	4	0.47	0.17	0.5
(1,1004)	1:244:A:GLN:HG3	1:322:A:ILE:HG13	4	0.47	0.17	0.5
(1,1015)	1:246:A:GLU:HG2	1:325:A:ARG:HG2	4	0.33	0.21	0.24
(1,1015)	1:246:A:GLU:HG3	1:325:A:ARG:HG2	4	0.33	0.21	0.24
(1,18)	1:245:A:TYR:H	1:273:A:ALA:HA	4	0.29	0.11	0.28
(1,190)	1:245:A:TYR:H	1:274:A:ASN:H	4	0.28	0.08	0.26
(1,1155)	1:285:A:LEU:HD11	1:315:A:ILE:HD11	4	0.26	0.08	0.23
(1,1155)	1:285:A:LEU:HD11	1:315:A:ILE:HD12	4	0.26	0.08	0.23
(1,1155)	1:285:A:LEU:HD11	1:315:A:ILE:HD13	4	0.26	0.08	0.23
(1,1155)	1:285:A:LEU:HD12	1:315:A:ILE:HD11	4	0.26	0.08	0.23
(1,1155)	1:285:A:LEU:HD12	1:315:A:ILE:HD12	4	0.26	0.08	0.23
(1,1155)	1:285:A:LEU:HD12	1:315:A:ILE:HD13	4	0.26	0.08	0.23
(1,1155)	1:285:A:LEU:HD13	1:315:A:ILE:HD11	4	0.26	0.08	0.23
(1,1155)	1:285:A:LEU:HD13	1:315:A:ILE:HD12	4	0.26	0.08	0.23
(1,1155)	1:285:A:LEU:HD13	1:315:A:ILE:HD13	4	0.26	0.08	0.23
(1,1155)	1:285:A:LEU:HD21	1:315:A:ILE:HD11	4	0.26	0.08	0.23
(1,1155)	1:285:A:LEU:HD21	1:315:A:ILE:HD12	4	0.26	0.08	0.23
(1,1155)	1:285:A:LEU:HD21	1:315:A:ILE:HD13	4	0.26	0.08	0.23
(1,1155)	1:285:A:LEU:HD22	1:315:A:ILE:HD11	4	0.26	0.08	0.23
(1,1155)	1:285:A:LEU:HD22	1:315:A:ILE:HD12	4	0.26	0.08	0.23
(1,1155)	1:285:A:LEU:HD22	1:315:A:ILE:HD13	4	0.26	0.08	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1155)	1:285:A:LEU:HD23	1:315:A:ILE:HD11	4	0.26	0.08	0.23
(1,1155)	1:285:A:LEU:HD23	1:315:A:ILE:HD12	4	0.26	0.08	0.23
(1,1155)	1:285:A:LEU:HD23	1:315:A:ILE:HD13	4	0.26	0.08	0.23
(1,1245)	1:325:A:ARG:HD2	1:326:A:SER:H	4	0.23	0.03	0.23
(1,1245)	1:325:A:ARG:HD3	1:326:A:SER:H	4	0.23	0.03	0.23
(1,441)	1:246:A:GLU:HB2	1:324:A:THR:H	4	0.21	0.07	0.22
(1,441)	1:246:A:GLU:HB3	1:324:A:THR:H	4	0.21	0.07	0.22
(1,849)	1:285:A:LEU:HB2	1:313:A:THR:HG21	4	0.21	0.12	0.15
(1,849)	1:285:A:LEU:HB2	1:313:A:THR:HG22	4	0.21	0.12	0.15
(1,849)	1:285:A:LEU:HB2	1:313:A:THR:HG23	4	0.21	0.12	0.15
(1,849)	1:285:A:LEU:HB3	1:313:A:THR:HG21	4	0.21	0.12	0.15
(1,849)	1:285:A:LEU:HB3	1:313:A:THR:HG22	4	0.21	0.12	0.15
(1,849)	1:285:A:LEU:HB3	1:313:A:THR:HG23	4	0.21	0.12	0.15
(1,513)	1:333:A:ILE:HB	1:334:A:THR:H	4	0.2	0.06	0.2
(1,285)	1:295:A:ALA:HB1	1:301:A:PHE:H	4	0.19	0.08	0.16
(1,285)	1:295:A:ALA:HB2	1:301:A:PHE:H	4	0.19	0.08	0.16
(1,285)	1:295:A:ALA:HB3	1:301:A:PHE:H	4	0.19	0.08	0.16
(1,871)	1:315:A:ILE:HD11	1:328:A:GLN:HB3	4	0.19	0.09	0.16
(1,871)	1:315:A:ILE:HD12	1:328:A:GLN:HB3	4	0.19	0.09	0.16
(1,871)	1:315:A:ILE:HD13	1:328:A:GLN:HB3	4	0.19	0.09	0.16
(1,632)	1:251:A:ILE:HG21	1:328:A:GLN:HA	4	0.18	0.05	0.21
(1,632)	1:251:A:ILE:HG22	1:328:A:GLN:HA	4	0.18	0.05	0.21
(1,632)	1:251:A:ILE:HG23	1:328:A:GLN:HA	4	0.18	0.05	0.21
(1,1146)	1:281:A:HIS:HB2	1:317:A:GLU:HB3	4	0.18	0.07	0.18
(1,1146)	1:281:A:HIS:HB3	1:317:A:GLU:HB3	4	0.18	0.07	0.18
(1,541)	1:251:A:ILE:HG21	1:269:A:CYS:HB2	4	0.18	0.04	0.17
(1,541)	1:251:A:ILE:HG22	1:269:A:CYS:HB2	4	0.18	0.04	0.17
(1,541)	1:251:A:ILE:HG23	1:269:A:CYS:HB2	4	0.18	0.04	0.17
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG11	4	0.17	0.05	0.16
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG12	4	0.17	0.05	0.16
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG13	4	0.17	0.05	0.16
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG21	4	0.17	0.05	0.16
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG22	4	0.17	0.05	0.16
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG23	4	0.17	0.05	0.16
(1,480)	1:313:A:THR:HG21	1:329:A:VAL:H	4	0.17	0.02	0.17
(1,480)	1:313:A:THR:HG22	1:329:A:VAL:H	4	0.17	0.02	0.17
(1,480)	1:313:A:THR:HG23	1:329:A:VAL:H	4	0.17	0.02	0.17
(1,532)	1:266:A:LYS:H	1:301:A:PHE:HA	4	0.16	0.02	0.16
(1,839)	1:302:A:PHE:HE1	1:306:A:ILE:HD11	4	0.16	0.05	0.14
(1,839)	1:302:A:PHE:HE1	1:306:A:ILE:HD12	4	0.16	0.05	0.14
(1,839)	1:302:A:PHE:HE1	1:306:A:ILE:HD13	4	0.16	0.05	0.14
(1,870)	1:285:A:LEU:HB2	1:315:A:ILE:HD11	4	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,870)	1:285:A:LEU:HB2	1:315:A:ILE:HD12	4	0.15	0.02	0.15
(1,870)	1:285:A:LEU:HB2	1:315:A:ILE:HD13	4	0.15	0.02	0.15
(1,870)	1:285:A:LEU:HB3	1:315:A:ILE:HD11	4	0.15	0.02	0.15
(1,870)	1:285:A:LEU:HB3	1:315:A:ILE:HD12	4	0.15	0.02	0.15
(1,870)	1:285:A:LEU:HB3	1:315:A:ILE:HD13	4	0.15	0.02	0.15
(1,403)	1:281:A:HIS:H	1:319:A:THR:H	4	0.12	0.01	0.12
(1,609)	1:250:A:THR:HB	1:270:A:LYS:HA	4	0.11	0.01	0.11
(1,768)	1:244:A:GLN:HB2	1:274:A:ASN:HB3	3	0.5	0.37	0.36
(1,1095)	1:262:A:ARG:HG2	1:264:A:ASP:HB3	3	0.49	0.37	0.37
(1,1095)	1:262:A:ARG:HG3	1:264:A:ASP:HB3	3	0.49	0.37	0.37
(1,528)	1:324:A:THR:H	1:325:A:ARG:HG2	3	0.43	0.26	0.38
(1,820)	1:300:A:LEU:HG	1:314:A:TYR:HE2	3	0.41	0.29	0.26
(1,1048)	1:252:A:GLU:HB2	1:270:A:LYS:HD2	3	0.39	0.03	0.39
(1,1048)	1:252:A:GLU:HB2	1:270:A:LYS:HD3	3	0.39	0.03	0.39
(1,1048)	1:252:A:GLU:HB3	1:270:A:LYS:HD2	3	0.39	0.03	0.39
(1,1048)	1:252:A:GLU:HB3	1:270:A:LYS:HD3	3	0.39	0.03	0.39
(1,1003)	1:244:A:GLN:HG2	1:274:A:ASN:HB3	3	0.32	0.26	0.16
(1,1003)	1:244:A:GLN:HG3	1:274:A:ASN:HB3	3	0.32	0.26	0.16
(1,1116)	1:267:A:LEU:HD11	1:329:A:VAL:HG21	3	0.29	0.05	0.32
(1,1116)	1:267:A:LEU:HD11	1:329:A:VAL:HG22	3	0.29	0.05	0.32
(1,1116)	1:267:A:LEU:HD11	1:329:A:VAL:HG23	3	0.29	0.05	0.32
(1,1116)	1:267:A:LEU:HD12	1:329:A:VAL:HG21	3	0.29	0.05	0.32
(1,1116)	1:267:A:LEU:HD12	1:329:A:VAL:HG22	3	0.29	0.05	0.32
(1,1116)	1:267:A:LEU:HD12	1:329:A:VAL:HG23	3	0.29	0.05	0.32
(1,1116)	1:267:A:LEU:HD13	1:329:A:VAL:HG21	3	0.29	0.05	0.32
(1,1116)	1:267:A:LEU:HD13	1:329:A:VAL:HG22	3	0.29	0.05	0.32
(1,1116)	1:267:A:LEU:HD13	1:329:A:VAL:HG23	3	0.29	0.05	0.32
(1,1116)	1:267:A:LEU:HD21	1:329:A:VAL:HG21	3	0.29	0.05	0.32
(1,1116)	1:267:A:LEU:HD21	1:329:A:VAL:HG22	3	0.29	0.05	0.32
(1,1116)	1:267:A:LEU:HD21	1:329:A:VAL:HG23	3	0.29	0.05	0.32
(1,1116)	1:267:A:LEU:HD22	1:329:A:VAL:HG21	3	0.29	0.05	0.32
(1,1116)	1:267:A:LEU:HD22	1:329:A:VAL:HG22	3	0.29	0.05	0.32
(1,1116)	1:267:A:LEU:HD22	1:329:A:VAL:HG23	3	0.29	0.05	0.32
(1,1116)	1:267:A:LEU:HD23	1:329:A:VAL:HG21	3	0.29	0.05	0.32
(1,1116)	1:267:A:LEU:HD23	1:329:A:VAL:HG22	3	0.29	0.05	0.32
(1,1116)	1:267:A:LEU:HD23	1:329:A:VAL:HG23	3	0.29	0.05	0.32
(1,790)	1:284:A:THR:HG21	1:314:A:TYR:HD2	3	0.2	0.05	0.22
(1,790)	1:284:A:THR:HG22	1:314:A:TYR:HD2	3	0.2	0.05	0.22
(1,790)	1:284:A:THR:HG23	1:314:A:TYR:HD2	3	0.2	0.05	0.22
(1,77)	1:258:A:TRP:H	1:333:A:ILE:HD11	3	0.19	0.07	0.2
(1,77)	1:258:A:TRP:H	1:333:A:ILE:HD12	3	0.19	0.07	0.2
(1,77)	1:258:A:TRP:H	1:333:A:ILE:HD13	3	0.19	0.07	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,765)	1:245:A:TYR:HD1	1:273:A:ALA:HB1	3	0.19	0.05	0.18
(1,765)	1:245:A:TYR:HD1	1:273:A:ALA:HB2	3	0.19	0.05	0.18
(1,765)	1:245:A:TYR:HD1	1:273:A:ALA:HB3	3	0.19	0.05	0.18
(1,1154)	1:285:A:LEU:HD11	1:313:A:THR:HB	3	0.19	0.0	0.19
(1,1154)	1:285:A:LEU:HD12	1:313:A:THR:HB	3	0.19	0.0	0.19
(1,1154)	1:285:A:LEU:HD13	1:313:A:THR:HB	3	0.19	0.0	0.19
(1,1154)	1:285:A:LEU:HD21	1:313:A:THR:HB	3	0.19	0.0	0.19
(1,1154)	1:285:A:LEU:HD22	1:313:A:THR:HB	3	0.19	0.0	0.19
(1,1154)	1:285:A:LEU:HD23	1:313:A:THR:HB	3	0.19	0.0	0.19
(1,703)	1:265:A:VAL:HG21	1:306:A:ILE:HD11	3	0.18	0.03	0.18
(1,703)	1:265:A:VAL:HG21	1:306:A:ILE:HD12	3	0.18	0.03	0.18
(1,703)	1:265:A:VAL:HG21	1:306:A:ILE:HD13	3	0.18	0.03	0.18
(1,703)	1:265:A:VAL:HG22	1:306:A:ILE:HD11	3	0.18	0.03	0.18
(1,703)	1:265:A:VAL:HG22	1:306:A:ILE:HD12	3	0.18	0.03	0.18
(1,703)	1:265:A:VAL:HG22	1:306:A:ILE:HD13	3	0.18	0.03	0.18
(1,703)	1:265:A:VAL:HG23	1:306:A:ILE:HD11	3	0.18	0.03	0.18
(1,703)	1:265:A:VAL:HG23	1:306:A:ILE:HD12	3	0.18	0.03	0.18
(1,703)	1:265:A:VAL:HG23	1:306:A:ILE:HD13	3	0.18	0.03	0.18
(1,778)	1:277:A:ALA:HB1	1:320:A:ASN:HA	3	0.18	0.03	0.16
(1,778)	1:277:A:ALA:HB2	1:320:A:ASN:HA	3	0.18	0.03	0.16
(1,778)	1:277:A:ALA:HB3	1:320:A:ASN:HA	3	0.18	0.03	0.16
(1,295)	1:302:A:PHE:H	1:303:A:ARG:HA	3	0.17	0.07	0.16
(1,382)	1:315:A:ILE:H	1:328:A:GLN:HB3	3	0.16	0.05	0.15
(1,542)	1:268:A:THR:HG21	1:269:A:CYS:HB2	3	0.15	0.04	0.14
(1,542)	1:268:A:THR:HG22	1:269:A:CYS:HB2	3	0.15	0.04	0.14
(1,542)	1:268:A:THR:HG23	1:269:A:CYS:HB2	3	0.15	0.04	0.14
(1,1081)	1:260:A:LEU:HD11	1:308:A:TYR:HB2	3	0.14	0.01	0.15
(1,1081)	1:260:A:LEU:HD11	1:308:A:TYR:HB3	3	0.14	0.01	0.15
(1,1081)	1:260:A:LEU:HD12	1:308:A:TYR:HB2	3	0.14	0.01	0.15
(1,1081)	1:260:A:LEU:HD12	1:308:A:TYR:HB3	3	0.14	0.01	0.15
(1,1081)	1:260:A:LEU:HD13	1:308:A:TYR:HB2	3	0.14	0.01	0.15
(1,1081)	1:260:A:LEU:HD13	1:308:A:TYR:HB3	3	0.14	0.01	0.15
(1,1081)	1:260:A:LEU:HD21	1:308:A:TYR:HB2	3	0.14	0.01	0.15
(1,1081)	1:260:A:LEU:HD21	1:308:A:TYR:HB3	3	0.14	0.01	0.15
(1,1081)	1:260:A:LEU:HD22	1:308:A:TYR:HB2	3	0.14	0.01	0.15
(1,1081)	1:260:A:LEU:HD22	1:308:A:TYR:HB3	3	0.14	0.01	0.15
(1,1081)	1:260:A:LEU:HD23	1:308:A:TYR:HB2	3	0.14	0.01	0.15
(1,1081)	1:260:A:LEU:HD23	1:308:A:TYR:HB3	3	0.14	0.01	0.15
(1,136)	1:264:A:ASP:HB2	1:266:A:LYS:H	3	0.14	0.02	0.13
(1,301)	1:299:A:THR:HG21	1:302:A:PHE:H	3	0.13	0.02	0.11
(1,301)	1:299:A:THR:HG22	1:302:A:PHE:H	3	0.13	0.02	0.11
(1,301)	1:299:A:THR:HG23	1:302:A:PHE:H	3	0.13	0.02	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,437)	1:246:A:GLU:HB2	1:323:A:GLY:H	3	0.12	0.03	0.11
(1,437)	1:246:A:GLU:HB3	1:323:A:GLY:H	3	0.12	0.03	0.11
(1,1119)	1:270:A:LYS:H	1:270:A:LYS:HD2	3	0.11	0.01	0.11
(1,1119)	1:270:A:LYS:H	1:270:A:LYS:HD3	3	0.11	0.01	0.11
(1,1133)	1:277:A:ALA:HA	1:320:A:ASN:HB2	3	0.11	0.0	0.11
(1,1133)	1:277:A:ALA:HA	1:320:A:ASN:HB3	3	0.11	0.0	0.11
(1,657)	1:308:A:TYR:HE1	1:333:A:ILE:HB	2	0.44	0.1	0.44
(1,111)	1:263:A:THR:H	1:264:A:ASP:HB3	2	0.42	0.05	0.42
(1,111)	1:263:A:THR:H	1:264:A:ASP:HB2	2	0.42	0.05	0.42
(1,982)	1:308:A:TYR:HA	1:308:A:TYR:HD1	2	0.4	0.08	0.4
(1,566)	1:243:A:VAL:HA	1:244:A:GLN:HG2	2	0.38	0.22	0.38
(1,691)	1:264:A:ASP:HB3	1:265:A:VAL:HA	2	0.36	0.05	0.36
(1,1047)	1:252:A:GLU:H	1:270:A:LYS:HD2	2	0.24	0.06	0.24
(1,1047)	1:252:A:GLU:H	1:270:A:LYS:HD3	2	0.24	0.06	0.24
(1,614)	1:251:A:ILE:HA	1:268:A:THR:H	2	0.23	0.02	0.23
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD11	2	0.23	0.02	0.23
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD12	2	0.23	0.02	0.23
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD13	2	0.23	0.02	0.23
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD21	2	0.23	0.02	0.23
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD22	2	0.23	0.02	0.23
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD23	2	0.23	0.02	0.23
(1,999)	1:243:A:VAL:HG11	1:245:A:TYR:HB2	2	0.22	0.05	0.22
(1,999)	1:243:A:VAL:HG11	1:245:A:TYR:HB3	2	0.22	0.05	0.22
(1,999)	1:243:A:VAL:HG12	1:245:A:TYR:HB2	2	0.22	0.05	0.22
(1,999)	1:243:A:VAL:HG12	1:245:A:TYR:HB3	2	0.22	0.05	0.22
(1,999)	1:243:A:VAL:HG13	1:245:A:TYR:HB2	2	0.22	0.05	0.22
(1,999)	1:243:A:VAL:HG13	1:245:A:TYR:HB3	2	0.22	0.05	0.22
(1,999)	1:243:A:VAL:HG21	1:245:A:TYR:HB2	2	0.22	0.05	0.22
(1,999)	1:243:A:VAL:HG21	1:245:A:TYR:HB3	2	0.22	0.05	0.22
(1,999)	1:243:A:VAL:HG22	1:245:A:TYR:HB2	2	0.22	0.05	0.22
(1,999)	1:243:A:VAL:HG22	1:245:A:TYR:HB3	2	0.22	0.05	0.22
(1,999)	1:243:A:VAL:HG23	1:245:A:TYR:HB2	2	0.22	0.05	0.22
(1,999)	1:243:A:VAL:HG23	1:245:A:TYR:HB3	2	0.22	0.05	0.22
(1,805)	1:290:A:PRO:HD3	1:314:A:TYR:HE1	2	0.22	0.08	0.22
(1,805)	1:290:A:PRO:HD2	1:314:A:TYR:HE1	2	0.22	0.08	0.22
(1,942)	1:251:A:ILE:HD11	1:327:A:GLY:HA3	2	0.21	0.01	0.21
(1,942)	1:251:A:ILE:HD12	1:327:A:GLY:HA3	2	0.21	0.01	0.21
(1,942)	1:251:A:ILE:HD13	1:327:A:GLY:HA3	2	0.21	0.01	0.21
(1,1112)	1:267:A:LEU:HD11	1:302:A:PHE:HZ	2	0.2	0.02	0.2
(1,1112)	1:267:A:LEU:HD12	1:302:A:PHE:HZ	2	0.2	0.02	0.2
(1,1112)	1:267:A:LEU:HD13	1:302:A:PHE:HZ	2	0.2	0.02	0.2
(1,1112)	1:267:A:LEU:HD21	1:302:A:PHE:HZ	2	0.2	0.02	0.2

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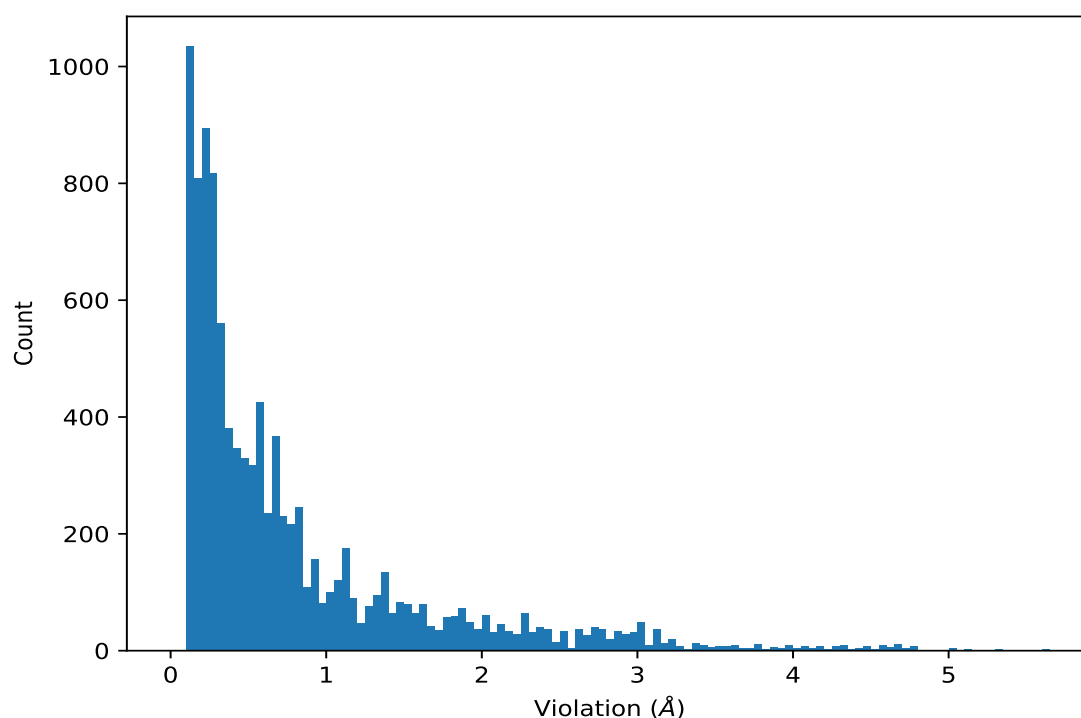
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1112)	1:267:A:LEU:HD22	1:302:A:PHE:HZ	2	0.2	0.02	0.2
(1,1112)	1:267:A:LEU:HD23	1:302:A:PHE:HZ	2	0.2	0.02	0.2
(1,1130)	1:273:A:ALA:HB1	1:320:A:ASN:HB2	2	0.2	0.02	0.2
(1,1130)	1:273:A:ALA:HB1	1:320:A:ASN:HB3	2	0.2	0.02	0.2
(1,1130)	1:273:A:ALA:HB2	1:320:A:ASN:HB2	2	0.2	0.02	0.2
(1,1130)	1:273:A:ALA:HB2	1:320:A:ASN:HB3	2	0.2	0.02	0.2
(1,1130)	1:273:A:ALA:HB3	1:320:A:ASN:HB2	2	0.2	0.02	0.2
(1,1130)	1:273:A:ALA:HB3	1:320:A:ASN:HB3	2	0.2	0.02	0.2
(1,787)	1:283:A:THR:HA	1:284:A:THR:HG21	2	0.16	0.01	0.16
(1,787)	1:283:A:THR:HA	1:284:A:THR:HG22	2	0.16	0.01	0.16
(1,787)	1:283:A:THR:HA	1:284:A:THR:HG23	2	0.16	0.01	0.16
(1,1076)	1:260:A:LEU:HD11	1:306:A:ILE:H	2	0.16	0.04	0.16
(1,1076)	1:260:A:LEU:HD12	1:306:A:ILE:H	2	0.16	0.04	0.16
(1,1076)	1:260:A:LEU:HD13	1:306:A:ILE:H	2	0.16	0.04	0.16
(1,1076)	1:260:A:LEU:HD21	1:306:A:ILE:H	2	0.16	0.04	0.16
(1,1076)	1:260:A:LEU:HD22	1:306:A:ILE:H	2	0.16	0.04	0.16
(1,1076)	1:260:A:LEU:HD23	1:306:A:ILE:H	2	0.16	0.04	0.16
(1,953)	1:251:A:ILE:HB	1:329:A:VAL:HB	2	0.15	0.0	0.15
(1,15)	1:251:A:ILE:HD11	1:316:A:CYS:H	2	0.15	0.03	0.15
(1,15)	1:251:A:ILE:HD12	1:316:A:CYS:H	2	0.15	0.03	0.15
(1,15)	1:251:A:ILE:HD13	1:316:A:CYS:H	2	0.15	0.03	0.15
(1,865)	1:285:A:LEU:HA	1:315:A:ILE:HG21	2	0.12	0.02	0.12
(1,865)	1:285:A:LEU:HA	1:315:A:ILE:HG22	2	0.12	0.02	0.12
(1,865)	1:285:A:LEU:HA	1:315:A:ILE:HG23	2	0.12	0.02	0.12
(1,997)	1:243:A:VAL:HG11	1:244:A:GLN:HA	2	0.11	0.01	0.11
(1,997)	1:243:A:VAL:HG12	1:244:A:GLN:HA	2	0.11	0.01	0.11
(1,997)	1:243:A:VAL:HG13	1:244:A:GLN:HA	2	0.11	0.01	0.11
(1,997)	1:243:A:VAL:HG21	1:244:A:GLN:HA	2	0.11	0.01	0.11
(1,997)	1:243:A:VAL:HG22	1:244:A:GLN:HA	2	0.11	0.01	0.11
(1,997)	1:243:A:VAL:HG23	1:244:A:GLN:HA	2	0.11	0.01	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	19	5.61
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	19	5.61
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	4	5.53
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	1	5.31
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	1	5.31
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	15	5.28
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	15	5.12
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	15	5.12
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	10	5.04
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	10	5.04
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	8	5.02
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	8	5.02
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	14	4.83
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	2	4.8
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	2	4.8
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	19	4.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	19	4.8
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	14	4.75
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	4	4.75
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	8	4.75
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	1	4.74
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	16	4.73
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	16	4.73
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	3	4.71
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	2	4.71
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	3	4.69
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	13	4.69
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	19	4.68
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	3	4.67
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	3	4.67
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	5	4.67
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	5	4.67
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	5	4.67
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	7	4.67
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	7	4.66
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	7	4.66
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	12	4.64
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	12	4.64
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	13	4.64
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	1	4.62
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	1	4.62
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	16	4.61
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	6	4.6
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	6	4.6
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	10	4.6
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	11	4.6
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	20	4.6
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	10	4.59
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	18	4.59
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	4	4.58
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	4	4.58
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	19	4.53
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	9	4.51
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	13	4.48
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	15	4.48
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	17	4.48
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	5	4.47
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	5	4.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	3	4.47
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	17	4.46
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	17	4.46
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	8	4.44
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	12	4.44
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	15	4.43
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	15	4.43
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	5	4.4
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	11	4.37
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	11	4.37
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	10	4.35
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	10	4.35
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	10	4.34
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	10	4.34
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	8	4.33
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	8	4.33
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	2	4.33
(1,98)	1:261:A:GLN:H	1:308:A:TYR:HA	6	4.31
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	20	4.3
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	20	4.3
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	13	4.29
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	13	4.29
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	19	4.29
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	18	4.27
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	18	4.27
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	14	4.25
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	14	4.25
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	14	4.24
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	14	4.24
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	11	4.2
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	7	4.19
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	7	4.19
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	7	4.18
(1,1090)	1:261:A:GLN:HG2	1:308:A:TYR:H	9	4.17
(1,1090)	1:261:A:GLN:HG3	1:308:A:TYR:H	9	4.17
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	4	4.15
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	4	4.15
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	13	4.12
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	2	4.11
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	2	4.11
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	19	4.11
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	19	4.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	13	4.1
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	17	4.09
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	5	4.08
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	6	4.05
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	11	4.05
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	11	4.05
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	8	4.05
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	16	4.04
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	16	4.04
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	3	4.03
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	7	4.01
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	16	3.99
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	3	3.99
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	3	3.98
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	3	3.98
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	13	3.97
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	13	3.97
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	3	3.96
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	3	3.96
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	12	3.95
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	12	3.95
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	12	3.94
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	16	3.94
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	16	3.94
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	6	3.91
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	6	3.91
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	4	3.89
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	4	3.89
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	20	3.89
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	19	3.89
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	8	3.88
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	7	3.87
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	9	3.83
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	1	3.82
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	20	3.79
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	5	3.78
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	5	3.78
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	17	3.77
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	17	3.77
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	1	3.76
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	1	3.76
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	18	3.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	18	3.75
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	17	3.75
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	17	3.75
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	8	3.74
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	8	3.74
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	7	3.73
(1,563)	1:243:A:VAL:HA	1:245:A:TYR:HD1	15	3.72
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	11	3.68
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	11	3.68
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	9	3.68
(1,563)	1:243:A:VAL:HA	1:245:A:TYR:HD1	7	3.67
(1,563)	1:243:A:VAL:HA	1:245:A:TYR:HD1	6	3.65
(1,563)	1:243:A:VAL:HA	1:245:A:TYR:HD1	17	3.65
(1,563)	1:243:A:VAL:HA	1:245:A:TYR:HD1	20	3.64
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	17	3.64
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	12	3.62
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	20	3.61
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	20	3.61
(1,563)	1:243:A:VAL:HA	1:245:A:TYR:HD1	12	3.61
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	13	3.6
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	13	3.6
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	2	3.59
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	12	3.59
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	18	3.58
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	18	3.58
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	18	3.58
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	18	3.58
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	18	3.56
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	15	3.56
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	14	3.55
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	14	3.55
(1,563)	1:243:A:VAL:HA	1:245:A:TYR:HD1	2	3.54
(1,568)	1:243:A:VAL:HB	1:245:A:TYR:HD1	18	3.53
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	1	3.52
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	7	3.5
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	7	3.5
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	12	3.5
(1,675)	1:261:A:GLN:HG3	1:308:A:TYR:H	9	3.48
(1,675)	1:261:A:GLN:HG2	1:308:A:TYR:H	9	3.48
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	17	3.48
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	11	3.48
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	8	3.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	4	3.46
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	12	3.44
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	12	3.44
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	11	3.44
(1,563)	1:243:A:VAL:HA	1:245:A:TYR:HD1	9	3.42
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	1	3.42
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	8	3.41
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	8	3.41
(1,563)	1:243:A:VAL:HA	1:245:A:TYR:HD1	19	3.41
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	17	3.41
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	17	3.4
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	9	3.4
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	18	3.4
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	20	3.39
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	20	3.39
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	20	3.39
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	20	3.39
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	20	3.39
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	20	3.39
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	1	3.38
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	11	3.38
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	18	3.38
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	2	3.34
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	13	3.31
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	20	3.28
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	12	3.27
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	12	3.27
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	7	3.27
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	7	3.27
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	5	3.27
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	9	3.25
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	13	3.25
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	14	3.24
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	15	3.24
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	18	3.24
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	15	3.23
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	1	3.22
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	7	3.21
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	7	3.21
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	7	3.21
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	7	3.21
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	7	3.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	7	3.21
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	10	3.21
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	6	3.21
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	6	3.21
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	10	3.21
(1,567)	1:243:A:VAL:HB	1:245:A:TYR:HE1	18	3.2
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	7	3.2
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	19	3.2
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	9	3.2
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	13	3.19
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	13	3.19
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	13	3.19
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	10	3.19
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	16	3.19
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	15	3.18
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	15	3.18
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	17	3.18
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	17	3.18
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	2	3.17
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	2	3.17
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	1	3.16
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	11	3.14
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	11	3.14
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	11	3.14
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	11	3.14
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	11	3.14
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	11	3.14
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	1	3.14
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	4	3.14
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	6	3.13
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	6	3.13
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	6	3.13
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	6	3.13
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	6	3.13
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	6	3.13
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	20	3.13
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	8	3.12
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	14	3.12
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	17	3.11
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	17	3.11
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	17	3.11
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	17	3.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	17	3.11
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	17	3.11
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	20	3.11
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	20	3.11
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	20	3.11
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	20	3.11
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	20	3.11
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	20	3.11
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	15	3.11
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	16	3.1
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	16	3.1
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	16	3.1
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	16	3.1
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	16	3.1
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	16	3.1
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	6	3.08
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	16	3.07
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	16	3.07
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	5	3.06
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	5	3.06
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	5	3.06
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	5	3.06
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	5	3.06
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	5	3.06
(1,563)	1:243:A:VAL:HA	1:245:A:TYR:HD1	18	3.06
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	12	3.05
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	12	3.05
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	12	3.05
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	12	3.05
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	12	3.05
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	12	3.05
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	9	3.05
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	9	3.05
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	9	3.05
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	9	3.05
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	9	3.05
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	9	3.05
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	19	3.05
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	19	3.05
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	2	3.05
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	6	3.05
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	1	3.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	1	3.04
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	1	3.04
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	1	3.04
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	1	3.04
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	1	3.04
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	6	3.04
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	6	3.04
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	6	3.04
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	6	3.04
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	6	3.04
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	6	3.04
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	10	3.03
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	10	3.03
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	10	3.03
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	10	3.03
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	10	3.03
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	10	3.03
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	7	3.03
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	9	3.02
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	9	3.02
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	9	3.02
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	9	3.02
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	9	3.02
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	9	3.02
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	5	3.01
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	5	3.01
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	5	3.01
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	5	3.01
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	5	3.01
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	5	3.01
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	4	3.01
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	6	2.99
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	5	2.99
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	18	2.98
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	18	2.98
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	18	2.98
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	18	2.98
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	18	2.98
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	18	2.98
(1,568)	1:243:A:VAL:HB	1:245:A:TYR:HD1	20	2.98
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	20	2.98
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	10	2.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	10	2.97
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	10	2.97
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	10	2.97
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	10	2.97
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	10	2.97
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	3	2.97
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	1	2.96
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	1	2.96
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	1	2.96
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	1	2.96
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	1	2.96
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	1	2.96
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	10	2.96
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	10	2.96
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	10	2.96
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	10	2.96
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	10	2.96
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	10	2.96
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	19	2.95
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	19	2.95
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	20	2.95
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	3	2.93
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	3	2.93
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	3	2.93
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	3	2.93
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	3	2.93
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	3	2.93
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	5	2.93
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	5	2.93
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	5	2.93
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	5	2.93
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	5	2.93
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	5	2.93
(1,1000)	1:243:A:VAL:HG11	1:245:A:TYR:HD1	20	2.93
(1,1000)	1:243:A:VAL:HG12	1:245:A:TYR:HD1	20	2.93
(1,1000)	1:243:A:VAL:HG13	1:245:A:TYR:HD1	20	2.93
(1,1000)	1:243:A:VAL:HG21	1:245:A:TYR:HD1	20	2.93
(1,1000)	1:243:A:VAL:HG22	1:245:A:TYR:HD1	20	2.93
(1,1000)	1:243:A:VAL:HG23	1:245:A:TYR:HD1	20	2.93
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	19	2.93
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	2	2.92
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	2	2.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	2	2.92
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	2	2.92
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	2	2.92
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	2	2.92
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	1	2.92
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	1	2.92
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	5	2.91
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	11	2.9
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	11	2.9
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	2	2.89
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	5	2.88
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	5	2.88
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	5	2.88
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	5	2.88
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	5	2.88
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	5	2.88
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	19	2.88
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	19	2.88
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	19	2.88
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	19	2.88
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	19	2.88
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	19	2.88
(1,567)	1:243:A:VAL:HB	1:245:A:TYR:HE1	20	2.88
(1,1000)	1:243:A:VAL:HG11	1:245:A:TYR:HD1	9	2.86
(1,1000)	1:243:A:VAL:HG12	1:245:A:TYR:HD1	9	2.86
(1,1000)	1:243:A:VAL:HG13	1:245:A:TYR:HD1	9	2.86
(1,1000)	1:243:A:VAL:HG21	1:245:A:TYR:HD1	9	2.86
(1,1000)	1:243:A:VAL:HG22	1:245:A:TYR:HD1	9	2.86
(1,1000)	1:243:A:VAL:HG23	1:245:A:TYR:HD1	9	2.86
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	8	2.85
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	8	2.85
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	8	2.85
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	8	2.85
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	8	2.85
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	8	2.85
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	19	2.85
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	19	2.85
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	19	2.85
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	19	2.85
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	19	2.85
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	19	2.85
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	16	2.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	16	2.84
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	13	2.84
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	13	2.84
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	13	2.84
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	13	2.84
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	13	2.84
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	13	2.84
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	7	2.83
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	7	2.83
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	4	2.82
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	4	2.82
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	4	2.82
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	4	2.82
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	4	2.82
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	4	2.82
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	19	2.82
(1,567)	1:243:A:VAL:HB	1:245:A:TYR:HE1	15	2.81
(1,351)	1:260:A:LEU:HG	1:311:A:ALA:H	12	2.81
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	12	2.8
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	12	2.8
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	12	2.8
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	12	2.8
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	12	2.8
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	12	2.8
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	7	2.8
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	10	2.8
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	6	2.79
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	6	2.79
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	6	2.79
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	6	2.79
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	6	2.79
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	6	2.79
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	20	2.79
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	20	2.79
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	4	2.79
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	15	2.78
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	15	2.78
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	4	2.78
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	5	2.78
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	15	2.77
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	15	2.77
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	15	2.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	15	2.77
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	15	2.77
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	15	2.77
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	14	2.77
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	10	2.76
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	10	2.76
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	10	2.76
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	10	2.76
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	10	2.76
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	10	2.76
(1,816)	1:299:A:THR:HG21	1:301:A:PHE:HZ	3	2.76
(1,816)	1:299:A:THR:HG22	1:301:A:PHE:HZ	3	2.76
(1,816)	1:299:A:THR:HG23	1:301:A:PHE:HZ	3	2.76
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	12	2.74
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	12	2.74
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	12	2.74
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	12	2.74
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	12	2.74
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	12	2.74
(1,816)	1:299:A:THR:HG21	1:301:A:PHE:HZ	11	2.74
(1,816)	1:299:A:THR:HG22	1:301:A:PHE:HZ	11	2.74
(1,816)	1:299:A:THR:HG23	1:301:A:PHE:HZ	11	2.74
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	7	2.73
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	7	2.73
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	7	2.73
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	7	2.73
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	7	2.73
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	7	2.73
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	15	2.73
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	15	2.73
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	1	2.73
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	6	2.72
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	6	2.72
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	6	2.72
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	6	2.72
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	6	2.72
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	6	2.72
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	18	2.72
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	18	2.72
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	18	2.72
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	18	2.72
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	18	2.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	18	2.72
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	6	2.71
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	17	2.7
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	17	2.7
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	17	2.7
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	17	2.7
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	17	2.7
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	17	2.7
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	6	2.7
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	7	2.7
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	17	2.7
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	16	2.69
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	16	2.69
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB2	19	2.69
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB3	19	2.69
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB2	19	2.69
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB3	19	2.69
(1,568)	1:243:A:VAL:HB	1:245:A:TYR:HD1	7	2.69
(1,1086)	1:260:A:LEU:HD11	1:311:A:ALA:HA	14	2.68
(1,1086)	1:260:A:LEU:HD12	1:311:A:ALA:HA	14	2.68
(1,1086)	1:260:A:LEU:HD13	1:311:A:ALA:HA	14	2.68
(1,1086)	1:260:A:LEU:HD21	1:311:A:ALA:HA	14	2.68
(1,1086)	1:260:A:LEU:HD22	1:311:A:ALA:HA	14	2.68
(1,1086)	1:260:A:LEU:HD23	1:311:A:ALA:HA	14	2.68
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	3	2.68
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	3	2.68
(1,568)	1:243:A:VAL:HB	1:245:A:TYR:HD1	6	2.67
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	14	2.67
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	14	2.67
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	16	2.67
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	16	2.67
(1,1000)	1:243:A:VAL:HG11	1:245:A:TYR:HD1	17	2.66
(1,1000)	1:243:A:VAL:HG12	1:245:A:TYR:HD1	17	2.66
(1,1000)	1:243:A:VAL:HG13	1:245:A:TYR:HD1	17	2.66
(1,1000)	1:243:A:VAL:HG21	1:245:A:TYR:HD1	17	2.66
(1,1000)	1:243:A:VAL:HG22	1:245:A:TYR:HD1	17	2.66
(1,1000)	1:243:A:VAL:HG23	1:245:A:TYR:HD1	17	2.66
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	6	2.66
(1,567)	1:243:A:VAL:HB	1:245:A:TYR:HE1	6	2.65
(1,1000)	1:243:A:VAL:HG11	1:245:A:TYR:HD1	7	2.64
(1,1000)	1:243:A:VAL:HG12	1:245:A:TYR:HD1	7	2.64
(1,1000)	1:243:A:VAL:HG13	1:245:A:TYR:HD1	7	2.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1000)	1:243:A:VAL:HG21	1:245:A:TYR:HD1	7	2.64
(1,1000)	1:243:A:VAL:HG22	1:245:A:TYR:HD1	7	2.64
(1,1000)	1:243:A:VAL:HG23	1:245:A:TYR:HD1	7	2.64
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	12	2.64
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	12	2.64
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	6	2.63
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	6	2.63
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	6	2.63
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	6	2.63
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	6	2.63
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	6	2.63
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	7	2.63
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	7	2.63
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	7	2.63
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	7	2.63
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	7	2.63
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	7	2.63
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	15	2.63
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	15	2.63
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	15	2.63
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	15	2.63
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	15	2.63
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	15	2.63
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	11	2.63
(1,567)	1:243:A:VAL:HB	1:245:A:TYR:HE1	7	2.63
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	11	2.62
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	11	2.62
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	18	2.62
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	18	2.62
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	11	2.6
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	8	2.6
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	8	2.6
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	8	2.6
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	12	2.59
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	9	2.58
(1,567)	1:243:A:VAL:HB	1:245:A:TYR:HE1	17	2.58
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	18	2.57
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	14	2.57
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	3	2.55
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	3	2.55
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	3	2.55
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	3	2.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	3	2.55
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	3	2.55
(1,1000)	1:243:A:VAL:HG11	1:245:A:TYR:HD1	6	2.55
(1,1000)	1:243:A:VAL:HG12	1:245:A:TYR:HD1	6	2.55
(1,1000)	1:243:A:VAL:HG13	1:245:A:TYR:HD1	6	2.55
(1,1000)	1:243:A:VAL:HG21	1:245:A:TYR:HD1	6	2.55
(1,1000)	1:243:A:VAL:HG22	1:245:A:TYR:HD1	6	2.55
(1,1000)	1:243:A:VAL:HG23	1:245:A:TYR:HD1	6	2.55
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	3	2.55
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	19	2.55
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	19	2.55
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	4	2.54
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	4	2.54
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	4	2.54
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	4	2.54
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	4	2.54
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	4	2.54
(1,1000)	1:243:A:VAL:HG11	1:245:A:TYR:HD1	15	2.53
(1,1000)	1:243:A:VAL:HG12	1:245:A:TYR:HD1	15	2.53
(1,1000)	1:243:A:VAL:HG13	1:245:A:TYR:HD1	15	2.53
(1,1000)	1:243:A:VAL:HG21	1:245:A:TYR:HD1	15	2.53
(1,1000)	1:243:A:VAL:HG22	1:245:A:TYR:HD1	15	2.53
(1,1000)	1:243:A:VAL:HG23	1:245:A:TYR:HD1	15	2.53
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	19	2.52
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	14	2.52
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	10	2.51
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	10	2.51
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	10	2.51
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	19	2.5
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	1	2.47
(1,568)	1:243:A:VAL:HB	1:245:A:TYR:HD1	12	2.47
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	4	2.47
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	4	2.47
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	5	2.46
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	1	2.46
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	9	2.45
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	9	2.45
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	9	2.45
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	1	2.45
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	12	2.45
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	9	2.45
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	9	2.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,567)	1:243:A:VAL:HB	1:245:A:TYR:HE1	12	2.45
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	19	2.44
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	19	2.44
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	19	2.44
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	19	2.44
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	19	2.44
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	19	2.44
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	12	2.44
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	10	2.44
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	20	2.43
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	20	2.43
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	20	2.43
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	20	2.43
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	20	2.43
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	20	2.43
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	1	2.43
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	1	2.43
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	1	2.43
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	1	2.43
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	1	2.43
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	1	2.43
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	3	2.43
(1,816)	1:299:A:THR:HG21	1:301:A:PHE:HZ	20	2.43
(1,816)	1:299:A:THR:HG22	1:301:A:PHE:HZ	20	2.43
(1,816)	1:299:A:THR:HG23	1:301:A:PHE:HZ	20	2.43
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	5	2.43
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	13	2.42
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	13	2.42
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	13	2.42
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	13	2.42
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	13	2.42
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	13	2.42
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	16	2.42
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	5	2.41
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	1	2.41
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	1	2.41
(1,568)	1:243:A:VAL:HB	1:245:A:TYR:HD1	9	2.41
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	9	2.4
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	11	2.4
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	13	2.4
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	2	2.4
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	2	2.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	7	2.39
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	10	2.39
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	5	2.38
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	5	2.38
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	1	2.38
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	1	2.38
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	1	2.38
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	2	2.38
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	4	2.38
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	11	2.38
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	18	2.38
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	16	2.37
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	2	2.37
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	16	2.36
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	16	2.36
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	16	2.36
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	16	2.36
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	16	2.36
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	16	2.36
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	14	2.36
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	14	2.36
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	14	2.36
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	14	2.36
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	14	2.36
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	14	2.36
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	1	2.36
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	1	2.36
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	1	2.36
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	1	2.36
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	1	2.36
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	1	2.36
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	2	2.36
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	12	2.36
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	5	2.36
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	5	2.36
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	19	2.34
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	6	2.33
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	6	2.33
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	7	2.33
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	7	2.33
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	7	2.33
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	7	2.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	7	2.33
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	7	2.33
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	8	2.33
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	8	2.33
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	8	2.33
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	8	2.33
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	8	2.33
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	8	2.33
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	2	2.33
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	2	2.33
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	2	2.33
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	2	2.33
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	2	2.33
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	2	2.33
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	10	2.33
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	16	2.33
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	17	2.32
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	12	2.31
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	12	2.31
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	12	2.31
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	12	2.31
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	12	2.31
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	12	2.31
(1,662)	1:259:A:TYR:HA	1:308:A:TYR:HD1	12	2.31
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	17	2.3
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	17	2.3
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	17	2.3
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	17	2.3
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	17	2.3
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	17	2.3
(1,1000)	1:243:A:VAL:HG11	1:245:A:TYR:HD1	2	2.3
(1,1000)	1:243:A:VAL:HG12	1:245:A:TYR:HD1	2	2.3
(1,1000)	1:243:A:VAL:HG13	1:245:A:TYR:HD1	2	2.3
(1,1000)	1:243:A:VAL:HG21	1:245:A:TYR:HD1	2	2.3
(1,1000)	1:243:A:VAL:HG22	1:245:A:TYR:HD1	2	2.3
(1,1000)	1:243:A:VAL:HG23	1:245:A:TYR:HD1	2	2.3
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	8	2.3
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	4	2.29
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	14	2.29
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	3	2.29
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	15	2.29
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	11	2.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	11	2.28
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	11	2.28
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	11	2.28
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	11	2.28
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	11	2.28
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	8	2.28
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	8	2.28
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	8	2.28
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	8	2.28
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	8	2.28
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	8	2.28
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	20	2.27
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	20	2.27
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	20	2.27
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	20	2.27
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	20	2.27
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	20	2.27
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	16	2.27
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	18	2.27
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	20	2.27
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	18	2.26
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	18	2.26
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	18	2.26
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	18	2.26
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	18	2.26
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	18	2.26
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	14	2.26
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	14	2.26
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	14	2.26
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	14	2.26
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	14	2.26
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	14	2.26
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	9	2.26
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	9	2.26
(1,568)	1:243:A:VAL:HB	1:245:A:TYR:HD1	15	2.26
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	1	2.25
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	1	2.25
(1,1000)	1:243:A:VAL:HG11	1:245:A:TYR:HD1	19	2.25
(1,1000)	1:243:A:VAL:HG12	1:245:A:TYR:HD1	19	2.25
(1,1000)	1:243:A:VAL:HG13	1:245:A:TYR:HD1	19	2.25
(1,1000)	1:243:A:VAL:HG21	1:245:A:TYR:HD1	19	2.25
(1,1000)	1:243:A:VAL:HG22	1:245:A:TYR:HD1	19	2.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1000)	1:243:A:VAL:HG23	1:245:A:TYR:HD1	19	2.25
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	6	2.25
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	10	2.25
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	10	2.25
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	12	2.24
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	12	2.24
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	12	2.24
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	15	2.24
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	1	2.23
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	1	2.23
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	1	2.23
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	1	2.23
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	1	2.23
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	1	2.23
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	8	2.23
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	4	2.23
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	14	2.23
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	5	2.22
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	12	2.21
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	12	2.21
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	12	2.21
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	12	2.21
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	12	2.21
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	12	2.21
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	15	2.21
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	9	2.2
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	9	2.2
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	9	2.2
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	9	2.2
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	9	2.2
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	9	2.2
(1,832)	1:306:A:ILE:HB	1:308:A:TYR:HA	10	2.2
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	13	2.19
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	13	2.19
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	4	2.19
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	9	2.18
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	9	2.18
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	15	2.18
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	15	2.18
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	15	2.18
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	15	2.18
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	15	2.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	15	2.18
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	20	2.18
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	3	2.17
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	3	2.17
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	3	2.17
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	3	2.17
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	3	2.17
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	3	2.17
(1,1000)	1:243:A:VAL:HG11	1:245:A:TYR:HD1	12	2.17
(1,1000)	1:243:A:VAL:HG12	1:245:A:TYR:HD1	12	2.17
(1,1000)	1:243:A:VAL:HG13	1:245:A:TYR:HD1	12	2.17
(1,1000)	1:243:A:VAL:HG21	1:245:A:TYR:HD1	12	2.17
(1,1000)	1:243:A:VAL:HG22	1:245:A:TYR:HD1	12	2.17
(1,1000)	1:243:A:VAL:HG23	1:245:A:TYR:HD1	12	2.17
(1,567)	1:243:A:VAL:HB	1:245:A:TYR:HE1	2	2.17
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	20	2.16
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	20	2.16
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	20	2.16
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	20	2.16
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	20	2.16
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	20	2.16
(1,568)	1:243:A:VAL:HB	1:245:A:TYR:HD1	17	2.15
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	7	2.15
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	9	2.14
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	9	2.14
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	9	2.14
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	9	2.14
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	9	2.14
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	9	2.14
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	8	2.13
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	8	2.13
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	8	2.13
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	8	2.13
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	8	2.13
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	8	2.13
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	13	2.13
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	13	2.13
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	13	2.13
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	13	2.13
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	13	2.13
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	13	2.13
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB3	18	2.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB2	18	2.12
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	20	2.12
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	20	2.12
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	6	2.12
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	2	2.11
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	2	2.11
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	2	2.11
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	2	2.11
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	2	2.11
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	2	2.11
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	10	2.11
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	10	2.11
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	10	2.11
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	10	2.11
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	10	2.11
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	10	2.11
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	13	2.11
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	13	2.11
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	20	2.11
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	11	2.1
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	11	2.1
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	11	2.1
(1,816)	1:299:A:THR:HG21	1:301:A:PHE:HZ	7	2.1
(1,816)	1:299:A:THR:HG22	1:301:A:PHE:HZ	7	2.1
(1,816)	1:299:A:THR:HG23	1:301:A:PHE:HZ	7	2.1
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	11	2.1
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	9	2.09
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	3	2.08
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	3	2.08
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	3	2.08
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	3	2.08
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	17	2.08
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	17	2.08
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	15	2.07
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	15	2.07
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	15	2.07
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	15	2.07
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	15	2.07
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	15	2.07
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	8	2.07
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	8	2.07
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	8	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	4	2.07
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	4	2.07
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	8	2.06
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	10	2.06
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	18	2.06
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	18	2.06
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	18	2.06
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	16	2.06
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	5	2.06
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	5	2.06
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	7	2.06
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	7	2.06
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	10	2.06
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	10	2.06
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	6	2.06
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	4	2.05
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	4	2.05
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	4	2.05
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	4	2.05
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	4	2.05
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	4	2.05
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	2	2.05
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	14	2.05
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	17	2.05
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	17	2.05
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	15	2.05
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	1	2.04
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	1	2.04
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	1	2.04
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	1	2.04
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	1	2.04
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	1	2.04
(1,816)	1:299:A:THR:HG21	1:301:A:PHE:HZ	10	2.04
(1,816)	1:299:A:THR:HG22	1:301:A:PHE:HZ	10	2.04
(1,816)	1:299:A:THR:HG23	1:301:A:PHE:HZ	10	2.04
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	20	2.04
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	13	2.04
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	16	2.04
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	9	2.03
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	4	2.03
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	4	2.03
(1,567)	1:243:A:VAL:HB	1:245:A:TYR:HE1	9	2.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	1	2.03
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	7	2.02
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	7	2.02
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	7	2.02
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	7	2.02
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	7	2.02
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	7	2.02
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	16	2.02
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	16	2.02
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	16	2.02
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	16	2.02
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	16	2.02
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	16	2.02
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	17	2.02
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	17	2.02
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	17	2.02
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	17	2.02
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	17	2.02
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	17	2.02
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	7	2.02
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	7	2.02
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	7	2.02
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	15	2.02
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	15	2.02
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	15	2.02
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	12	2.02
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	12	2.02
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	11	2.02
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	4	2.01
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	4	2.0
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	2	2.0
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	8	2.0
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	18	2.0
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	1	1.99
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG21	4	1.99
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG22	4	1.99
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG23	4	1.99
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	19	1.99
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	17	1.98
(1,568)	1:243:A:VAL:HB	1:245:A:TYR:HD1	19	1.98
(1,567)	1:243:A:VAL:HB	1:245:A:TYR:HE1	19	1.98
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	10	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	10	1.98
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	10	1.98
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	11	1.98
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	11	1.98
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	5	1.97
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	5	1.97
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	5	1.97
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	5	1.97
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	5	1.97
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	5	1.97
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	4	1.97
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	4	1.97
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	4	1.97
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	4	1.97
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	4	1.97
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	4	1.97
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	16	1.97
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	18	1.96
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	18	1.96
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	18	1.96
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	18	1.96
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	18	1.96
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	18	1.96
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	4	1.96
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	4	1.96
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	4	1.96
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	5	1.96
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	6	1.96
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	3	1.95
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	3	1.95
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	3	1.95
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	3	1.95
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	3	1.95
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	3	1.95
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	9	1.94
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	2	1.93
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	2	1.93
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	2	1.93
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	2	1.93
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	2	1.93
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	2	1.93
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	14	1.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	14	1.92
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	14	1.92
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	14	1.92
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	14	1.92
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	14	1.92
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	8	1.92
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	7	1.92
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	11	1.91
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	11	1.91
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	11	1.91
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	11	1.91
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	11	1.91
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	11	1.91
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	12	1.91
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	12	1.91
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	12	1.91
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	12	1.91
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	12	1.91
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	12	1.91
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	4	1.91
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	4	1.91
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	4	1.91
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	4	1.91
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	4	1.91
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	4	1.91
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	5	1.91
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	5	1.91
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	5	1.91
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	7	1.91
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	7	1.91
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	7	1.91
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	12	1.91
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	12	1.91
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	12	1.91
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	8	1.9
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	8	1.9
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	8	1.9
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	8	1.9
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	8	1.9
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	8	1.9
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	17	1.9
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	17	1.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	17	1.9
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	17	1.9
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	17	1.9
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	17	1.9
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	12	1.9
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	12	1.9
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	12	1.9
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	12	1.9
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	12	1.9
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	12	1.9
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	19	1.9
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	2	1.9
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	2	1.9
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	17	1.9
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	17	1.9
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	17	1.9
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	5	1.89
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	5	1.89
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	19	1.89
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	19	1.89
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	19	1.89
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	19	1.89
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	19	1.89
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	19	1.89
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	18	1.89
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	18	1.89
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	18	1.89
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	18	1.89
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	18	1.89
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	18	1.89
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	8	1.89
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	8	1.89
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	8	1.89
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	8	1.89
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	8	1.89
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	8	1.89
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	1	1.89
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	1	1.89
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	1	1.89
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	14	1.89
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	14	1.89
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	14	1.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	11	1.87
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	13	1.87
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	15	1.87
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	15	1.87
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	3	1.86
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	3	1.86
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	3	1.86
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	3	1.86
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	3	1.86
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	3	1.86
(1,723)	1:266:A:LYS:HD2	1:301:A:PHE:HZ	11	1.86
(1,723)	1:266:A:LYS:HD3	1:301:A:PHE:HZ	11	1.86
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	17	1.86
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	17	1.86
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	17	1.86
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	1	1.85
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	1	1.85
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	9	1.85
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	9	1.85
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	9	1.85
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	9	1.85
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	9	1.85
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	9	1.85
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	13	1.84
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	13	1.84
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	13	1.84
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	13	1.84
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	13	1.84
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	13	1.84
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	15	1.84
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	15	1.84
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	15	1.84
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	15	1.84
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	15	1.84
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	15	1.84
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	15	1.84
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	6	1.83
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	6	1.83
(1,1085)	1:260:A:LEU:HD11	1:311:A:ALA:H	6	1.83
(1,1085)	1:260:A:LEU:HD12	1:311:A:ALA:H	6	1.83
(1,1085)	1:260:A:LEU:HD13	1:311:A:ALA:H	6	1.83
(1,1085)	1:260:A:LEU:HD21	1:311:A:ALA:H	6	1.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1085)	1:260:A:LEU:HD22	1:311:A:ALA:H	6	1.83
(1,1085)	1:260:A:LEU:HD23	1:311:A:ALA:H	6	1.83
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	2	1.82
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	10	1.81
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	10	1.81
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	10	1.81
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	10	1.81
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	10	1.81
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	10	1.81
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	3	1.81
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	3	1.81
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	3	1.81
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	3	1.81
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	3	1.81
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	3	1.81
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	8	1.81
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	8	1.81
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	8	1.81
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	14	1.81
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	9	1.81
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	9	1.81
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	9	1.81
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	7	1.8
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	7	1.8
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	7	1.8
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	7	1.8
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	7	1.8
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	7	1.8
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	13	1.8
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	13	1.8
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	13	1.8
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	13	1.8
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	13	1.8
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	13	1.8
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	18	1.8
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	3	1.8
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	3	1.8
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	13	1.8
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	13	1.8
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	13	1.8
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	11	1.79
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	11	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	11	1.79
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	11	1.79
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	11	1.79
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	11	1.79
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	2	1.79
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	2	1.79
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	2	1.79
(1,816)	1:299:A:THR:HG21	1:301:A:PHE:HZ	15	1.79
(1,816)	1:299:A:THR:HG22	1:301:A:PHE:HZ	15	1.79
(1,816)	1:299:A:THR:HG23	1:301:A:PHE:HZ	15	1.79
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	2	1.78
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	2	1.78
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	2	1.78
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	2	1.78
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	2	1.78
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	2	1.78
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	13	1.78
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	13	1.78
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	13	1.78
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	13	1.78
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	13	1.78
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	13	1.78
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	9	1.78
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	9	1.78
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	9	1.78
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	5	1.78
(1,813)	1:299:A:THR:HB	1:301:A:PHE:HE1	17	1.78
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	11	1.78
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	11	1.78
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	11	1.78
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	1	1.78
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	1	1.78
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	5	1.78
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	5	1.78
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	5	1.78
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	4	1.77
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	4	1.77
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	4	1.77
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	4	1.77
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	4	1.77
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	4	1.77
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	19	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	19	1.77
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	19	1.77
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	7	1.76
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	17	1.76
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	1	1.76
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	1	1.76
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	14	1.76
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB2	10	1.75
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB3	10	1.75
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB2	10	1.75
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB3	10	1.75
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	12	1.75
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	12	1.75
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	12	1.75
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	11	1.74
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	11	1.74
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	10	1.74
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	14	1.74
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	14	1.74
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	14	1.74
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	10	1.74
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG11	16	1.73
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG12	16	1.73
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG13	16	1.73
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG21	16	1.73
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG22	16	1.73
(1,1056)	1:255:A:ASP:H	1:331:A:VAL:HG23	16	1.73
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	3	1.73
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	9	1.73
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	15	1.73
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	14	1.72
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	14	1.72
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	14	1.72
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	14	1.72
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	14	1.72
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	14	1.72
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	4	1.72
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	4	1.72
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	4	1.72
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	6	1.72
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	1	1.72
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	1	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	1	1.72
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	2	1.72
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG21	4	1.71
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG22	4	1.71
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG23	4	1.71
(1,568)	1:243:A:VAL:HB	1:245:A:TYR:HD1	2	1.71
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	11	1.71
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	5	1.7
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	5	1.7
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	5	1.7
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	5	1.7
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	5	1.7
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	5	1.7
(1,723)	1:266:A:LYS:HD2	1:301:A:PHE:HZ	3	1.7
(1,723)	1:266:A:LYS:HD3	1:301:A:PHE:HZ	3	1.7
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	2	1.7
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	2	1.68
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	2	1.68
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	12	1.68
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	12	1.68
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	12	1.68
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	11	1.68
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	6	1.68
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	6	1.68
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	6	1.68
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	7	1.67
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	7	1.67
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	7	1.67
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	7	1.67
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	7	1.67
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	7	1.67
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	1	1.67
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	1	1.67
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	1	1.67
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	13	1.67
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	13	1.67
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	13	1.67
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	14	1.67
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	9	1.66
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	9	1.66
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB2	4	1.66
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB3	4	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB2	4	1.66
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB3	4	1.66
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	14	1.66
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	14	1.66
(1,65)	1:251:A:ILE:HG21	1:254:A:PHE:H	5	1.66
(1,65)	1:251:A:ILE:HG22	1:254:A:PHE:H	5	1.66
(1,65)	1:251:A:ILE:HG23	1:254:A:PHE:H	5	1.66
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	2	1.65
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	2	1.65
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	16	1.65
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	16	1.65
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	16	1.65
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	18	1.65
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	18	1.65
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	18	1.65
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	9	1.65
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	9	1.65
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	9	1.65
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	16	1.65
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	16	1.65
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	16	1.65
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	20	1.65
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	15	1.65
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	15	1.65
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	15	1.65
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	13	1.64
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	19	1.64
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	19	1.64
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	20	1.64
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	20	1.64
(1,816)	1:299:A:THR:HG21	1:301:A:PHE:HZ	18	1.63
(1,816)	1:299:A:THR:HG22	1:301:A:PHE:HZ	18	1.63
(1,816)	1:299:A:THR:HG23	1:301:A:PHE:HZ	18	1.63
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB3	7	1.63
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB2	7	1.63
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	2	1.63
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	2	1.63
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	15	1.63
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	15	1.63
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	6	1.63
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	6	1.63
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	6	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	7	1.63
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	7	1.63
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	7	1.63
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	20	1.62
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	20	1.62
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	20	1.62
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	20	1.62
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	20	1.62
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	20	1.62
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	18	1.62
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	18	1.62
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	18	1.62
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	18	1.62
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	18	1.62
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	18	1.62
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	18	1.62
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	18	1.62
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	11	1.62
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	11	1.62
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	18	1.62
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	18	1.62
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	19	1.62
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	19	1.62
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	19	1.62
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	13	1.62
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	13	1.62
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	1	1.61
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	1	1.61
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	1	1.61
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	7	1.61
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	7	1.61
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	7	1.61
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	14	1.6
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	14	1.6
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	14	1.6
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	14	1.6
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	14	1.6
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	14	1.6
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB3	6	1.6
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB2	6	1.6
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	17	1.6
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	17	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	4	1.6
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	4	1.6
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	4	1.6
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	10	1.59
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	10	1.59
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	10	1.59
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	2	1.59
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	2	1.59
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	2	1.59
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	13	1.59
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	13	1.59
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	13	1.59
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	15	1.59
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	15	1.59
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	15	1.59
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	7	1.59
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	7	1.59
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	7	1.59
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	16	1.59
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	16	1.59
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	14	1.59
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	14	1.59
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	13	1.58
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	13	1.58
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	20	1.58
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	17	1.57
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	17	1.57
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	17	1.57
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	3	1.57
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	3	1.57
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	3	1.57
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	8	1.57
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	8	1.57
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	10	1.56
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	10	1.56
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	2	1.56
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	2	1.56
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	2	1.56
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	19	1.56
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	18	1.56
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	3	1.56
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	3	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	3	1.56
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	19	1.55
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	19	1.55
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	19	1.55
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	19	1.55
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	19	1.55
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	19	1.55
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	16	1.55
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	16	1.55
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	16	1.55
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	19	1.55
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	19	1.55
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	19	1.55
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	2	1.55
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	2	1.55
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	2	1.55
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	15	1.55
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	15	1.55
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	15	1.55
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	16	1.55
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	16	1.55
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	16	1.55
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	19	1.55
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	19	1.55
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	19	1.55
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	11	1.54
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	11	1.54
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	11	1.54
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	13	1.54
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	13	1.54
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	13	1.54
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	16	1.54
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	16	1.54
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	16	1.54
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	18	1.54
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	18	1.54
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	18	1.54
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	16	1.54
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	16	1.54
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	16	1.54
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	16	1.54
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	15	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	15	1.54
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	15	1.54
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	6	1.53
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	6	1.53
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	6	1.53
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	11	1.53
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	14	1.53
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	14	1.53
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	20	1.53
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	20	1.53
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	20	1.53
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	2	1.53
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	2	1.53
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	2	1.53
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	12	1.53
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	12	1.53
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	12	1.53
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	17	1.53
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	17	1.53
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	17	1.53
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	20	1.53
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	20	1.53
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	20	1.53
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	16	1.53
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	16	1.53
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	11	1.52
(1,1082)	1:260:A:LEU:HD11	1:308:A:TYR:HD1	4	1.51
(1,1082)	1:260:A:LEU:HD12	1:308:A:TYR:HD1	4	1.51
(1,1082)	1:260:A:LEU:HD13	1:308:A:TYR:HD1	4	1.51
(1,1082)	1:260:A:LEU:HD21	1:308:A:TYR:HD1	4	1.51
(1,1082)	1:260:A:LEU:HD22	1:308:A:TYR:HD1	4	1.51
(1,1082)	1:260:A:LEU:HD23	1:308:A:TYR:HD1	4	1.51
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG21	15	1.51
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG22	15	1.51
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG23	15	1.51
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	4	1.51
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	4	1.51
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	4	1.51
(1,900)	1:244:A:GLN:HB3	1:322:A:ILE:HA	20	1.51
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	13	1.51
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	13	1.51
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	13	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB3	2	1.51
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB2	2	1.51
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	1	1.51
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	1	1.51
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	1	1.51
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	9	1.51
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	9	1.51
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	9	1.51
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	18	1.5
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	18	1.5
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	14	1.5
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	14	1.5
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	14	1.5
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	11	1.5
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	11	1.5
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	11	1.5
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	18	1.5
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	18	1.5
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	18	1.5
(1,67)	1:255:A:ASP:H	1:257:A:ASN:H	13	1.5
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	15	1.49
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	15	1.49
(1,1000)	1:243:A:VAL:HG11	1:245:A:TYR:HD1	18	1.49
(1,1000)	1:243:A:VAL:HG12	1:245:A:TYR:HD1	18	1.49
(1,1000)	1:243:A:VAL:HG13	1:245:A:TYR:HD1	18	1.49
(1,1000)	1:243:A:VAL:HG21	1:245:A:TYR:HD1	18	1.49
(1,1000)	1:243:A:VAL:HG22	1:245:A:TYR:HD1	18	1.49
(1,1000)	1:243:A:VAL:HG23	1:245:A:TYR:HD1	18	1.49
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	6	1.49
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	6	1.49
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	6	1.49
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	20	1.49
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	20	1.49
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	20	1.49
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	15	1.49
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	15	1.49
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	15	1.49
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	9	1.49
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	9	1.49
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	15	1.49
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	15	1.49
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	15	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	12	1.49
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB2	5	1.48
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB3	5	1.48
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB2	5	1.48
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB3	5	1.48
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	3	1.48
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	4	1.48
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	4	1.48
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	4	1.48
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	14	1.48
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	14	1.48
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	14	1.48
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	12	1.47
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	12	1.47
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	6	1.47
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	2	1.47
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	2	1.47
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	2	1.47
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	5	1.47
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	5	1.47
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	8	1.47
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	8	1.47
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	8	1.47
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	15	1.47
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	15	1.47
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	15	1.47
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	3	1.47
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	3	1.47
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	3	1.47
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	9	1.46
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	9	1.46
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	9	1.46
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	9	1.46
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	9	1.46
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	9	1.46
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	17	1.46
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	17	1.46
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	17	1.46
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	17	1.46
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	17	1.46
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	17	1.46
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	12	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	12	1.46
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	12	1.46
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB2	7	1.46
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB3	7	1.46
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB2	7	1.46
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB3	7	1.46
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	17	1.46
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	8	1.46
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	8	1.46
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	8	1.46
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	17	1.46
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	17	1.46
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	17	1.46
(1,65)	1:251:A:ILE:HG21	1:254:A:PHE:H	6	1.46
(1,65)	1:251:A:ILE:HG22	1:254:A:PHE:H	6	1.46
(1,65)	1:251:A:ILE:HG23	1:254:A:PHE:H	6	1.46
(1,65)	1:251:A:ILE:HG21	1:254:A:PHE:H	10	1.46
(1,65)	1:251:A:ILE:HG22	1:254:A:PHE:H	10	1.46
(1,65)	1:251:A:ILE:HG23	1:254:A:PHE:H	10	1.46
(1,900)	1:244:A:GLN:HB3	1:322:A:ILE:HA	1	1.45
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	10	1.45
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	10	1.45
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	10	1.45
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	10	1.45
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	10	1.45
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	9	1.45
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	10	1.45
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	10	1.45
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	10	1.45
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	14	1.45
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	14	1.45
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	14	1.45
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	12	1.44
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	12	1.44
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	12	1.44
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	18	1.44
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	18	1.44
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	11	1.43
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	11	1.43
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	11	1.43
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	11	1.43
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	11	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	11	1.43
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	7	1.43
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	7	1.43
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	7	1.43
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	10	1.43
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	10	1.43
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	10	1.43
(1,1083)	1:260:A:LEU:HD11	1:310:A:LEU:H	6	1.42
(1,1083)	1:260:A:LEU:HD12	1:310:A:LEU:H	6	1.42
(1,1083)	1:260:A:LEU:HD13	1:310:A:LEU:H	6	1.42
(1,1083)	1:260:A:LEU:HD21	1:310:A:LEU:H	6	1.42
(1,1083)	1:260:A:LEU:HD22	1:310:A:LEU:H	6	1.42
(1,1083)	1:260:A:LEU:HD23	1:310:A:LEU:H	6	1.42
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	8	1.42
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	8	1.42
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	8	1.42
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	11	1.42
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	11	1.42
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	11	1.42
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB3	19	1.42
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB2	19	1.42
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	20	1.42
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	20	1.42
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	20	1.42
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	15	1.41
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	15	1.41
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	15	1.41
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	15	1.41
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	15	1.41
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	15	1.41
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	11	1.41
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	11	1.41
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	5	1.41
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	5	1.41
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	5	1.41
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	14	1.41
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	14	1.41
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	14	1.41
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	20	1.41
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	20	1.41
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	20	1.41
(1,67)	1:255:A:ASP:H	1:257:A:ASN:H	6	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	1	1.4
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	1	1.4
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	18	1.4
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	18	1.4
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	18	1.4
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	18	1.4
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	18	1.4
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	18	1.4
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	9	1.4
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	9	1.4
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	9	1.4
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB2	17	1.4
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB3	17	1.4
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB2	17	1.4
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB3	17	1.4
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	13	1.4
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	13	1.4
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	14	1.4
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	14	1.4
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	14	1.4
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	11	1.4
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	11	1.4
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	11	1.4
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	1	1.39
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	1	1.39
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	1	1.39
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	6	1.39
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	6	1.39
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	6	1.39
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	6	1.39
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	6	1.39
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	12	1.39
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	12	1.39
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	12	1.39
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	16	1.39
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	16	1.39
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	16	1.39
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	10	1.38
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	10	1.38
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	10	1.38
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	10	1.38
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	10	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	10	1.38
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	18	1.38
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	18	1.38
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	18	1.38
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	18	1.38
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	18	1.38
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	18	1.38
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	13	1.38
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	13	1.38
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	13	1.38
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	14	1.38
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	14	1.38
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	14	1.38
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	4	1.38
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	4	1.38
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	4	1.38
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	16	1.38
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	16	1.38
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	16	1.38
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	18	1.38
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	18	1.38
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	18	1.38
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	4	1.38
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	4	1.38
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	4	1.38
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	10	1.38
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	10	1.38
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	19	1.38
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	11	1.37
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	11	1.37
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	11	1.37
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	3	1.37
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	3	1.37
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	3	1.37
(1,811)	1:296:A:GLN:HG2	1:301:A:PHE:HD1	20	1.37
(1,811)	1:296:A:GLN:HG3	1:301:A:PHE:HD1	20	1.37
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	18	1.37
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	18	1.37
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	18	1.37
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	19	1.37
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	2	1.37
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	2	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	2	1.37
(1,67)	1:255:A:ASP:H	1:257:A:ASN:H	1	1.37
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	16	1.36
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	16	1.36
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	16	1.36
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	16	1.36
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	16	1.36
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	16	1.36
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	1	1.36
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	1	1.36
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	1	1.36
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	1	1.36
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	1	1.36
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	1	1.36
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	10	1.36
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	10	1.36
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	10	1.36
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	1	1.36
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	1	1.36
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	1	1.36
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	8	1.36
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	8	1.36
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	8	1.36
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	6	1.36
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	6	1.36
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	20	1.36
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	20	1.36
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	20	1.36
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	2	1.35
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	2	1.35
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	2	1.35
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	2	1.35
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	2	1.35
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	2	1.35
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	11	1.35
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	11	1.35
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	11	1.35
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	11	1.35
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	11	1.35
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	11	1.35
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	16	1.35
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	16	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	16	1.35
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB2	11	1.35
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB3	11	1.35
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB2	11	1.35
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB3	11	1.35
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	18	1.35
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	18	1.35
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	18	1.35
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	12	1.34
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	12	1.34
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	9	1.34
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	9	1.34
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	9	1.34
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	9	1.34
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	9	1.34
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	9	1.34
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	2	1.34
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	2	1.34
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	2	1.34
(1,900)	1:244:A:GLN:HB3	1:322:A:ILE:HA	4	1.34
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	7	1.34
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	7	1.34
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	7	1.34
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	19	1.34
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	19	1.34
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	19	1.34
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB3	9	1.34
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB2	9	1.34
(1,722)	1:266:A:LYS:HD2	1:301:A:PHE:HD1	16	1.34
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	6	1.34
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	6	1.34
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	16	1.33
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	16	1.33
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	16	1.33
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	16	1.33
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	16	1.33
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	16	1.33
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	18	1.33
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	18	1.33
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	18	1.33
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	8	1.33
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	8	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	8	1.33
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	11	1.33
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	11	1.33
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	11	1.33
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	11	1.33
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	11	1.33
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	11	1.33
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB3	12	1.33
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB2	12	1.33
(1,483)	1:315:A:ILE:HD11	1:329:A:VAL:H	5	1.33
(1,483)	1:315:A:ILE:HD12	1:329:A:VAL:H	5	1.33
(1,483)	1:315:A:ILE:HD13	1:329:A:VAL:H	5	1.33
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	7	1.33
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	1	1.32
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	1	1.32
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	1	1.32
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	1	1.32
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	1	1.32
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	1	1.32
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	16	1.32
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	16	1.32
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	16	1.32
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	3	1.32
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	3	1.32
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	3	1.32
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	20	1.32
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	20	1.32
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	20	1.32
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	4	1.32
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	14	1.32
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	14	1.32
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	12	1.31
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	12	1.31
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	12	1.31
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	18	1.31
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	18	1.31
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	18	1.31
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB3	20	1.31
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB2	20	1.31
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	4	1.31
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	4	1.31
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	4	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,623)	1:251:A:ILE:HG12	1:268:A:THR:H	7	1.31
(1,623)	1:251:A:ILE:HG13	1:268:A:THR:H	7	1.31
(1,574)	1:244:A:GLN:HA	1:245:A:TYR:HE1	2	1.31
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	4	1.31
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	1	1.31
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	1	1.31
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	1	1.31
(1,65)	1:251:A:ILE:HG21	1:254:A:PHE:H	7	1.31
(1,65)	1:251:A:ILE:HG22	1:254:A:PHE:H	7	1.31
(1,65)	1:251:A:ILE:HG23	1:254:A:PHE:H	7	1.31
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	3	1.3
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	3	1.3
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	16	1.3
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	16	1.3
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	16	1.3
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	1	1.3
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	1	1.3
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	1	1.3
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	15	1.3
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	9	1.29
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	9	1.29
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	13	1.29
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	13	1.29
(1,984)	1:260:A:LEU:HG	1:308:A:TYR:HA	12	1.29
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG21	1	1.29
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG22	1	1.29
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG23	1	1.29
(1,678)	1:262:A:ARG:HB2	1:264:A:ASP:HB3	15	1.29
(1,678)	1:262:A:ARG:HB3	1:264:A:ASP:HB3	15	1.29
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	18	1.29
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	5	1.29
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	10	1.29
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	10	1.29
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	10	1.29
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	11	1.29
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	11	1.29
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	11	1.29
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	10	1.29
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	10	1.29
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	10	1.29
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	19	1.28
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	19	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	19	1.28
(1,723)	1:266:A:LYS:HD2	1:301:A:PHE:HZ	20	1.28
(1,723)	1:266:A:LYS:HD3	1:301:A:PHE:HZ	20	1.28
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	8	1.28
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	8	1.28
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	2	1.28
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	2	1.28
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	2	1.28
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	4	1.27
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	4	1.27
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	4	1.27
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	4	1.27
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	4	1.27
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	4	1.27
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	1	1.27
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	1	1.27
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	1	1.27
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	4	1.27
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	4	1.27
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	4	1.27
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB3	15	1.27
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB2	15	1.27
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB3	17	1.27
(1,773)	1:245:A:TYR:HE1	1:274:A:ASN:HB2	17	1.27
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	10	1.27
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	10	1.27
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	10	1.27
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	6	1.27
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	19	1.27
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	14	1.26
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	14	1.26
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	14	1.26
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB2	15	1.26
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB3	15	1.26
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB2	15	1.26
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB3	15	1.26
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	7	1.26
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	13	1.25
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	13	1.25
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	13	1.25
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	13	1.25
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	13	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	13	1.25
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	7	1.25
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	7	1.25
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG21	20	1.25
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG22	20	1.25
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG23	20	1.25
(1,900)	1:244:A:GLN:HB3	1:322:A:ILE:HA	12	1.25
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	15	1.25
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	19	1.25
(1,67)	1:255:A:ASP:H	1:257:A:ASN:H	4	1.25
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	12	1.25
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	5	1.24
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	5	1.24
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	19	1.24
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	19	1.24
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	17	1.24
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	17	1.24
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	17	1.24
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	20	1.24
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	20	1.24
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	20	1.24
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB3	18	1.24
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB2	18	1.24
(1,574)	1:244:A:GLN:HA	1:245:A:TYR:HE1	15	1.24
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	16	1.24
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	16	1.24
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	16	1.24
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	2	1.24
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	20	1.24
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	5	1.23
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	5	1.23
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	5	1.23
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	5	1.23
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	5	1.23
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	5	1.23
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	8	1.23
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	8	1.23
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	9	1.23
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	13	1.22
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	13	1.22
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	13	1.22
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	13	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	13	1.22
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	13	1.22
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	20	1.22
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	20	1.22
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	20	1.22
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD11	5	1.22
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD12	5	1.22
(1,878)	1:314:A:TYR:H	1:315:A:ILE:HD13	5	1.22
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	8	1.22
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	8	1.22
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	8	1.22
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	9	1.21
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	10	1.21
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	19	1.21
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	13	1.21
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	16	1.21
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	5	1.2
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	5	1.2
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	5	1.2
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	5	1.2
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	5	1.2
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	5	1.2
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	10	1.2
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	5	1.2
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	5	1.2
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	5	1.2
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	15	1.2
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	17	1.2
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	19	1.2
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	19	1.2
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	19	1.2
(1,65)	1:251:A:ILE:HG21	1:254:A:PHE:H	1	1.2
(1,65)	1:251:A:ILE:HG22	1:254:A:PHE:H	1	1.2
(1,65)	1:251:A:ILE:HG23	1:254:A:PHE:H	1	1.2
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	3	1.2
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	11	1.2
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	12	1.19
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	12	1.19
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	12	1.19
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	12	1.19
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	12	1.19
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	12	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	4	1.19
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	4	1.19
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	9	1.19
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	9	1.19
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	9	1.19
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	20	1.19
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	8	1.19
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	16	1.19
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	1	1.19
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	4	1.18
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	4	1.18
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	4	1.18
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	4	1.18
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	4	1.18
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	4	1.18
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	16	1.18
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	16	1.18
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	8	1.18
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	12	1.18
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	12	1.18
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	12	1.18
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	8	1.18
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	2	1.17
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	2	1.17
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	2	1.17
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	2	1.17
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	2	1.17
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	2	1.17
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	18	1.17
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	18	1.17
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	18	1.17
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	18	1.17
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	18	1.17
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	18	1.17
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	20	1.17
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	20	1.17
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	20	1.17
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	20	1.17
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	20	1.17
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	3	1.17
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	3	1.17
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	3	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	8	1.17
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	8	1.17
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	8	1.17
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	19	1.17
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	19	1.17
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	19	1.17
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	1	1.17
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	7	1.17
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	7	1.17
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	7	1.17
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	13	1.17
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	13	1.17
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	13	1.17
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	10	1.17
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	18	1.17
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	15	1.16
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	15	1.16
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	14	1.16
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	14	1.16
(1,816)	1:299:A:THR:HG21	1:301:A:PHE:HZ	17	1.16
(1,816)	1:299:A:THR:HG22	1:301:A:PHE:HZ	17	1.16
(1,816)	1:299:A:THR:HG23	1:301:A:PHE:HZ	17	1.16
(1,1082)	1:260:A:LEU:HD11	1:308:A:TYR:HD1	10	1.15
(1,1082)	1:260:A:LEU:HD12	1:308:A:TYR:HD1	10	1.15
(1,1082)	1:260:A:LEU:HD13	1:308:A:TYR:HD1	10	1.15
(1,1082)	1:260:A:LEU:HD21	1:308:A:TYR:HD1	10	1.15
(1,1082)	1:260:A:LEU:HD22	1:308:A:TYR:HD1	10	1.15
(1,1082)	1:260:A:LEU:HD23	1:308:A:TYR:HD1	10	1.15
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	3	1.15
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	3	1.15
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	3	1.15
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	3	1.15
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	3	1.15
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	3	1.15
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	7	1.15
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	7	1.15
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	7	1.15
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	7	1.15
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	7	1.15
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	7	1.15
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	5	1.15
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	5	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	5	1.15
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	13	1.15
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	13	1.15
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	13	1.15
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	16	1.15
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	12	1.15
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	20	1.15
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	20	1.14
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	20	1.14
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	20	1.14
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	20	1.14
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	20	1.14
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	20	1.14
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	17	1.14
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	17	1.14
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	17	1.14
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	5	1.14
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	5	1.14
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	5	1.14
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	17	1.14
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	17	1.14
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	17	1.14
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	20	1.14
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	18	1.14
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	3	1.14
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	3	1.14
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	3	1.14
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	19	1.14
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG21	20	1.14
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG22	20	1.14
(1,66)	1:254:A:PHE:H	1:329:A:VAL:HG23	20	1.14
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	5	1.14
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	6	1.13
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	6	1.13
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	6	1.13
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	15	1.13
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	15	1.13
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	15	1.13
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	10	1.13
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	10	1.13
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	10	1.13
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	3	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	3	1.13
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	3	1.13
(1,65)	1:251:A:ILE:HG21	1:254:A:PHE:H	8	1.13
(1,65)	1:251:A:ILE:HG22	1:254:A:PHE:H	8	1.13
(1,65)	1:251:A:ILE:HG23	1:254:A:PHE:H	8	1.13
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	12	1.12
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	12	1.12
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	8	1.12
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	8	1.12
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	8	1.12
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	8	1.12
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	8	1.12
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	8	1.12
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	10	1.12
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	10	1.12
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	10	1.12
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	10	1.12
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	10	1.12
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	10	1.12
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	4	1.12
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	4	1.12
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	4	1.12
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	7	1.12
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	7	1.12
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	7	1.12
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	13	1.12
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	13	1.12
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	13	1.12
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	20	1.12
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	20	1.12
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	20	1.12
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD11	6	1.12
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD12	6	1.12
(1,840)	1:302:A:PHE:HD1	1:306:A:ILE:HD13	6	1.12
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	14	1.12
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	16	1.12
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	13	1.12
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	13	1.12
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	11	1.12
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	11	1.12
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	11	1.12
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	18	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	18	1.12
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	18	1.12
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	11	1.12
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	20	1.12
(1,67)	1:255:A:ASP:H	1:257:A:ASN:H	7	1.12
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	7	1.11
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	7	1.11
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	20	1.11
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	20	1.11
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	20	1.11
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	20	1.11
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	20	1.11
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	20	1.11
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	20	1.11
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	20	1.11
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	20	1.11
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	20	1.11
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	20	1.11
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	20	1.11
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	20	1.11
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	20	1.11
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	3	1.11
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	3	1.11
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	3	1.11
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	13	1.11
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	13	1.11
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	13	1.11
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	12	1.11
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	12	1.11
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	12	1.11
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	18	1.11
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	18	1.11
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	18	1.11
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG21	12	1.11
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG22	12	1.11
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG23	12	1.11
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	8	1.11
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	5	1.11
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	16	1.11
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	16	1.11
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	16	1.11
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	11	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	11	1.11
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	11	1.11
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	13	1.11
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	13	1.11
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	13	1.11
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	3	1.11
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	10	1.1
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	10	1.1
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	10	1.1
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	10	1.1
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	10	1.1
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	10	1.1
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	10	1.1
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	10	1.1
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	10	1.1
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	10	1.1
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	10	1.1
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	10	1.1
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	1	1.1
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	1	1.1
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	1	1.1
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	16	1.1
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	16	1.1
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	16	1.1
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	9	1.1
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	9	1.1
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	9	1.1
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	4	1.1
(1,63)	1:251:A:ILE:HG13	1:252:A:GLU:H	17	1.1
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG21	19	1.09
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG22	19	1.09
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG23	19	1.09
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	19	1.09
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	19	1.09
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	19	1.09
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	4	1.09
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	4	1.09
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	4	1.09
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	14	1.08
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	14	1.08
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	14	1.08
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	14	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	14	1.08
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	14	1.08
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	17	1.08
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	17	1.08
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	3	1.08
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	3	1.08
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	3	1.08
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	3	1.08
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	3	1.08
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	3	1.08
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	11	1.08
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	11	1.08
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	11	1.08
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	18	1.08
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	18	1.08
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	18	1.08
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	2	1.08
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	2	1.08
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	2	1.08
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	11	1.08
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	11	1.08
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	11	1.08
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB2	8	1.08
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB3	8	1.08
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB2	8	1.08
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB3	8	1.08
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	16	1.08
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	3	1.08
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	4	1.08
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	4	1.08
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	4	1.08
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	19	1.08
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	19	1.08
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	19	1.08
(1,65)	1:251:A:ILE:HG21	1:254:A:PHE:H	12	1.08
(1,65)	1:251:A:ILE:HG22	1:254:A:PHE:H	12	1.08
(1,65)	1:251:A:ILE:HG23	1:254:A:PHE:H	12	1.08
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	2	1.08
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	5	1.07
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	5	1.07
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	5	1.07
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	10	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	10	1.07
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	10	1.07
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	17	1.07
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	17	1.07
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	17	1.07
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG21	11	1.07
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG22	11	1.07
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG23	11	1.07
(1,900)	1:244:A:GLN:HB3	1:322:A:ILE:HA	9	1.07
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB3	2	1.07
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB2	2	1.07
(1,726)	1:266:A:LYS:HG3	1:301:A:PHE:HD1	16	1.07
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	17	1.07
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	17	1.07
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	17	1.07
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	18	1.07
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	18	1.07
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	18	1.07
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	9	1.07
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	2	1.06
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	2	1.06
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	9	1.06
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	9	1.06
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	9	1.06
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	5	1.06
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	5	1.06
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	5	1.06
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	14	1.06
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	14	1.06
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	14	1.06
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	5	1.06
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	5	1.06
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	5	1.06
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	17	1.06
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	17	1.06
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	17	1.06
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	6	1.06
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	6	1.05
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	6	1.05
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	6	1.05
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	6	1.05
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	6	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	6	1.05
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	19	1.05
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	19	1.05
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	3	1.05
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	3	1.05
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	3	1.05
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	9	1.05
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	9	1.05
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	9	1.05
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG21	4	1.05
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG22	4	1.05
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG23	4	1.05
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	2	1.05
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	2	1.05
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	2	1.05
(1,574)	1:244:A:GLN:HA	1:245:A:TYR:HE1	6	1.05
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	15	1.05
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	5	1.05
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	9	1.05
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	17	1.05
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	17	1.05
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	17	1.05
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	17	1.05
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	19	1.04
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	19	1.04
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	19	1.04
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	19	1.04
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	19	1.04
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	19	1.04
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	8	1.04
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	8	1.04
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	8	1.04
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG21	2	1.04
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG22	2	1.04
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG23	2	1.04
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	7	1.04
(1,317)	1:294:A:GLU:HG2	1:304:A:GLY:H	16	1.04
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	2	1.04
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	2	1.04
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	2	1.04
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	14	1.03
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	14	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	15	1.03
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	15	1.03
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD11	15	1.03
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD12	15	1.03
(1,914)	1:322:A:ILE:HA	1:322:A:ILE:HD13	15	1.03
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	14	1.03
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	14	1.03
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	14	1.03
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	5	1.03
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	5	1.03
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	5	1.03
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	1	1.02
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	1	1.02
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	1	1.02
(1,723)	1:266:A:LYS:HD2	1:301:A:PHE:HZ	10	1.02
(1,723)	1:266:A:LYS:HD3	1:301:A:PHE:HZ	10	1.02
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	9	1.02
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	9	1.02
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	9	1.02
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	3	1.02
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	13	1.02
(1,1077)	1:260:A:LEU:HD11	1:306:A:ILE:HB	6	1.01
(1,1077)	1:260:A:LEU:HD12	1:306:A:ILE:HB	6	1.01
(1,1077)	1:260:A:LEU:HD13	1:306:A:ILE:HB	6	1.01
(1,1077)	1:260:A:LEU:HD21	1:306:A:ILE:HB	6	1.01
(1,1077)	1:260:A:LEU:HD22	1:306:A:ILE:HB	6	1.01
(1,1077)	1:260:A:LEU:HD23	1:306:A:ILE:HB	6	1.01
(1,1072)	1:260:A:LEU:HB2	1:308:A:TYR:H	6	1.01
(1,1072)	1:260:A:LEU:HB3	1:308:A:TYR:H	6	1.01
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	14	1.01
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	14	1.01
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	14	1.01
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	14	1.01
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	14	1.01
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	14	1.01
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD11	7	1.01
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD12	7	1.01
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD13	7	1.01
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG21	15	1.01
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG22	15	1.01
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG23	15	1.01
(1,768)	1:244:A:GLN:HB2	1:274:A:ASN:HB3	15	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	7	1.01
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	15	1.01
(1,658)	1:308:A:TYR:HD1	1:333:A:ILE:HB	7	1.01
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	14	1.01
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	1	1.01
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	8	1.01
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	18	1.01
(1,1095)	1:262:A:ARG:HG2	1:264:A:ASP:HB3	14	1.0
(1,1095)	1:262:A:ARG:HG3	1:264:A:ASP:HB3	14	1.0
(1,1082)	1:260:A:LEU:HD11	1:308:A:TYR:HD1	16	1.0
(1,1082)	1:260:A:LEU:HD12	1:308:A:TYR:HD1	16	1.0
(1,1082)	1:260:A:LEU:HD13	1:308:A:TYR:HD1	16	1.0
(1,1082)	1:260:A:LEU:HD21	1:308:A:TYR:HD1	16	1.0
(1,1082)	1:260:A:LEU:HD22	1:308:A:TYR:HD1	16	1.0
(1,1082)	1:260:A:LEU:HD23	1:308:A:TYR:HD1	16	1.0
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	1	1.0
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	1	1.0
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	1	1.0
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	1	1.0
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	1	1.0
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	1	1.0
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	1	1.0
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	1	1.0
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	1	1.0
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	1	1.0
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	1	1.0
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	1	1.0
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	12	1.0
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	12	1.0
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	12	1.0
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	12	1.0
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	12	1.0
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	12	1.0
(1,900)	1:244:A:GLN:HB3	1:322:A:ILE:HA	11	1.0
(1,574)	1:244:A:GLN:HA	1:245:A:TYR:HE1	12	1.0
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	7	1.0
(1,65)	1:251:A:ILE:HG21	1:254:A:PHE:H	14	1.0
(1,65)	1:251:A:ILE:HG22	1:254:A:PHE:H	14	1.0
(1,65)	1:251:A:ILE:HG23	1:254:A:PHE:H	14	1.0
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	13	0.99
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	13	0.99
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	1	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	1	0.99
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	15	0.99
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	15	0.99
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	15	0.99
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	10	0.99
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	10	0.99
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	10	0.99
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	12	0.99
(1,658)	1:308:A:TYR:HD1	1:333:A:ILE:HB	4	0.99
(1,539)	1:267:A:LEU:HB2	1:269:A:CYS:HB2	5	0.99
(1,539)	1:267:A:LEU:HB3	1:269:A:CYS:HB2	5	0.99
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	17	0.99
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	8	0.99
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	8	0.99
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	8	0.99
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	9	0.99
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	9	0.99
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	9	0.99
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	10	0.99
(1,1082)	1:260:A:LEU:HD11	1:308:A:TYR:HD1	15	0.98
(1,1082)	1:260:A:LEU:HD12	1:308:A:TYR:HD1	15	0.98
(1,1082)	1:260:A:LEU:HD13	1:308:A:TYR:HD1	15	0.98
(1,1082)	1:260:A:LEU:HD21	1:308:A:TYR:HD1	15	0.98
(1,1082)	1:260:A:LEU:HD22	1:308:A:TYR:HD1	15	0.98
(1,1082)	1:260:A:LEU:HD23	1:308:A:TYR:HD1	15	0.98
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB2	13	0.98
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB3	13	0.98
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB2	13	0.98
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB3	13	0.98
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB2	14	0.98
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB3	14	0.98
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB2	14	0.98
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB3	14	0.98
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	4	0.98
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	18	0.98
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	18	0.98
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	18	0.98
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	2	0.97
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	2	0.97
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	17	0.97
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	17	0.97
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	17	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG21	16	0.97
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG22	16	0.97
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG23	16	0.97
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	20	0.97
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	20	0.97
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	20	0.97
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	17	0.97
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	17	0.97
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	17	0.97
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	17	0.97
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	9	0.97
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	9	0.97
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	19	0.97
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	19	0.97
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	19	0.97
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	9	0.97
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	9	0.97
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	9	0.97
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	13	0.97
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG21	2	0.97
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG22	2	0.97
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG23	2	0.97
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	19	0.97
(1,816)	1:299:A:THR:HG21	1:301:A:PHE:HZ	16	0.96
(1,816)	1:299:A:THR:HG22	1:301:A:PHE:HZ	16	0.96
(1,816)	1:299:A:THR:HG23	1:301:A:PHE:HZ	16	0.96
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	11	0.96
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	11	0.96
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	11	0.96
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	7	0.96
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	7	0.96
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	7	0.96
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	13	0.96
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	13	0.96
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	13	0.96
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	18	0.96
(1,539)	1:267:A:LEU:HB2	1:269:A:CYS:HB2	6	0.95
(1,539)	1:267:A:LEU:HB3	1:269:A:CYS:HB2	6	0.95
(1,539)	1:267:A:LEU:HB2	1:269:A:CYS:HB2	16	0.95
(1,539)	1:267:A:LEU:HB3	1:269:A:CYS:HB2	16	0.95
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	16	0.95
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	16	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	16	0.95
(1,157)	1:268:A:THR:H	1:269:A:CYS:HB2	16	0.95
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	16	0.95
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	16	0.95
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	16	0.95
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	2	0.94
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	2	0.94
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	16	0.94
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	16	0.94
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	16	0.94
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	16	0.94
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	16	0.94
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	16	0.94
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	16	0.94
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	16	0.94
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	16	0.94
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	16	0.94
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	16	0.94
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	16	0.94
(1,900)	1:244:A:GLN:HB3	1:322:A:ILE:HA	2	0.94
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	2	0.94
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	18	0.94
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	6	0.94
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	5	0.93
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	5	0.93
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	1	0.93
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	1	0.93
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	1	0.93
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	1	0.93
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	1	0.93
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	1	0.93
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	1	0.93
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	1	0.93
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	1	0.93
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	1	0.93
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	1	0.93
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	1	0.93
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	20	0.93
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	20	0.93
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	20	0.93
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	20	0.93
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	20	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	20	0.93
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	18	0.93
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	18	0.93
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG21	9	0.93
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG22	9	0.93
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG23	9	0.93
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB2	1	0.93
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB3	1	0.93
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB2	1	0.93
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB3	1	0.93
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB2	5	0.93
(1,677)	1:294:A:GLU:HG2	1:303:A:ARG:HB3	5	0.93
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	6	0.93
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	9	0.93
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	9	0.93
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	9	0.93
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	9	0.93
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	9	0.93
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	9	0.93
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	9	0.93
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	9	0.93
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	9	0.93
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	19	0.93
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	16	0.93
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	2	0.93
(1,67)	1:255:A:ASP:H	1:257:A:ASN:H	5	0.93
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	6	0.92
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	6	0.92
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	17	0.92
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	17	0.92
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	17	0.92
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	17	0.92
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	20	0.92
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	20	0.92
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG21	14	0.92
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG22	14	0.92
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG23	14	0.92
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	9	0.92
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	20	0.92
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	6	0.92
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	6	0.92
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	6	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	7	0.92
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	7	0.92
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	7	0.92
(1,678)	1:262:A:ARG:HB2	1:264:A:ASP:HB3	19	0.92
(1,678)	1:262:A:ARG:HB3	1:264:A:ASP:HB3	19	0.92
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	19	0.92
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	19	0.92
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	19	0.92
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	5	0.92
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	7	0.92
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	7	0.92
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	7	0.92
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	16	0.92
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	3	0.91
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	3	0.91
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	5	0.91
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	5	0.91
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	10	0.91
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	10	0.91
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	17	0.91
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	17	0.91
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	17	0.91
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	17	0.91
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	17	0.91
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	17	0.91
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	6	0.91
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	6	0.91
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	8	0.91
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	8	0.91
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	9	0.91
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	9	0.91
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	16	0.91
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	16	0.91
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	18	0.91
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	18	0.91
(1,1082)	1:260:A:LEU:HD11	1:308:A:TYR:HD1	14	0.91
(1,1082)	1:260:A:LEU:HD12	1:308:A:TYR:HD1	14	0.91
(1,1082)	1:260:A:LEU:HD13	1:308:A:TYR:HD1	14	0.91
(1,1082)	1:260:A:LEU:HD21	1:308:A:TYR:HD1	14	0.91
(1,1082)	1:260:A:LEU:HD22	1:308:A:TYR:HD1	14	0.91
(1,1082)	1:260:A:LEU:HD23	1:308:A:TYR:HD1	14	0.91
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	2	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	2	0.91
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	8	0.91
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	8	0.91
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	3	0.91
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	3	0.91
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	3	0.91
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	1	0.91
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	14	0.91
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	12	0.91
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	4	0.91
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	4	0.91
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	4	0.91
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	16	0.91
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	13	0.9
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	13	0.9
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB3	7	0.9
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB2	7	0.9
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	3	0.9
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	3	0.9
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	3	0.9
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	18	0.9
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	15	0.9
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	15	0.9
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	15	0.9
(1,1093)	1:262:A:ARG:HA	1:262:A:ARG:HD2	4	0.89
(1,1093)	1:262:A:ARG:HA	1:262:A:ARG:HD3	4	0.89
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	17	0.89
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	17	0.89
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	17	0.89
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	17	0.89
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	17	0.89
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	17	0.89
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	17	0.89
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	17	0.89
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	17	0.89
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	17	0.89
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	17	0.89
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	17	0.89
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	20	0.89
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	20	0.89
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG21	10	0.89
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG22	10	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG23	10	0.89
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	10	0.89
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	13	0.89
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	17	0.89
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	17	0.89
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	17	0.89
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	6	0.89
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	15	0.88
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	15	0.88
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	19	0.88
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	19	0.88
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	4	0.88
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	4	0.88
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	3	0.88
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	3	0.88
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	12	0.88
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	12	0.88
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	6	0.88
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	6	0.88
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	8	0.88
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	8	0.88
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	8	0.88
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	8	0.88
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	8	0.88
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	8	0.88
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	10	0.88
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	10	0.88
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	10	0.88
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	15	0.88
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	10	0.88
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB3	6	0.88
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB2	6	0.88
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	12	0.88
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	19	0.88
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	9	0.88
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	11	0.88
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	13	0.88
(1,539)	1:267:A:LEU:HB2	1:269:A:CYS:HB2	15	0.88
(1,539)	1:267:A:LEU:HB3	1:269:A:CYS:HB2	15	0.88
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	15	0.88
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	14	0.87
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	14	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	6	0.87
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	6	0.87
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	6	0.87
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG21	18	0.87
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG22	18	0.87
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG23	18	0.87
(1,816)	1:299:A:THR:HG21	1:301:A:PHE:HZ	5	0.87
(1,816)	1:299:A:THR:HG22	1:301:A:PHE:HZ	5	0.87
(1,816)	1:299:A:THR:HG23	1:301:A:PHE:HZ	5	0.87
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	19	0.87
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	19	0.87
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	19	0.87
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	1	0.87
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	1	0.87
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	1	0.87
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	1	0.86
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	1	0.86
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	1	0.86
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	1	0.86
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	4	0.86
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	4	0.86
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	6	0.86
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	6	0.86
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	6	0.86
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	6	0.86
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	6	0.86
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	6	0.86
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	6	0.86
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	6	0.86
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	6	0.86
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	6	0.86
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	6	0.86
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	6	0.86
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	13	0.86
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	13	0.86
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	13	0.86
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG21	8	0.86
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG22	8	0.86
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG23	8	0.86
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG21	13	0.86
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG22	13	0.86
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG23	13	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB3	19	0.86
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB2	19	0.86
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	10	0.86
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	15	0.86
(1,539)	1:267:A:LEU:HB2	1:269:A:CYS:HB2	11	0.86
(1,539)	1:267:A:LEU:HB3	1:269:A:CYS:HB2	11	0.86
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	10	0.85
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	10	0.85
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	9	0.85
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	9	0.85
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	9	0.85
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	9	0.85
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	9	0.85
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	9	0.85
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	9	0.85
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	9	0.85
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	9	0.85
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	9	0.85
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	9	0.85
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	9	0.85
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	16	0.85
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	16	0.85
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	14	0.85
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	14	0.85
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	14	0.85
(1,723)	1:266:A:LYS:HD2	1:301:A:PHE:HZ	15	0.85
(1,723)	1:266:A:LYS:HD3	1:301:A:PHE:HZ	15	0.85
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	9	0.85
(1,309)	1:294:A:GLU:HG2	1:303:A:ARG:H	16	0.85
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	8	0.85
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	8	0.85
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	8	0.85
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	7	0.85
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	3	0.84
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	3	0.84
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	16	0.84
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	16	0.84
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	15	0.84
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	15	0.84
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG21	5	0.84
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG22	5	0.84
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG23	5	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,722)	1:266:A:LYS:HD2	1:301:A:PHE:HD1	5	0.84
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	3	0.84
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	4	0.84
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	1	0.84
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	4	0.84
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	4	0.84
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	4	0.84
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	5	0.84
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	5	0.84
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	5	0.84
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	11	0.84
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	16	0.84
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	2	0.84
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	2	0.84
(1,157)	1:268:A:THR:H	1:269:A:CYS:HB2	4	0.84
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	6	0.84
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	6	0.84
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	6	0.84
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG21	15	0.84
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG22	15	0.84
(1,103)	1:261:A:GLN:H	1:333:A:ILE:HG23	15	0.84
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	10	0.84
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	10	0.84
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	10	0.84
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	11	0.84
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	12	0.83
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	12	0.83
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	7	0.83
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	7	0.83
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	8	0.83
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	8	0.83
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	8	0.83
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	8	0.83
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	8	0.83
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	8	0.83
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	8	0.83
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	8	0.83
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	8	0.83
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	8	0.83
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	8	0.83
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	8	0.83
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	8	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	8	0.83
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	8	0.83
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	8	0.83
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD11	6	0.83
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD12	6	0.83
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD13	6	0.83
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	1	0.83
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	1	0.83
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	1	0.83
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	5	0.83
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	5	0.83
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	5	0.83
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	3	0.83
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	7	0.83
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	13	0.83
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	13	0.83
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	13	0.83
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	1	0.83
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	12	0.83
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	18	0.83
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	20	0.83
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	20	0.83
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	20	0.83
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	4	0.83
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	14	0.83
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	6	0.82
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	6	0.82
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	18	0.82
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	18	0.82
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	10	0.82
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	10	0.82
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	9	0.82
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	9	0.82
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	9	0.82
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	9	0.82
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	9	0.82
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	9	0.82
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	18	0.82
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	18	0.82
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	18	0.82
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	20	0.82
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	20	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	20	0.82
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	14	0.82
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	14	0.82
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	14	0.82
(1,900)	1:244:A:GLN:HB3	1:322:A:ILE:HA	18	0.82
(1,820)	1:300:A:LEU:HG	1:314:A:TYR:HE2	2	0.82
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	4	0.82
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	5	0.82
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	20	0.82
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	4	0.82
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	14	0.82
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	14	0.82
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	14	0.82
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	5	0.82
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	12	0.82
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	12	0.82
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	1	0.82
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	7	0.82
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	10	0.82
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	10	0.82
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	10	0.82
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	18	0.82
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	19	0.82
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	14	0.82
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	16	0.82
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	15	0.81
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	15	0.81
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	15	0.81
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	15	0.81
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	15	0.81
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	15	0.81
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	15	0.81
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	15	0.81
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	15	0.81
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	15	0.81
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	15	0.81
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	15	0.81
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD11	16	0.81
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD12	16	0.81
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD13	16	0.81
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD21	16	0.81
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD22	16	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD23	16	0.81
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	4	0.81
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	4	0.81
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	4	0.81
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	4	0.81
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	4	0.81
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	4	0.81
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	2	0.81
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	2	0.81
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	2	0.81
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	2	0.81
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	18	0.81
(1,539)	1:267:A:LEU:HB2	1:269:A:CYS:HB2	14	0.81
(1,539)	1:267:A:LEU:HB3	1:269:A:CYS:HB2	14	0.81
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	1	0.81
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	1	0.81
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	1	0.81
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	9	0.81
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	9	0.81
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	9	0.81
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	15	0.81
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	15	0.81
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	15	0.81
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	2	0.81
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	20	0.81
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	2	0.81
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	5	0.81
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	15	0.81
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	10	0.8
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	10	0.8
(1,1093)	1:262:A:ARG:HA	1:262:A:ARG:HD2	20	0.8
(1,1093)	1:262:A:ARG:HA	1:262:A:ARG:HD3	20	0.8
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	2	0.8
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	2	0.8
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	2	0.8
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	2	0.8
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	2	0.8
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	2	0.8
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	2	0.8
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	2	0.8
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	2	0.8
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	2	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	2	0.8
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	2	0.8
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	18	0.8
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	18	0.8
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	18	0.8
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	18	0.8
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	18	0.8
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	18	0.8
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	18	0.8
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	18	0.8
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	18	0.8
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	18	0.8
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	18	0.8
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	18	0.8
(1,1082)	1:260:A:LEU:HD11	1:308:A:TYR:HD1	8	0.8
(1,1082)	1:260:A:LEU:HD12	1:308:A:TYR:HD1	8	0.8
(1,1082)	1:260:A:LEU:HD13	1:308:A:TYR:HD1	8	0.8
(1,1082)	1:260:A:LEU:HD21	1:308:A:TYR:HD1	8	0.8
(1,1082)	1:260:A:LEU:HD22	1:308:A:TYR:HD1	8	0.8
(1,1082)	1:260:A:LEU:HD23	1:308:A:TYR:HD1	8	0.8
(1,1082)	1:260:A:LEU:HD11	1:308:A:TYR:HD1	19	0.8
(1,1082)	1:260:A:LEU:HD12	1:308:A:TYR:HD1	19	0.8
(1,1082)	1:260:A:LEU:HD13	1:308:A:TYR:HD1	19	0.8
(1,1082)	1:260:A:LEU:HD21	1:308:A:TYR:HD1	19	0.8
(1,1082)	1:260:A:LEU:HD22	1:308:A:TYR:HD1	19	0.8
(1,1082)	1:260:A:LEU:HD23	1:308:A:TYR:HD1	19	0.8
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	10	0.8
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	10	0.8
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	10	0.8
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	17	0.8
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	13	0.8
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	13	0.8
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	13	0.8
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	17	0.8
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	6	0.8
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	6	0.8
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	6	0.8
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	12	0.8
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	12	0.8
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	12	0.8
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	3	0.8
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	18	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	18	0.79
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	11	0.79
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	11	0.79
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	19	0.79
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	19	0.79
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	19	0.79
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	19	0.79
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	19	0.79
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	19	0.79
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	4	0.79
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	4	0.79
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	4	0.79
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	8	0.79
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	9	0.79
(1,722)	1:266:A:LYS:HD2	1:301:A:PHE:HD1	6	0.79
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	14	0.79
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	8	0.79
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	4	0.79
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	4	0.79
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	2	0.79
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	4	0.79
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	6	0.79
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	15	0.79
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	15	0.79
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	15	0.79
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	3	0.79
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	3	0.79
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	3	0.79
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	20	0.78
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	20	0.78
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	4	0.78
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	4	0.78
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	12	0.78
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	12	0.78
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	12	0.78
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	12	0.78
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	12	0.78
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	12	0.78
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	12	0.78
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	12	0.78
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	12	0.78
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	12	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	12	0.78
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	12	0.78
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	6	0.78
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	6	0.78
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	6	0.78
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	8	0.78
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	8	0.78
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	8	0.78
(1,723)	1:266:A:LYS:HD2	1:301:A:PHE:HZ	7	0.78
(1,723)	1:266:A:LYS:HD3	1:301:A:PHE:HZ	7	0.78
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	17	0.78
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	17	0.78
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	8	0.78
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	8	0.78
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	8	0.78
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	10	0.78
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	10	0.78
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	10	0.78
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	11	0.78
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	11	0.78
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	11	0.78
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	16	0.78
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	16	0.78
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	16	0.78
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	19	0.78
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	19	0.78
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	19	0.78
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	13	0.78
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	13	0.78
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	13	0.78
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	17	0.78
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	14	0.77
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	14	0.77
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	15	0.77
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	15	0.77
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	7	0.77
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	7	0.77
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	12	0.77
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	12	0.77
(1,816)	1:299:A:THR:HG21	1:301:A:PHE:HZ	12	0.77
(1,816)	1:299:A:THR:HG22	1:301:A:PHE:HZ	12	0.77
(1,816)	1:299:A:THR:HG23	1:301:A:PHE:HZ	12	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	6	0.77
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	19	0.77
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	15	0.77
(1,574)	1:244:A:GLN:HA	1:245:A:TYR:HE1	18	0.77
(1,539)	1:267:A:LEU:HB2	1:269:A:CYS:HB2	20	0.77
(1,539)	1:267:A:LEU:HB3	1:269:A:CYS:HB2	20	0.77
(1,528)	1:324:A:THR:H	1:325:A:ARG:HG2	13	0.77
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	8	0.77
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	2	0.77
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	2	0.77
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	2	0.77
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	4	0.77
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	4	0.77
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	4	0.77
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	7	0.77
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	7	0.77
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	7	0.77
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	8	0.77
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	11	0.77
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	10	0.77
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	2	0.77
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	2	0.77
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	2	0.77
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	4	0.77
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	4	0.77
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	4	0.77
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	6	0.77
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	6	0.77
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	6	0.77
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	16	0.76
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	16	0.76
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	11	0.76
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	11	0.76
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	11	0.76
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	11	0.76
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	11	0.76
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	11	0.76
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	11	0.76
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	11	0.76
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	11	0.76
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	11	0.76
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	11	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	11	0.76
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	13	0.76
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	13	0.76
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	13	0.76
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	13	0.76
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	13	0.76
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	13	0.76
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	13	0.76
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	13	0.76
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	13	0.76
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	13	0.76
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	13	0.76
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	13	0.76
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	19	0.76
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	19	0.76
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	19	0.76
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	19	0.76
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	19	0.76
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	19	0.76
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	15	0.76
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	15	0.76
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	15	0.76
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	15	0.76
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	15	0.76
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	15	0.76
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	4	0.76
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	4	0.76
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	3	0.76
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	3	0.76
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	3	0.76
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	16	0.76
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	3	0.76
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	3	0.76
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	3	0.76
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	16	0.76
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	16	0.76
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	16	0.76
(1,539)	1:267:A:LEU:HB2	1:269:A:CYS:HB2	2	0.76
(1,539)	1:267:A:LEU:HB3	1:269:A:CYS:HB2	2	0.76
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	19	0.76
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	10	0.76
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	3	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	14	0.76
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	14	0.76
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	14	0.76
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	8	0.76
(1,67)	1:255:A:ASP:H	1:257:A:ASN:H	14	0.76
(1,21)	1:244:A:GLN:HB3	1:245:A:TYR:H	1	0.76
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	16	0.75
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	16	0.75
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	16	0.75
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	16	0.75
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	16	0.75
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	16	0.75
(1,1102)	1:266:A:LYS:HE2	1:300:A:LEU:H	19	0.75
(1,1102)	1:266:A:LYS:HE3	1:300:A:LEU:H	19	0.75
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	10	0.75
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	10	0.75
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	10	0.75
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	10	0.75
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	10	0.75
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	10	0.75
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	10	0.75
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	10	0.75
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	10	0.75
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	10	0.75
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	10	0.75
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	10	0.75
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	8	0.75
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	8	0.75
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	8	0.75
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	8	0.75
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	8	0.75
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	8	0.75
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	6	0.75
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	6	0.75
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	6	0.75
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	6	0.75
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	6	0.75
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	6	0.75
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	11	0.75
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	13	0.75
(1,722)	1:266:A:LYS:HD2	1:301:A:PHE:HD1	1	0.75
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	6	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,574)	1:244:A:GLN:HA	1:245:A:TYR:HE1	20	0.75
(1,537)	1:251:A:ILE:HD11	1:316:A:CYS:HB2	12	0.75
(1,537)	1:251:A:ILE:HD12	1:316:A:CYS:HB2	12	0.75
(1,537)	1:251:A:ILE:HD13	1:316:A:CYS:HB2	12	0.75
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	2	0.75
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	5	0.74
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	5	0.74
(1,1109)	1:267:A:LEU:HD11	1:268:A:THR:H	16	0.74
(1,1109)	1:267:A:LEU:HD12	1:268:A:THR:H	16	0.74
(1,1109)	1:267:A:LEU:HD13	1:268:A:THR:H	16	0.74
(1,1109)	1:267:A:LEU:HD21	1:268:A:THR:H	16	0.74
(1,1109)	1:267:A:LEU:HD22	1:268:A:THR:H	16	0.74
(1,1109)	1:267:A:LEU:HD23	1:268:A:THR:H	16	0.74
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	3	0.74
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	3	0.74
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	3	0.74
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	3	0.74
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	3	0.74
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	3	0.74
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	3	0.74
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	3	0.74
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	3	0.74
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	3	0.74
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	3	0.74
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	3	0.74
(1,1082)	1:260:A:LEU:HD11	1:308:A:TYR:HD1	2	0.74
(1,1082)	1:260:A:LEU:HD12	1:308:A:TYR:HD1	2	0.74
(1,1082)	1:260:A:LEU:HD13	1:308:A:TYR:HD1	2	0.74
(1,1082)	1:260:A:LEU:HD21	1:308:A:TYR:HD1	2	0.74
(1,1082)	1:260:A:LEU:HD22	1:308:A:TYR:HD1	2	0.74
(1,1082)	1:260:A:LEU:HD23	1:308:A:TYR:HD1	2	0.74
(1,1082)	1:260:A:LEU:HD11	1:308:A:TYR:HD1	13	0.74
(1,1082)	1:260:A:LEU:HD12	1:308:A:TYR:HD1	13	0.74
(1,1082)	1:260:A:LEU:HD13	1:308:A:TYR:HD1	13	0.74
(1,1082)	1:260:A:LEU:HD21	1:308:A:TYR:HD1	13	0.74
(1,1082)	1:260:A:LEU:HD22	1:308:A:TYR:HD1	13	0.74
(1,1082)	1:260:A:LEU:HD23	1:308:A:TYR:HD1	13	0.74
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	5	0.74
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	5	0.74
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	5	0.74
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	5	0.74
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	5	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	5	0.74
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	5	0.74
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	5	0.74
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	5	0.74
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	5	0.74
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	5	0.74
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	5	0.74
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	3	0.74
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	3	0.74
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	3	0.74
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	3	0.74
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	3	0.74
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	3	0.74
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	7	0.74
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	7	0.74
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	7	0.74
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	7	0.74
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	7	0.74
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	7	0.74
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	7	0.74
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	7	0.74
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	7	0.74
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	17	0.74
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	17	0.74
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	17	0.74
(1,731)	1:267:A:LEU:HB2	1:314:A:TYR:HE2	2	0.74
(1,731)	1:267:A:LEU:HB3	1:314:A:TYR:HE2	2	0.74
(1,573)	1:244:A:GLN:HA	1:245:A:TYR:HD1	2	0.74
(1,539)	1:267:A:LEU:HB2	1:269:A:CYS:HB2	4	0.74
(1,539)	1:267:A:LEU:HB3	1:269:A:CYS:HB2	4	0.74
(1,522)	1:255:A:ASP:H	1:258:A:TRP:H	11	0.74
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	3	0.74
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	3	0.74
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	3	0.74
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	11	0.74
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	14	0.73
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	14	0.73
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	19	0.73
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	19	0.73
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	19	0.73
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	19	0.73
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	19	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	19	0.73
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	8	0.73
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	8	0.73
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	8	0.73
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD11	9	0.73
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD12	9	0.73
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD13	9	0.73
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD11	9	0.73
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD12	9	0.73
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD13	9	0.73
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	7	0.73
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	7	0.73
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	7	0.73
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	12	0.73
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	12	0.73
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	12	0.73
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	14	0.73
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	14	0.73
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	14	0.73
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	19	0.73
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	19	0.73
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	19	0.73
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	3	0.73
(1,739)	1:268:A:THR:HG21	1:269:A:CYS:HB3	16	0.73
(1,739)	1:268:A:THR:HG22	1:269:A:CYS:HB3	16	0.73
(1,739)	1:268:A:THR:HG23	1:269:A:CYS:HB3	16	0.73
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	14	0.73
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	14	0.73
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	14	0.73
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	4	0.73
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	4	0.73
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	4	0.73
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	4	0.73
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	4	0.73
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	4	0.73
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	4	0.73
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	4	0.73
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	4	0.73
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	8	0.73
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	8	0.73
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	9	0.73
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	9	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	16	0.73
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	16	0.73
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	8	0.73
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	6	0.73
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	6	0.73
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	6	0.73
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	20	0.73
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	20	0.73
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	20	0.73
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	14	0.73
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	18	0.73
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	18	0.73
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	18	0.73
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	1	0.73
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	1	0.73
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	1	0.73
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	9	0.72
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	9	0.72
(1,1093)	1:262:A:ARG:HA	1:262:A:ARG:HD2	9	0.72
(1,1093)	1:262:A:ARG:HA	1:262:A:ARG:HD3	9	0.72
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	4	0.72
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	4	0.72
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	4	0.72
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	19	0.72
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	19	0.72
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	19	0.72
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	7	0.72
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	7	0.72
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	7	0.72
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB3	12	0.72
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB2	12	0.72
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	13	0.72
(1,739)	1:268:A:THR:HG21	1:269:A:CYS:HB3	6	0.72
(1,739)	1:268:A:THR:HG22	1:269:A:CYS:HB3	6	0.72
(1,739)	1:268:A:THR:HG23	1:269:A:CYS:HB3	6	0.72
(1,722)	1:266:A:LYS:HD2	1:301:A:PHE:HD1	9	0.72
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	19	0.72
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	19	0.72
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	19	0.72
(1,574)	1:244:A:GLN:HA	1:245:A:TYR:HE1	19	0.72
(1,573)	1:244:A:GLN:HA	1:245:A:TYR:HD1	15	0.72
(1,537)	1:251:A:ILE:HD11	1:316:A:CYS:HB2	18	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,537)	1:251:A:ILE:HD12	1:316:A:CYS:HB2	18	0.72
(1,537)	1:251:A:ILE:HD13	1:316:A:CYS:HB2	18	0.72
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	19	0.72
(1,67)	1:255:A:ASP:H	1:257:A:ASN:H	8	0.72
(1,67)	1:255:A:ASP:H	1:257:A:ASN:H	10	0.72
(1,21)	1:244:A:GLN:HB3	1:245:A:TYR:H	12	0.72
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	7	0.71
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	7	0.71
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	18	0.71
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	18	0.71
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	12	0.71
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	12	0.71
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	12	0.71
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	12	0.71
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	12	0.71
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	12	0.71
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	4	0.71
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	4	0.71
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	4	0.71
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	4	0.71
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	4	0.71
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	4	0.71
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	4	0.71
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	4	0.71
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	4	0.71
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	4	0.71
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	4	0.71
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	4	0.71
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	14	0.71
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	14	0.71
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	14	0.71
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	14	0.71
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	14	0.71
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	14	0.71
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	14	0.71
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	14	0.71
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	14	0.71
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	14	0.71
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	14	0.71
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	14	0.71
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	19	0.71
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	19	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	19	0.71
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	19	0.71
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	19	0.71
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	19	0.71
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	19	0.71
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	19	0.71
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	19	0.71
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	19	0.71
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	19	0.71
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	19	0.71
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	8	0.71
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	8	0.71
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	8	0.71
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	12	0.71
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	12	0.71
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	12	0.71
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	17	0.71
(1,739)	1:268:A:THR:HG21	1:269:A:CYS:HB3	2	0.71
(1,739)	1:268:A:THR:HG22	1:269:A:CYS:HB3	2	0.71
(1,739)	1:268:A:THR:HG23	1:269:A:CYS:HB3	2	0.71
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	14	0.71
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	14	0.71
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	14	0.71
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	12	0.71
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	3	0.71
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	1	0.71
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	11	0.7
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	11	0.7
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	11	0.7
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	11	0.7
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	11	0.7
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	11	0.7
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	1	0.7
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	1	0.7
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	1	0.7
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	1	0.7
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	1	0.7
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	1	0.7
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	18	0.7
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	18	0.7
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	18	0.7
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	9	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	9	0.7
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	9	0.7
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	9	0.7
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	9	0.7
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	9	0.7
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	9	0.7
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	9	0.7
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	9	0.7
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	11	0.7
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	11	0.7
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	11	0.7
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	16	0.7
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	16	0.7
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	16	0.7
(1,816)	1:299:A:THR:HG21	1:301:A:PHE:HZ	6	0.7
(1,816)	1:299:A:THR:HG22	1:301:A:PHE:HZ	6	0.7
(1,816)	1:299:A:THR:HG23	1:301:A:PHE:HZ	6	0.7
(1,739)	1:268:A:THR:HG21	1:269:A:CYS:HB3	20	0.7
(1,739)	1:268:A:THR:HG22	1:269:A:CYS:HB3	20	0.7
(1,739)	1:268:A:THR:HG23	1:269:A:CYS:HB3	20	0.7
(1,574)	1:244:A:GLN:HA	1:245:A:TYR:HE1	17	0.7
(1,333)	1:306:A:ILE:HB	1:307:A:THR:H	7	0.7
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	13	0.7
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	20	0.69
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	20	0.69
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	20	0.69
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	20	0.69
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	20	0.69
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	20	0.69
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	14	0.69
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	14	0.69
(1,1015)	1:246:A:GLU:HG2	1:325:A:ARG:HG2	13	0.69
(1,1015)	1:246:A:GLU:HG3	1:325:A:ARG:HG2	13	0.69
(1,1003)	1:244:A:GLN:HG2	1:274:A:ASN:HB3	1	0.69
(1,1003)	1:244:A:GLN:HG3	1:274:A:ASN:HB3	1	0.69
(1,939)	1:327:A:GLY:HA3	1:328:A:GLN:HG2	8	0.69
(1,939)	1:327:A:GLY:HA3	1:328:A:GLN:HG3	8	0.69
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	15	0.69
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	15	0.69
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	15	0.69
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	15	0.69
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	15	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	15	0.69
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	15	0.69
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	15	0.69
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	15	0.69
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	18	0.69
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	18	0.69
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	18	0.69
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	11	0.69
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	18	0.69
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	19	0.69
(1,574)	1:244:A:GLN:HA	1:245:A:TYR:HE1	7	0.69
(1,564)	1:243:A:VAL:HA	1:244:A:GLN:HG3	14	0.69
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	5	0.69
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	5	0.69
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	15	0.69
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	15	0.69
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	8	0.69
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	11	0.69
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	4	0.69
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	3	0.69
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	3	0.69
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	3	0.69
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	12	0.69
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	12	0.69
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	12	0.69
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	17	0.69
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	17	0.69
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	17	0.69
(1,65)	1:251:A:ILE:HG21	1:254:A:PHE:H	18	0.69
(1,65)	1:251:A:ILE:HG22	1:254:A:PHE:H	18	0.69
(1,65)	1:251:A:ILE:HG23	1:254:A:PHE:H	18	0.69
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	1	0.68
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	1	0.68
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	4	0.68
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	4	0.68
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	8	0.68
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	8	0.68
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	11	0.68
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	11	0.68
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	3	0.68
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	3	0.68
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	3	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	3	0.68
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	3	0.68
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	3	0.68
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	3	0.68
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	3	0.68
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	3	0.68
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	3	0.68
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	3	0.68
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	3	0.68
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	5	0.68
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	5	0.68
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	2	0.68
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	2	0.68
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	2	0.68
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	2	0.68
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	2	0.68
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	2	0.68
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	2	0.68
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	2	0.68
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	2	0.68
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	8	0.68
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	8	0.68
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	8	0.68
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	14	0.68
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	14	0.68
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	14	0.68
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	2	0.68
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	2	0.68
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	2	0.68
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	3	0.68
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	11	0.68
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	19	0.68
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	19	0.68
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	19	0.68
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	11	0.68
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	10	0.68
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	10	0.68
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	7	0.68
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	7	0.68
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	7	0.68
(1,347)	1:306:A:ILE:HG21	1:310:A:LEU:H	18	0.68
(1,347)	1:306:A:ILE:HG22	1:310:A:LEU:H	18	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:306:A:ILE:HG23	1:310:A:LEU:H	18	0.68
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	2	0.68
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	2	0.68
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	2	0.68
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	9	0.68
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	14	0.68
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	14	0.68
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	14	0.68
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	20	0.68
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	20	0.68
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	20	0.68
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	2	0.68
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	2	0.68
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	2	0.68
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	9	0.68
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	13	0.67
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	13	0.67
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	19	0.67
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	19	0.67
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	12	0.67
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	12	0.67
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	12	0.67
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	12	0.67
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	12	0.67
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	12	0.67
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	12	0.67
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	12	0.67
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	12	0.67
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	12	0.67
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	12	0.67
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	12	0.67
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	7	0.67
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	7	0.67
(1,1004)	1:244:A:GLN:HG2	1:322:A:ILE:HG13	18	0.67
(1,1004)	1:244:A:GLN:HG3	1:322:A:ILE:HG13	18	0.67
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD11	4	0.67
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD12	4	0.67
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD13	4	0.67
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	12	0.67
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	12	0.67
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	12	0.67
(1,939)	1:327:A:GLY:HA3	1:328:A:GLN:HG2	1	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,939)	1:327:A:GLY:HA3	1:328:A:GLN:HG3	1	0.67
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	2	0.67
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	9	0.67
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	15	0.67
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	19	0.67
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	18	0.67
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	18	0.67
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	18	0.67
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	18	0.67
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	18	0.67
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	18	0.67
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	18	0.67
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	18	0.67
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	18	0.67
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	6	0.67
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	6	0.67
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	7	0.67
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	7	0.67
(1,549)	1:300:A:LEU:HA	1:301:A:PHE:HD1	17	0.67
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	13	0.67
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	13	0.67
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	8	0.67
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	8	0.67
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	8	0.67
(1,157)	1:268:A:THR:H	1:269:A:CYS:HB2	5	0.67
(1,65)	1:251:A:ILE:HG21	1:254:A:PHE:H	4	0.67
(1,65)	1:251:A:ILE:HG22	1:254:A:PHE:H	4	0.67
(1,65)	1:251:A:ILE:HG23	1:254:A:PHE:H	4	0.67
(1,65)	1:251:A:ILE:HG21	1:254:A:PHE:H	13	0.67
(1,65)	1:251:A:ILE:HG22	1:254:A:PHE:H	13	0.67
(1,65)	1:251:A:ILE:HG23	1:254:A:PHE:H	13	0.67
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	17	0.66
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	17	0.66
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	20	0.66
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	20	0.66
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	7	0.66
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	7	0.66
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	5	0.66
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	5	0.66
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	5	0.66
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	5	0.66
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	5	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	5	0.66
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	5	0.66
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	5	0.66
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	5	0.66
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	5	0.66
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	5	0.66
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	5	0.66
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	17	0.66
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	17	0.66
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	17	0.66
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	17	0.66
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	17	0.66
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	17	0.66
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	10	0.66
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	10	0.66
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	10	0.66
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	13	0.66
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	13	0.66
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	13	0.66
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD11	18	0.66
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD12	18	0.66
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD13	18	0.66
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD11	18	0.66
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD12	18	0.66
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD13	18	0.66
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	8	0.66
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	8	0.66
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	8	0.66
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	8	0.66
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	8	0.66
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	8	0.66
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	8	0.66
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	8	0.66
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	8	0.66
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	11	0.66
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	11	0.66
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	11	0.66
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	11	0.66
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	11	0.66
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	11	0.66
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	11	0.66
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	11	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	11	0.66
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	14	0.66
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	14	0.66
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	14	0.66
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	14	0.66
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	14	0.66
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	14	0.66
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	14	0.66
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	14	0.66
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	14	0.66
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	20	0.66
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	20	0.66
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	20	0.66
(1,770)	1:274:A:ASN:HB2	1:322:A:ILE:HG13	11	0.66
(1,770)	1:274:A:ASN:HB3	1:322:A:ILE:HG13	11	0.66
(1,722)	1:266:A:LYS:HD2	1:301:A:PHE:HD1	13	0.66
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	10	0.66
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	10	0.66
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	10	0.66
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	5	0.66
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	7	0.66
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	10	0.66
(1,538)	1:251:A:ILE:HG13	1:316:A:CYS:HB2	6	0.66
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	3	0.66
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	3	0.66
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	3	0.66
(1,21)	1:244:A:GLN:HB3	1:245:A:TYR:H	11	0.66
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	15	0.65
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	15	0.65
(1,1093)	1:262:A:ARG:HA	1:262:A:ARG:HD2	1	0.65
(1,1093)	1:262:A:ARG:HA	1:262:A:ARG:HD3	1	0.65
(1,1082)	1:260:A:LEU:HD11	1:308:A:TYR:HD1	3	0.65
(1,1082)	1:260:A:LEU:HD12	1:308:A:TYR:HD1	3	0.65
(1,1082)	1:260:A:LEU:HD13	1:308:A:TYR:HD1	3	0.65
(1,1082)	1:260:A:LEU:HD21	1:308:A:TYR:HD1	3	0.65
(1,1082)	1:260:A:LEU:HD22	1:308:A:TYR:HD1	3	0.65
(1,1082)	1:260:A:LEU:HD23	1:308:A:TYR:HD1	3	0.65
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	9	0.65
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	9	0.65
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	7	0.65
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	7	0.65
(1,911)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	6	0.65
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	6	0.65
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	6	0.65
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	6	0.65
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	6	0.65
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	6	0.65
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	6	0.65
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	6	0.65
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	6	0.65
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	16	0.65
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	16	0.65
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	16	0.65
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	16	0.65
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	16	0.65
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	16	0.65
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	16	0.65
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	16	0.65
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	16	0.65
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	20	0.65
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	20	0.65
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	20	0.65
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	20	0.65
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	20	0.65
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	20	0.65
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	20	0.65
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	20	0.65
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	20	0.65
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	8	0.65
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	18	0.65
(1,739)	1:268:A:THR:HG21	1:269:A:CYS:HB3	11	0.65
(1,739)	1:268:A:THR:HG22	1:269:A:CYS:HB3	11	0.65
(1,739)	1:268:A:THR:HG23	1:269:A:CYS:HB3	11	0.65
(1,739)	1:268:A:THR:HG21	1:269:A:CYS:HB3	15	0.65
(1,739)	1:268:A:THR:HG22	1:269:A:CYS:HB3	15	0.65
(1,739)	1:268:A:THR:HG23	1:269:A:CYS:HB3	15	0.65
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	6	0.65
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	6	0.65
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	6	0.65
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	14	0.65
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	14	0.65
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	14	0.65
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	14	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	14	0.65
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	14	0.65
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	14	0.65
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	14	0.65
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	14	0.65
(1,537)	1:251:A:ILE:HD11	1:316:A:CYS:HB2	1	0.65
(1,537)	1:251:A:ILE:HD12	1:316:A:CYS:HB2	1	0.65
(1,537)	1:251:A:ILE:HD13	1:316:A:CYS:HB2	1	0.65
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	14	0.65
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	12	0.65
(1,157)	1:268:A:THR:H	1:269:A:CYS:HB2	6	0.65
(1,157)	1:268:A:THR:H	1:269:A:CYS:HB2	15	0.65
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	5	0.65
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	5	0.65
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	5	0.65
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	17	0.65
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD11	5	0.64
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD12	5	0.64
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD13	5	0.64
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD21	5	0.64
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD22	5	0.64
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD23	5	0.64
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	15	0.64
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	15	0.64
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	15	0.64
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	15	0.64
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	15	0.64
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	15	0.64
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	3	0.64
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	3	0.64
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	1	0.64
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	1	0.64
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	1	0.64
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	5	0.64
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	5	0.64
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	5	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	4	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	4	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	4	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	4	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	4	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	4	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	4	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	4	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	4	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	5	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	5	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	5	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	5	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	5	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	5	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	5	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	5	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	5	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	7	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	7	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	7	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	7	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	7	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	7	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	7	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	7	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	7	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	10	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	10	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	10	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	10	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	10	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	10	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	10	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	10	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	10	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	17	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	17	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	17	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	17	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	17	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	17	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	17	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	17	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	17	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	19	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	19	0.64
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	19	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	19	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	19	0.64
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	19	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	19	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	19	0.64
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	19	0.64
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB2	18	0.64
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB3	18	0.64
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB2	18	0.64
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB3	18	0.64
(1,770)	1:274:A:ASN:HB2	1:322:A:ILE:HG13	15	0.64
(1,770)	1:274:A:ASN:HB3	1:322:A:ILE:HG13	15	0.64
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	19	0.64
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	16	0.64
(1,678)	1:262:A:ARG:HB2	1:264:A:ASP:HB3	14	0.64
(1,678)	1:262:A:ARG:HB3	1:264:A:ASP:HB3	14	0.64
(1,537)	1:251:A:ILE:HD11	1:316:A:CYS:HB2	8	0.64
(1,537)	1:251:A:ILE:HD12	1:316:A:CYS:HB2	8	0.64
(1,537)	1:251:A:ILE:HD13	1:316:A:CYS:HB2	8	0.64
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	3	0.64
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	3	0.64
(1,157)	1:268:A:THR:H	1:269:A:CYS:HB2	11	0.64
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD11	19	0.64
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD12	19	0.64
(1,94)	1:260:A:LEU:H	1:333:A:ILE:HD13	19	0.64
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	14	0.64
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	14	0.64
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	14	0.64
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	18	0.63
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	18	0.63
(1,1093)	1:262:A:ARG:HA	1:262:A:ARG:HD2	6	0.63
(1,1093)	1:262:A:ARG:HA	1:262:A:ARG:HD3	6	0.63
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	13	0.63
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	13	0.63
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	13	0.63
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	13	0.63
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	13	0.63
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	13	0.63
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	13	0.63
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	13	0.63
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	13	0.63
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	18	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	18	0.63
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	18	0.63
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	18	0.63
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	18	0.63
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	18	0.63
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	18	0.63
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	18	0.63
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	18	0.63
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	13	0.63
(1,814)	1:299:A:THR:HB	1:301:A:PHE:HD1	20	0.63
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	6	0.63
(1,731)	1:267:A:LEU:HB2	1:314:A:TYR:HE2	17	0.63
(1,731)	1:267:A:LEU:HB3	1:314:A:TYR:HE2	17	0.63
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	9	0.63
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	9	0.63
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	9	0.63
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	1	0.63
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	19	0.63
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	9	0.63
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	9	0.63
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	9	0.63
(1,21)	1:244:A:GLN:HB3	1:245:A:TYR:H	4	0.63
(1,1093)	1:262:A:ARG:HA	1:262:A:ARG:HD2	15	0.62
(1,1093)	1:262:A:ARG:HA	1:262:A:ARG:HD3	15	0.62
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	11	0.62
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	11	0.62
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	11	0.62
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	11	0.62
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	11	0.62
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	11	0.62
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	2	0.62
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	2	0.62
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	2	0.62
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	12	0.62
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	12	0.62
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	12	0.62
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	12	0.62
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	12	0.62
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	12	0.62
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	12	0.62
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	12	0.62
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	12	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	17	0.62
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	17	0.62
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	17	0.62
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	15	0.62
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	15	0.62
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	15	0.62
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	2	0.62
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	10	0.62
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	4	0.62
(1,739)	1:268:A:THR:HG21	1:269:A:CYS:HB3	5	0.62
(1,739)	1:268:A:THR:HG22	1:269:A:CYS:HB3	5	0.62
(1,739)	1:268:A:THR:HG23	1:269:A:CYS:HB3	5	0.62
(1,731)	1:267:A:LEU:HB2	1:314:A:TYR:HE2	16	0.62
(1,731)	1:267:A:LEU:HB3	1:314:A:TYR:HE2	16	0.62
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	7	0.62
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	7	0.62
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	7	0.62
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	11	0.62
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	11	0.62
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	11	0.62
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	7	0.62
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	5	0.62
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	4	0.62
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	14	0.62
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	14	0.62
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	10	0.62
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	12	0.62
(1,157)	1:268:A:THR:H	1:269:A:CYS:HB2	14	0.62
(1,91)	1:260:A:LEU:H	1:306:A:ILE:HB	12	0.62
(1,65)	1:251:A:ILE:HG21	1:254:A:PHE:H	3	0.62
(1,65)	1:251:A:ILE:HG22	1:254:A:PHE:H	3	0.62
(1,65)	1:251:A:ILE:HG23	1:254:A:PHE:H	3	0.62
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	4	0.62
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	4	0.62
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	19	0.61
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	19	0.61
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	9	0.61
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	9	0.61
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	13	0.61
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	13	0.61
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	13	0.61
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	13	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	13	0.61
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	13	0.61
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	13	0.61
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	13	0.61
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	13	0.61
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	13	0.61
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	13	0.61
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	13	0.61
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	8	0.61
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	8	0.61
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	8	0.61
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	1	0.61
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	1	0.61
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	1	0.61
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	1	0.61
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	1	0.61
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	1	0.61
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	1	0.61
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	1	0.61
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	1	0.61
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	9	0.61
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	9	0.61
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	9	0.61
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB3	9	0.61
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB2	9	0.61
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	7	0.61
(1,739)	1:268:A:THR:HG21	1:269:A:CYS:HB3	4	0.61
(1,739)	1:268:A:THR:HG22	1:269:A:CYS:HB3	4	0.61
(1,739)	1:268:A:THR:HG23	1:269:A:CYS:HB3	4	0.61
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	1	0.61
(1,534)	1:251:A:ILE:HG12	1:316:A:CYS:HB3	3	0.61
(1,534)	1:251:A:ILE:HG13	1:316:A:CYS:HB3	3	0.61
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	12	0.61
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	12	0.61
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	12	0.61
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	1	0.61
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	11	0.61
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	10	0.61
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	4	0.61
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	7	0.61
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	10	0.61
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	16	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	16	0.6
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	16	0.6
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	16	0.6
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	16	0.6
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	16	0.6
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	17	0.6
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	17	0.6
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	17	0.6
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	17	0.6
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	17	0.6
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	17	0.6
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD11	3	0.6
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD12	3	0.6
(1,910)	1:322:A:ILE:HG21	1:322:A:ILE:HD13	3	0.6
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD11	3	0.6
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD12	3	0.6
(1,910)	1:322:A:ILE:HG22	1:322:A:ILE:HD13	3	0.6
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD11	3	0.6
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD12	3	0.6
(1,910)	1:322:A:ILE:HG23	1:322:A:ILE:HD13	3	0.6
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	9	0.6
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	9	0.6
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	9	0.6
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	12	0.6
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	7	0.6
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	7	0.6
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	7	0.6
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	20	0.6
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	8	0.6
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	8	0.6
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	8	0.6
(1,573)	1:244:A:GLN:HA	1:245:A:TYR:HD1	6	0.6
(1,566)	1:243:A:VAL:HA	1:244:A:GLN:HG2	6	0.6
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	12	0.6
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	12	0.6
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	20	0.6
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	3	0.6
(1,157)	1:268:A:THR:H	1:269:A:CYS:HB2	2	0.6
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	7	0.6
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	3	0.59
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	3	0.59
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	7	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	7	0.59
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	7	0.59
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	7	0.59
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	7	0.59
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	7	0.59
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	7	0.59
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	7	0.59
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	7	0.59
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	7	0.59
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	7	0.59
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	7	0.59
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	2	0.59
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	2	0.59
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	2	0.59
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	2	0.59
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	2	0.59
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	2	0.59
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	2	0.59
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	2	0.59
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	2	0.59
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	2	0.59
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	2	0.59
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	2	0.59
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	13	0.59
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	13	0.59
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	13	0.59
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	13	0.59
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	13	0.59
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	13	0.59
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG21	10	0.59
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG22	10	0.59
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG23	10	0.59
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB3	15	0.59
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB2	15	0.59
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	10	0.59
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	11	0.59
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	11	0.59
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	11	0.59
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	13	0.59
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	8	0.59
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	8	0.59
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	8	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	8	0.59
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	8	0.59
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	8	0.59
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	8	0.59
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	8	0.59
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	8	0.59
(1,573)	1:244:A:GLN:HA	1:245:A:TYR:HD1	12	0.59
(1,564)	1:243:A:VAL:HA	1:244:A:GLN:HG3	12	0.59
(1,537)	1:251:A:ILE:HD11	1:316:A:CYS:HB2	4	0.59
(1,537)	1:251:A:ILE:HD12	1:316:A:CYS:HB2	4	0.59
(1,537)	1:251:A:ILE:HD13	1:316:A:CYS:HB2	4	0.59
(1,537)	1:251:A:ILE:HD11	1:316:A:CYS:HB2	17	0.59
(1,537)	1:251:A:ILE:HD12	1:316:A:CYS:HB2	17	0.59
(1,537)	1:251:A:ILE:HD13	1:316:A:CYS:HB2	17	0.59
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	1	0.59
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	1	0.59
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	1	0.59
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	7	0.59
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	10	0.59
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	10	0.59
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	10	0.59
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	14	0.59
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	14	0.59
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	14	0.59
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	18	0.59
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	18	0.59
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	18	0.59
(1,397)	1:318:A:ALA:H	1:326:A:SER:HB3	11	0.59
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	20	0.59
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	19	0.59
(1,101)	1:261:A:GLN:H	1:305:A:PRO:HB2	19	0.59
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	15	0.59
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	11	0.58
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	11	0.58
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	10	0.58
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	10	0.58
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	10	0.58
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	10	0.58
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	10	0.58
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	10	0.58
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	7	0.58
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	7	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	7	0.58
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	7	0.58
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	7	0.58
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	7	0.58
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	7	0.58
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	7	0.58
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	7	0.58
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	7	0.58
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	7	0.58
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	7	0.58
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	17	0.58
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	17	0.58
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	17	0.58
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	17	0.58
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	17	0.58
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	17	0.58
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	10	0.58
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	10	0.58
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	10	0.58
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	10	0.58
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	10	0.58
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	10	0.58
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	15	0.58
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	15	0.58
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	15	0.58
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	2	0.58
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	4	0.58
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	4	0.58
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	4	0.58
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	1	0.58
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	1	0.58
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	1	0.58
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	14	0.58
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	14	0.58
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	14	0.58
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	14	0.58
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	11	0.58
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	11	0.58
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	11	0.58
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	7	0.58
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	7	0.58
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	7	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	8	0.58
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	9	0.58
(1,1122)	1:270:A:LYS:HB2	1:270:A:LYS:HD2	12	0.57
(1,1122)	1:270:A:LYS:HB2	1:270:A:LYS:HD3	12	0.57
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	9	0.57
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	9	0.57
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	9	0.57
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	9	0.57
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	9	0.57
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	9	0.57
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG21	16	0.57
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG22	16	0.57
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG23	16	0.57
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	12	0.57
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	12	0.57
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	12	0.57
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	18	0.57
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	18	0.57
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	18	0.57
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	12	0.57
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	12	0.57
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	12	0.57
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	20	0.57
(1,732)	1:267:A:LEU:HB2	1:302:A:PHE:HD1	16	0.57
(1,732)	1:267:A:LEU:HB3	1:302:A:PHE:HD1	16	0.57
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG11	16	0.57
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG12	16	0.57
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG13	16	0.57
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	1	0.57
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	11	0.57
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	2	0.57
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	2	0.57
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	2	0.57
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	11	0.57
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	11	0.57
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	11	0.57
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	17	0.57
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	17	0.57
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	17	0.57
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	3	0.57
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	3	0.57
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	10	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	10	0.57
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	10	0.57
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	1	0.57
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	10	0.57
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	17	0.57
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	13	0.57
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	13	0.57
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	13	0.57
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	18	0.57
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	17	0.57
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	20	0.57
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	19	0.57
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	19	0.57
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	19	0.57
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	13	0.57
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	13	0.57
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	13	0.57
(1,72)	1:258:A:TRP:H	1:334:A:THR:H	9	0.57
(1,72)	1:258:A:TRP:H	1:334:A:THR:H	19	0.57
(1,21)	1:244:A:GLN:HB3	1:245:A:TYR:H	2	0.57
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	17	0.56
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	17	0.56
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	17	0.56
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	17	0.56
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	17	0.56
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	17	0.56
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	17	0.56
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	17	0.56
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	17	0.56
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	17	0.56
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	17	0.56
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	17	0.56
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	20	0.56
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	20	0.56
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	20	0.56
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	20	0.56
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	20	0.56
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	20	0.56
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	20	0.56
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	20	0.56
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	20	0.56
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	20	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	20	0.56
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	20	0.56
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	12	0.56
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	12	0.56
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	12	0.56
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	12	0.56
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	12	0.56
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	12	0.56
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	12	0.56
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	12	0.56
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	12	0.56
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD11	13	0.56
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD12	13	0.56
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD13	13	0.56
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD11	13	0.56
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD12	13	0.56
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD13	13	0.56
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	11	0.56
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	11	0.56
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	11	0.56
(1,776)	1:273:A:ALA:HB1	1:277:A:ALA:HA	9	0.56
(1,776)	1:273:A:ALA:HB2	1:277:A:ALA:HA	9	0.56
(1,776)	1:273:A:ALA:HB3	1:277:A:ALA:HA	9	0.56
(1,776)	1:273:A:ALA:HB1	1:277:A:ALA:HA	11	0.56
(1,776)	1:273:A:ALA:HB2	1:277:A:ALA:HA	11	0.56
(1,776)	1:273:A:ALA:HB3	1:277:A:ALA:HA	11	0.56
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB3	17	0.56
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB2	17	0.56
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	1	0.56
(1,739)	1:268:A:THR:HG21	1:269:A:CYS:HB3	14	0.56
(1,739)	1:268:A:THR:HG22	1:269:A:CYS:HB3	14	0.56
(1,739)	1:268:A:THR:HG23	1:269:A:CYS:HB3	14	0.56
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	1	0.56
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	1	0.56
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	1	0.56
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	4	0.56
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	6	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	1	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	1	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	1	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	3	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	3	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	3	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	9	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	9	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	9	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	10	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	10	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	10	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	12	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	12	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	12	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	13	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	13	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	13	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	14	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	14	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	14	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	19	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	19	0.56
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	19	0.56
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	2	0.56
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	2	0.56
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	2	0.56
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	11	0.56
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	11	0.56
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	11	0.56
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	19	0.56
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	2	0.56
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	1	0.56
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	12	0.56
(1,270)	1:296:A:GLN:HG2	1:299:A:THR:H	18	0.56
(1,270)	1:296:A:GLN:HG3	1:299:A:THR:H	18	0.56
(1,157)	1:268:A:THR:H	1:269:A:CYS:HB2	20	0.56
(1,101)	1:261:A:GLN:H	1:305:A:PRO:HB2	10	0.56
(1,1208)	1:310:A:LEU:HD11	1:314:A:TYR:HE1	3	0.55
(1,1208)	1:310:A:LEU:HD12	1:314:A:TYR:HE1	3	0.55
(1,1208)	1:310:A:LEU:HD13	1:314:A:TYR:HE1	3	0.55
(1,1208)	1:310:A:LEU:HD21	1:314:A:TYR:HE1	3	0.55
(1,1208)	1:310:A:LEU:HD22	1:314:A:TYR:HE1	3	0.55
(1,1208)	1:310:A:LEU:HD23	1:314:A:TYR:HE1	3	0.55
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	9	0.55
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	9	0.55
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	9	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	9	0.55
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	9	0.55
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	9	0.55
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	16	0.55
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	16	0.55
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	16	0.55
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	16	0.55
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	16	0.55
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	16	0.55
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	18	0.55
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	18	0.55
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	18	0.55
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	18	0.55
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	18	0.55
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	18	0.55
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	18	0.55
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	18	0.55
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	18	0.55
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	18	0.55
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	18	0.55
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	18	0.55
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	14	0.55
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	14	0.55
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	14	0.55
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	14	0.55
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	14	0.55
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	14	0.55
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG21	3	0.55
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG22	3	0.55
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG23	3	0.55
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	4	0.55
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	4	0.55
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	4	0.55
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	5	0.55
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	5	0.55
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	5	0.55
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	15	0.55
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	15	0.55
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	15	0.55
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	15	0.55
(1,757)	1:245:A:TYR:HD1	1:273:A:ALA:HA	11	0.55
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	9	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	14	0.55
(1,659)	1:257:A:ASN:HA	1:334:A:THR:HA	3	0.55
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	11	0.55
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	11	0.55
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	11	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	4	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	4	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	4	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	5	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	5	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	5	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	6	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	6	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	6	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	7	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	7	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	7	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	8	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	8	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	8	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	15	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	15	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	15	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	18	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	18	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	18	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	20	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	20	0.55
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	20	0.55
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	9	0.55
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	13	0.55
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	5	0.55
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	5	0.55
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	5	0.55
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	6	0.55
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	12	0.55
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	19	0.55
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	15	0.55
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	16	0.55
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	16	0.55
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	16	0.55
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG21	16	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG22	16	0.55
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG23	16	0.55
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG21	20	0.55
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG22	20	0.55
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG23	20	0.55
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG2	6	0.54
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG3	6	0.54
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG2	6	0.54
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG3	6	0.54
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG2	6	0.54
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG3	6	0.54
(1,1208)	1:310:A:LEU:HD11	1:314:A:TYR:HE1	7	0.54
(1,1208)	1:310:A:LEU:HD12	1:314:A:TYR:HE1	7	0.54
(1,1208)	1:310:A:LEU:HD13	1:314:A:TYR:HE1	7	0.54
(1,1208)	1:310:A:LEU:HD21	1:314:A:TYR:HE1	7	0.54
(1,1208)	1:310:A:LEU:HD22	1:314:A:TYR:HE1	7	0.54
(1,1208)	1:310:A:LEU:HD23	1:314:A:TYR:HE1	7	0.54
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	2	0.54
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	2	0.54
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	2	0.54
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	2	0.54
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	2	0.54
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	2	0.54
(1,1117)	1:268:A:THR:HB	1:270:A:LYS:HG2	17	0.54
(1,1117)	1:268:A:THR:HB	1:270:A:LYS:HG3	17	0.54
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	20	0.54
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	20	0.54
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	20	0.54
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	20	0.54
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	20	0.54
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	20	0.54
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	11	0.54
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	11	0.54
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	11	0.54
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	11	0.54
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	11	0.54
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	11	0.54
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	11	0.54
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	11	0.54
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	11	0.54
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	11	0.54
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	11	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	11	0.54
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	17	0.54
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	17	0.54
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	17	0.54
(1,939)	1:327:A:GLY:HA3	1:328:A:GLN:HG2	7	0.54
(1,939)	1:327:A:GLY:HA3	1:328:A:GLN:HG3	7	0.54
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD11	3	0.54
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD12	3	0.54
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD13	3	0.54
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD11	3	0.54
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD12	3	0.54
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD13	3	0.54
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD11	10	0.54
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD12	10	0.54
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD13	10	0.54
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD11	10	0.54
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD12	10	0.54
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD13	10	0.54
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	5	0.54
(1,726)	1:266:A:LYS:HG3	1:301:A:PHE:HD1	9	0.54
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	10	0.54
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	10	0.54
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	10	0.54
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	15	0.54
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	15	0.54
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	15	0.54
(1,657)	1:308:A:TYR:HE1	1:333:A:ILE:HB	7	0.54
(1,641)	1:251:A:ILE:HD11	1:316:A:CYS:HA	17	0.54
(1,641)	1:251:A:ILE:HD12	1:316:A:CYS:HA	17	0.54
(1,641)	1:251:A:ILE:HD13	1:316:A:CYS:HA	17	0.54
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD11	16	0.54
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD12	16	0.54
(1,636)	1:251:A:ILE:HB	1:251:A:ILE:HD13	16	0.54
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	3	0.54
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	3	0.54
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	3	0.54
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	15	0.54
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	15	0.54
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	15	0.54
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	15	0.54
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	15	0.54
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	15	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	15	0.54
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	15	0.54
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	15	0.54
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	2	0.54
(1,397)	1:318:A:ALA:H	1:326:A:SER:HB3	14	0.54
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	7	0.54
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	12	0.54
(1,302)	1:293:A:VAL:HG21	1:302:A:PHE:H	4	0.54
(1,302)	1:293:A:VAL:HG22	1:302:A:PHE:H	4	0.54
(1,302)	1:293:A:VAL:HG23	1:302:A:PHE:H	4	0.54
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	20	0.54
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	3	0.54
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	3	0.54
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	3	0.54
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	1	0.54
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	2	0.53
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	2	0.53
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	2	0.53
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	2	0.53
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	2	0.53
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	2	0.53
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	11	0.53
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	11	0.53
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	11	0.53
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	11	0.53
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	11	0.53
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	11	0.53
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	19	0.53
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	19	0.53
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	19	0.53
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD11	11	0.53
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD12	11	0.53
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD13	11	0.53
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	19	0.53
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	19	0.53
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	19	0.53
(1,940)	1:251:A:ILE:HD11	1:327:A:GLY:HA2	6	0.53
(1,940)	1:251:A:ILE:HD12	1:327:A:GLY:HA2	6	0.53
(1,940)	1:251:A:ILE:HD13	1:327:A:GLY:HA2	6	0.53
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	1	0.53
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	1	0.53
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	1	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG21	13	0.53
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG22	13	0.53
(1,835)	1:302:A:PHE:HZ	1:306:A:ILE:HG23	13	0.53
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	6	0.53
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	5	0.53
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	5	0.53
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	5	0.53
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	2	0.53
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	2	0.53
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	2	0.53
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	2	0.53
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	2	0.53
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	2	0.53
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	18	0.53
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	18	0.53
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	18	0.53
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	12	0.53
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	5	0.53
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	17	0.53
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	15	0.53
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	12	0.53
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	12	0.53
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	12	0.53
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	2	0.53
(1,397)	1:318:A:ALA:H	1:326:A:SER:HB3	1	0.53
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	7	0.53
(1,250)	1:290:A:PRO:HD2	1:293:A:VAL:H	19	0.53
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	3	0.53
(1,72)	1:258:A:TRP:H	1:334:A:THR:H	20	0.53
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	12	0.53
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	19	0.52
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	19	0.52
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	19	0.52
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	19	0.52
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	19	0.52
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	19	0.52
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	19	0.52
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	19	0.52
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	19	0.52
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	19	0.52
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	19	0.52
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	19	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	18	0.52
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	18	0.52
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	18	0.52
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	18	0.52
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	18	0.52
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	18	0.52
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	8	0.52
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	8	0.52
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	8	0.52
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	8	0.52
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	8	0.52
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	8	0.52
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	19	0.52
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB2	16	0.52
(1,809)	1:296:A:GLN:HG2	1:301:A:PHE:HB3	16	0.52
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB2	16	0.52
(1,809)	1:296:A:GLN:HG3	1:301:A:PHE:HB3	16	0.52
(1,718)	1:266:A:LYS:HB2	1:301:A:PHE:HZ	19	0.52
(1,718)	1:266:A:LYS:HB3	1:301:A:PHE:HZ	19	0.52
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	9	0.52
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	9	0.52
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	9	0.52
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	8	0.52
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	16	0.52
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	11	0.52
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	14	0.52
(1,537)	1:251:A:ILE:HD11	1:316:A:CYS:HB2	10	0.52
(1,537)	1:251:A:ILE:HD12	1:316:A:CYS:HB2	10	0.52
(1,537)	1:251:A:ILE:HD13	1:316:A:CYS:HB2	10	0.52
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	17	0.52
(1,397)	1:318:A:ALA:H	1:326:A:SER:HB3	6	0.52
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	6	0.52
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	16	0.52
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	15	0.52
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	18	0.52
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	7	0.52
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	7	0.52
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	7	0.52
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	12	0.52
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	12	0.52
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	12	0.52
(1,1122)	1:270:A:LYS:HB2	1:270:A:LYS:HD2	1	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1122)	1:270:A:LYS:HB2	1:270:A:LYS:HD3	1	0.51
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	15	0.51
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	15	0.51
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	15	0.51
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	15	0.51
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	15	0.51
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	15	0.51
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	11	0.51
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	11	0.51
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	15	0.51
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	15	0.51
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	15	0.51
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	15	0.51
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	15	0.51
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	15	0.51
(1,1004)	1:244:A:GLN:HG2	1:322:A:ILE:HG13	10	0.51
(1,1004)	1:244:A:GLN:HG3	1:322:A:ILE:HG13	10	0.51
(1,810)	1:296:A:GLN:HG2	1:299:A:THR:HB	16	0.51
(1,810)	1:296:A:GLN:HG3	1:299:A:THR:HB	16	0.51
(1,743)	1:250:A:THR:HB	1:270:A:LYS:HB3	17	0.51
(1,731)	1:267:A:LEU:HB2	1:314:A:TYR:HE2	13	0.51
(1,731)	1:267:A:LEU:HB3	1:314:A:TYR:HE2	13	0.51
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	2	0.51
(1,638)	1:251:A:ILE:HD11	1:316:A:CYS:HB3	9	0.51
(1,638)	1:251:A:ILE:HD12	1:316:A:CYS:HB3	9	0.51
(1,638)	1:251:A:ILE:HD13	1:316:A:CYS:HB3	9	0.51
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	11	0.51
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	11	0.51
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	11	0.51
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	17	0.51
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	17	0.51
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	17	0.51
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	17	0.51
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	17	0.51
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	17	0.51
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	17	0.51
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	17	0.51
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	17	0.51
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	16	0.51
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	2	0.51
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	2	0.51
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	2	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	7	0.51
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	16	0.51
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	1	0.51
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	17	0.51
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	19	0.51
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	8	0.51
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	17	0.51
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	11	0.51
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	17	0.51
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	17	0.51
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	17	0.51
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG21	15	0.51
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG22	15	0.51
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG23	15	0.51
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	6	0.51
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	8	0.51
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	2	0.5
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	2	0.5
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB2	12	0.5
(1,1132)	1:277:A:ALA:H	1:320:A:ASN:HB3	12	0.5
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	13	0.5
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	13	0.5
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	4	0.5
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	4	0.5
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	4	0.5
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	4	0.5
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	4	0.5
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	4	0.5
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG21	19	0.5
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG22	19	0.5
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG23	19	0.5
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG21	10	0.5
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG22	10	0.5
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG23	10	0.5
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	9	0.5
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	9	0.5
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	9	0.5
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	7	0.5
(1,810)	1:296:A:GLN:HG2	1:299:A:THR:HB	14	0.5
(1,810)	1:296:A:GLN:HG3	1:299:A:THR:HB	14	0.5
(1,744)	1:269:A:CYS:HA	1:270:A:LYS:HB2	14	0.5
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	1	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	1	0.5
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	1	0.5
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	8	0.5
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	8	0.5
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	8	0.5
(1,678)	1:262:A:ARG:HB2	1:264:A:ASP:HB3	17	0.5
(1,678)	1:262:A:ARG:HB3	1:264:A:ASP:HB3	17	0.5
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	8	0.5
(1,537)	1:251:A:ILE:HD11	1:316:A:CYS:HB2	7	0.5
(1,537)	1:251:A:ILE:HD12	1:316:A:CYS:HB2	7	0.5
(1,537)	1:251:A:ILE:HD13	1:316:A:CYS:HB2	7	0.5
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	20	0.5
(1,495)	1:331:A:VAL:HB	1:332:A:ASN:H	5	0.5
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	18	0.5
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	18	0.5
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	18	0.5
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	6	0.5
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	16	0.5
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	15	0.5
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	13	0.5
(1,269)	1:269:A:CYS:HB3	1:299:A:THR:H	13	0.5
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	14	0.5
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	14	0.5
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	14	0.5
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	19	0.5
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	19	0.5
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	19	0.5
(1,67)	1:255:A:ASP:H	1:257:A:ASN:H	18	0.5
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG2	3	0.49
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG3	3	0.49
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG2	3	0.49
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG3	3	0.49
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG2	3	0.49
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG3	3	0.49
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	3	0.49
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	3	0.49
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	3	0.49
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	3	0.49
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	3	0.49
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	3	0.49
(1,1082)	1:260:A:LEU:HD11	1:308:A:TYR:HD1	5	0.49
(1,1082)	1:260:A:LEU:HD12	1:308:A:TYR:HD1	5	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1082)	1:260:A:LEU:HD13	1:308:A:TYR:HD1	5	0.49
(1,1082)	1:260:A:LEU:HD21	1:308:A:TYR:HD1	5	0.49
(1,1082)	1:260:A:LEU:HD22	1:308:A:TYR:HD1	5	0.49
(1,1082)	1:260:A:LEU:HD23	1:308:A:TYR:HD1	5	0.49
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	14	0.49
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	14	0.49
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	14	0.49
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	14	0.49
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	14	0.49
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	14	0.49
(1,1004)	1:244:A:GLN:HG2	1:322:A:ILE:HG13	13	0.49
(1,1004)	1:244:A:GLN:HG3	1:322:A:ILE:HG13	13	0.49
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG21	17	0.49
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG22	17	0.49
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG23	17	0.49
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	10	0.49
(1,810)	1:296:A:GLN:HG2	1:299:A:THR:HB	12	0.49
(1,810)	1:296:A:GLN:HG3	1:299:A:THR:HB	12	0.49
(1,810)	1:296:A:GLN:HG2	1:299:A:THR:HB	18	0.49
(1,810)	1:296:A:GLN:HG3	1:299:A:THR:HB	18	0.49
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB3	20	0.49
(1,774)	1:245:A:TYR:HD1	1:274:A:ASN:HB2	20	0.49
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	12	0.49
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	12	0.49
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	12	0.49
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	17	0.49
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	6	0.49
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	6	0.49
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	6	0.49
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	6	0.49
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	6	0.49
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	6	0.49
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	6	0.49
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	6	0.49
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	6	0.49
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	14	0.49
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	14	0.49
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	14	0.49
(1,537)	1:251:A:ILE:HD11	1:316:A:CYS:HB2	5	0.49
(1,537)	1:251:A:ILE:HD12	1:316:A:CYS:HB2	5	0.49
(1,537)	1:251:A:ILE:HD13	1:316:A:CYS:HB2	5	0.49
(1,537)	1:251:A:ILE:HD11	1:316:A:CYS:HB2	20	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,537)	1:251:A:ILE:HD12	1:316:A:CYS:HB2	20	0.49
(1,537)	1:251:A:ILE:HD13	1:316:A:CYS:HB2	20	0.49
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	8	0.49
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	8	0.49
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	8	0.49
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	3	0.49
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	5	0.49
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	5	0.49
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	5	0.49
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	5	0.49
(1,397)	1:318:A:ALA:H	1:326:A:SER:HB3	7	0.49
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	10	0.49
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	12	0.49
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	19	0.49
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	19	0.49
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	19	0.49
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	10	0.49
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	6	0.48
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	6	0.48
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	6	0.48
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	6	0.48
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	6	0.48
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	6	0.48
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	2	0.48
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	2	0.48
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	2	0.48
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	2	0.48
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	2	0.48
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	2	0.48
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	10	0.48
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	10	0.48
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	10	0.48
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	10	0.48
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	10	0.48
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	10	0.48
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	17	0.48
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	17	0.48
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	17	0.48
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	17	0.48
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	17	0.48
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	17	0.48
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	16	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	16	0.48
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	16	0.48
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	16	0.48
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	16	0.48
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	16	0.48
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	16	0.48
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	16	0.48
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	16	0.48
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	16	0.48
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	16	0.48
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	16	0.48
(1,982)	1:308:A:TYR:HA	1:308:A:TYR:HD1	7	0.48
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	14	0.48
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	14	0.48
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	14	0.48
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	15	0.48
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	15	0.48
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	15	0.48
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	20	0.48
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	20	0.48
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	20	0.48
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	5	0.48
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	4	0.48
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	4	0.48
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	4	0.48
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	10	0.48
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	18	0.48
(1,641)	1:251:A:ILE:HD11	1:316:A:CYS:HA	19	0.48
(1,641)	1:251:A:ILE:HD12	1:316:A:CYS:HA	19	0.48
(1,641)	1:251:A:ILE:HD13	1:316:A:CYS:HA	19	0.48
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	5	0.48
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	5	0.48
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	5	0.48
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	6	0.48
(1,495)	1:331:A:VAL:HB	1:332:A:ASN:H	6	0.48
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	5	0.48
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	8	0.48
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	8	0.48
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	8	0.48
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	8	0.48
(1,111)	1:263:A:THR:H	1:264:A:ASP:HB3	14	0.48
(1,111)	1:263:A:THR:H	1:264:A:ASP:HB2	14	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG21	9	0.48
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG22	9	0.48
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG23	9	0.48
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	5	0.48
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	3	0.48
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG2	11	0.47
(1,1223)	1:315:A:ILE:HB	1:328:A:GLN:HG3	11	0.47
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	18	0.47
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	18	0.47
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	18	0.47
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	18	0.47
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	18	0.47
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	18	0.47
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD11	4	0.47
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD12	4	0.47
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD13	4	0.47
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD21	4	0.47
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD22	4	0.47
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD23	4	0.47
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	5	0.47
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	5	0.47
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	5	0.47
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	5	0.47
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	5	0.47
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	5	0.47
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG21	2	0.47
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG22	2	0.47
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG23	2	0.47
(1,940)	1:251:A:ILE:HD11	1:327:A:GLY:HA2	9	0.47
(1,940)	1:251:A:ILE:HD12	1:327:A:GLY:HA2	9	0.47
(1,940)	1:251:A:ILE:HD13	1:327:A:GLY:HA2	9	0.47
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD11	5	0.47
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD12	5	0.47
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD13	5	0.47
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD11	5	0.47
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD12	5	0.47
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD13	5	0.47
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	6	0.47
(1,810)	1:296:A:GLN:HG2	1:299:A:THR:HB	19	0.47
(1,810)	1:296:A:GLN:HG3	1:299:A:THR:HB	19	0.47
(1,732)	1:267:A:LEU:HB2	1:302:A:PHE:HD1	8	0.47
(1,732)	1:267:A:LEU:HB3	1:302:A:PHE:HD1	8	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	17	0.47
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	19	0.47
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	19	0.47
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	19	0.47
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	1	0.47
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	1	0.47
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	20	0.47
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	20	0.47
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	17	0.47
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	17	0.47
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	17	0.47
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	9	0.47
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	11	0.47
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	3	0.47
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	7	0.47
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	10	0.47
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	5	0.47
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	5	0.47
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	5	0.47
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	16	0.47
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	16	0.47
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	16	0.47
(1,67)	1:255:A:ASP:H	1:257:A:ASN:H	3	0.47
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	8	0.46
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	8	0.46
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	8	0.46
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	8	0.46
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	8	0.46
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	8	0.46
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	8	0.46
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	8	0.46
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	8	0.46
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	8	0.46
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	8	0.46
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	8	0.46
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	14	0.46
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	14	0.46
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	14	0.46
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	14	0.46
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	14	0.46
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	14	0.46
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	14	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	14	0.46
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	14	0.46
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	14	0.46
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	14	0.46
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	14	0.46
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD11	3	0.46
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD12	3	0.46
(1,973)	1:260:A:LEU:HG	1:333:A:ILE:HD13	3	0.46
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG21	16	0.46
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG22	16	0.46
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG23	16	0.46
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	4	0.46
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	4	0.46
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	4	0.46
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	1	0.46
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	3	0.46
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	13	0.46
(1,810)	1:296:A:GLN:HG2	1:299:A:THR:HB	11	0.46
(1,810)	1:296:A:GLN:HG3	1:299:A:THR:HB	11	0.46
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	20	0.46
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	20	0.46
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	20	0.46
(1,770)	1:274:A:ASN:HB2	1:322:A:ILE:HG13	6	0.46
(1,770)	1:274:A:ASN:HB3	1:322:A:ILE:HG13	6	0.46
(1,723)	1:266:A:LYS:HD2	1:301:A:PHE:HZ	18	0.46
(1,723)	1:266:A:LYS:HD3	1:301:A:PHE:HZ	18	0.46
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	4	0.46
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	4	0.46
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	4	0.46
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	17	0.46
(1,672)	1:261:A:GLN:HB3	1:305:A:PRO:HB2	9	0.46
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	15	0.46
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	15	0.46
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	15	0.46
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	11	0.46
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	11	0.46
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	11	0.46
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	11	0.46
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	11	0.46
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	11	0.46
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	11	0.46
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	11	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	11	0.46
(1,574)	1:244:A:GLN:HA	1:245:A:TYR:HE1	9	0.46
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	4	0.46
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	9	0.46
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	5	0.46
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	19	0.46
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	10	0.46
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	10	0.46
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	10	0.46
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	11	0.45
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	11	0.45
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	11	0.45
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	11	0.45
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	11	0.45
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	11	0.45
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	9	0.45
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	9	0.45
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	9	0.45
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	17	0.45
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	17	0.45
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	17	0.45
(1,827)	1:261:A:GLN:HA	1:305:A:PRO:HB2	10	0.45
(1,816)	1:299:A:THR:HG21	1:301:A:PHE:HZ	13	0.45
(1,816)	1:299:A:THR:HG22	1:301:A:PHE:HZ	13	0.45
(1,816)	1:299:A:THR:HG23	1:301:A:PHE:HZ	13	0.45
(1,757)	1:245:A:TYR:HD1	1:273:A:ALA:HA	3	0.45
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	15	0.45
(1,641)	1:251:A:ILE:HD11	1:316:A:CYS:HA	1	0.45
(1,641)	1:251:A:ILE:HD12	1:316:A:CYS:HA	1	0.45
(1,641)	1:251:A:ILE:HD13	1:316:A:CYS:HA	1	0.45
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	12	0.45
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	12	0.45
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	12	0.45
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	12	0.45
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	12	0.45
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	12	0.45
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	12	0.45
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	12	0.45
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	12	0.45
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	16	0.45
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	16	0.45
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	16	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	16	0.45
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	16	0.45
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	16	0.45
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	16	0.45
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	16	0.45
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	16	0.45
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	7	0.45
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	13	0.45
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	15	0.45
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	15	0.45
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	15	0.45
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	9	0.45
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	7	0.45
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	9	0.45
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	20	0.45
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	10	0.45
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	10	0.45
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	10	0.45
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG21	10	0.45
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG22	10	0.45
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG23	10	0.45
(1,1125)	1:270:A:LYS:HB3	1:270:A:LYS:HE2	15	0.44
(1,1125)	1:270:A:LYS:HB3	1:270:A:LYS:HE3	15	0.44
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	19	0.44
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	19	0.44
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	19	0.44
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	19	0.44
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	19	0.44
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	19	0.44
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	10	0.44
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	10	0.44
(1,1093)	1:262:A:ARG:HA	1:262:A:ARG:HD2	8	0.44
(1,1093)	1:262:A:ARG:HA	1:262:A:ARG:HD3	8	0.44
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD11	16	0.44
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD12	16	0.44
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD13	16	0.44
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD11	16	0.44
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD12	16	0.44
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD13	16	0.44
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	16	0.44
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG21	19	0.44
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG22	19	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG23	19	0.44
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG21	19	0.44
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG22	19	0.44
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG23	19	0.44
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	15	0.44
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	15	0.44
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	15	0.44
(1,678)	1:262:A:ARG:HB2	1:264:A:ASP:HB3	10	0.44
(1,678)	1:262:A:ARG:HB3	1:264:A:ASP:HB3	10	0.44
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	2	0.44
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	2	0.44
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	2	0.44
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	2	0.44
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	2	0.44
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	2	0.44
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	2	0.44
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	2	0.44
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	2	0.44
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	19	0.44
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	19	0.44
(1,537)	1:251:A:ILE:HD11	1:316:A:CYS:HB2	19	0.44
(1,537)	1:251:A:ILE:HD12	1:316:A:CYS:HB2	19	0.44
(1,537)	1:251:A:ILE:HD13	1:316:A:CYS:HB2	19	0.44
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	1	0.44
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	4	0.44
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	10	0.44
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	16	0.44
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	12	0.44
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	6	0.44
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	13	0.44
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	6	0.44
(1,270)	1:296:A:GLN:HG2	1:299:A:THR:H	12	0.44
(1,270)	1:296:A:GLN:HG3	1:299:A:THR:H	12	0.44
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	20	0.44
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	20	0.44
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	20	0.44
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG21	19	0.44
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG22	19	0.44
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG23	19	0.44
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	6	0.43
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	6	0.43
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	11	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	11	0.43
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	11	0.43
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	11	0.43
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	11	0.43
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	11	0.43
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	13	0.43
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	13	0.43
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	13	0.43
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	13	0.43
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	13	0.43
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	13	0.43
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	20	0.43
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	20	0.43
(1,1048)	1:252:A:GLU:HB2	1:270:A:LYS:HD2	2	0.43
(1,1048)	1:252:A:GLU:HB2	1:270:A:LYS:HD3	2	0.43
(1,1048)	1:252:A:GLU:HB3	1:270:A:LYS:HD2	2	0.43
(1,1048)	1:252:A:GLU:HB3	1:270:A:LYS:HD3	2	0.43
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	19	0.43
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	19	0.43
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	19	0.43
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	19	0.43
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	19	0.43
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	19	0.43
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	3	0.43
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	3	0.43
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	3	0.43
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	3	0.43
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	3	0.43
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	3	0.43
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	5	0.43
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	5	0.43
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	5	0.43
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	16	0.43
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	16	0.43
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	16	0.43
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	5	0.43
(1,776)	1:273:A:ALA:HB1	1:277:A:ALA:HA	12	0.43
(1,776)	1:273:A:ALA:HB2	1:277:A:ALA:HA	12	0.43
(1,776)	1:273:A:ALA:HB3	1:277:A:ALA:HA	12	0.43
(1,770)	1:274:A:ASN:HB2	1:322:A:ILE:HG13	12	0.43
(1,770)	1:274:A:ASN:HB3	1:322:A:ILE:HG13	12	0.43
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG21	11	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG22	11	0.43
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG23	11	0.43
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG21	11	0.43
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG22	11	0.43
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG23	11	0.43
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	12	0.43
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	12	0.43
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	12	0.43
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	3	0.43
(1,678)	1:262:A:ARG:HB2	1:264:A:ASP:HB3	9	0.43
(1,678)	1:262:A:ARG:HB3	1:264:A:ASP:HB3	9	0.43
(1,658)	1:308:A:TYR:HD1	1:333:A:ILE:HB	15	0.43
(1,645)	1:251:A:ILE:HD11	1:314:A:TYR:H	8	0.43
(1,645)	1:251:A:ILE:HD12	1:314:A:TYR:H	8	0.43
(1,645)	1:251:A:ILE:HD13	1:314:A:TYR:H	8	0.43
(1,645)	1:251:A:ILE:HD11	1:314:A:TYR:H	12	0.43
(1,645)	1:251:A:ILE:HD12	1:314:A:TYR:H	12	0.43
(1,645)	1:251:A:ILE:HD13	1:314:A:TYR:H	12	0.43
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	14	0.43
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	14	0.43
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	14	0.43
(1,605)	1:250:A:THR:HA	1:270:A:LYS:HB2	20	0.43
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	12	0.43
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	18	0.43
(1,495)	1:331:A:VAL:HB	1:332:A:ASN:H	10	0.43
(1,495)	1:331:A:VAL:HB	1:332:A:ASN:H	18	0.43
(1,495)	1:331:A:VAL:HB	1:332:A:ASN:H	20	0.43
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	5	0.43
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	20	0.43
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	1	0.43
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	2	0.43
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	12	0.43
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	15	0.43
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	2	0.43
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG21	5	0.43
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG22	5	0.43
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG23	5	0.43
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	6	0.43
(1,18)	1:245:A:TYR:H	1:273:A:ALA:HA	15	0.43
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG2	8	0.42
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG3	8	0.42
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG2	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG3	8	0.42
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG2	8	0.42
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG3	8	0.42
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	14	0.42
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	14	0.42
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	3	0.42
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	3	0.42
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	3	0.42
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	3	0.42
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	3	0.42
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	3	0.42
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	8	0.42
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	8	0.42
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	8	0.42
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	8	0.42
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	8	0.42
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	8	0.42
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	20	0.42
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	20	0.42
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	20	0.42
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	20	0.42
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	20	0.42
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	20	0.42
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	16	0.42
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	16	0.42
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	16	0.42
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	16	0.42
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	16	0.42
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	16	0.42
(1,905)	1:247:A:PRO:HD2	1:322:A:ILE:HG12	10	0.42
(1,905)	1:247:A:PRO:HD3	1:322:A:ILE:HG12	10	0.42
(1,849)	1:285:A:LEU:HB2	1:313:A:THR:HG21	6	0.42
(1,849)	1:285:A:LEU:HB2	1:313:A:THR:HG22	6	0.42
(1,849)	1:285:A:LEU:HB2	1:313:A:THR:HG23	6	0.42
(1,849)	1:285:A:LEU:HB3	1:313:A:THR:HG21	6	0.42
(1,849)	1:285:A:LEU:HB3	1:313:A:THR:HG22	6	0.42
(1,849)	1:285:A:LEU:HB3	1:313:A:THR:HG23	6	0.42
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	7	0.42
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	7	0.42
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	7	0.42
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	7	0.42
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	7	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	7	0.42
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	7	0.42
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	7	0.42
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	7	0.42
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	7	0.42
(1,564)	1:243:A:VAL:HA	1:244:A:GLN:HG3	3	0.42
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	6	0.42
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	6	0.42
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	6	0.42
(1,537)	1:251:A:ILE:HD11	1:316:A:CYS:HB2	15	0.42
(1,537)	1:251:A:ILE:HD12	1:316:A:CYS:HB2	15	0.42
(1,537)	1:251:A:ILE:HD13	1:316:A:CYS:HB2	15	0.42
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	8	0.42
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	14	0.42
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	20	0.42
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	20	0.42
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	20	0.42
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	11	0.42
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	15	0.42
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	2	0.42
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	8	0.42
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	3	0.42
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	3	0.42
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	8	0.42
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	8	0.42
(1,157)	1:268:A:THR:H	1:269:A:CYS:HB2	3	0.42
(1,123)	1:265:A:VAL:H	1:266:A:LYS:HG2	3	0.42
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD11	20	0.41
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD12	20	0.41
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD13	20	0.41
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD11	20	0.41
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD12	20	0.41
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD13	20	0.41
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB2	6	0.41
(1,1084)	1:260:A:LEU:HD11	1:310:A:LEU:HB3	6	0.41
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB2	6	0.41
(1,1084)	1:260:A:LEU:HD12	1:310:A:LEU:HB3	6	0.41
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB2	6	0.41
(1,1084)	1:260:A:LEU:HD13	1:310:A:LEU:HB3	6	0.41
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB2	6	0.41
(1,1084)	1:260:A:LEU:HD21	1:310:A:LEU:HB3	6	0.41
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB2	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1084)	1:260:A:LEU:HD22	1:310:A:LEU:HB3	6	0.41
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB2	6	0.41
(1,1084)	1:260:A:LEU:HD23	1:310:A:LEU:HB3	6	0.41
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	1	0.41
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	1	0.41
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	1	0.41
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	1	0.41
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	1	0.41
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	1	0.41
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD11	13	0.41
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD12	13	0.41
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD13	13	0.41
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD21	13	0.41
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD22	13	0.41
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD23	13	0.41
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	2	0.41
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	2	0.41
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	2	0.41
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	2	0.41
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	2	0.41
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	2	0.41
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB2	9	0.41
(1,1043)	1:251:A:ILE:HG21	1:254:A:PHE:HB3	9	0.41
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB2	9	0.41
(1,1043)	1:251:A:ILE:HG22	1:254:A:PHE:HB3	9	0.41
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB2	9	0.41
(1,1043)	1:251:A:ILE:HG23	1:254:A:PHE:HB3	9	0.41
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	6	0.41
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	6	0.41
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	6	0.41
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD11	15	0.41
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD12	15	0.41
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD13	15	0.41
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG21	7	0.41
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG22	7	0.41
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG23	7	0.41
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG21	7	0.41
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG22	7	0.41
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG23	7	0.41
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	6	0.41
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	6	0.41
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	16	0.41
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	16	0.41
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	16	0.41
(1,691)	1:264:A:ASP:HB3	1:265:A:VAL:HA	15	0.41
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	2	0.41
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	2	0.41
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	2	0.41
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	3	0.41
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	18	0.41
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	12	0.41
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	13	0.41
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	4	0.41
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	14	0.41
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	16	0.41
(1,190)	1:245:A:TYR:H	1:274:A:ASN:H	15	0.41
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	8	0.41
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	18	0.41
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	18	0.41
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	18	0.41
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	16	0.4
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	16	0.4
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD11	6	0.4
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD12	6	0.4
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD13	6	0.4
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD21	6	0.4
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD22	6	0.4
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD23	6	0.4
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG21	15	0.4
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG22	15	0.4
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG23	15	0.4
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	19	0.4
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	19	0.4
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	19	0.4
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	9	0.4
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	9	0.4
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	9	0.4
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	7	0.4
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	7	0.4
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	7	0.4
(1,816)	1:299:A:THR:HG21	1:301:A:PHE:HZ	1	0.4
(1,816)	1:299:A:THR:HG22	1:301:A:PHE:HZ	1	0.4
(1,816)	1:299:A:THR:HG23	1:301:A:PHE:HZ	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,757)	1:245:A:TYR:HD1	1:273:A:ALA:HA	8	0.4
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	18	0.4
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	1	0.4
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	1	0.4
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	1	0.4
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	5	0.4
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	5	0.4
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	5	0.4
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	9	0.4
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	9	0.4
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	9	0.4
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	12	0.4
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	12	0.4
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	12	0.4
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	17	0.4
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	17	0.4
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	17	0.4
(1,573)	1:244:A:GLN:HA	1:245:A:TYR:HD1	17	0.4
(1,495)	1:331:A:VAL:HB	1:332:A:ASN:H	3	0.4
(1,495)	1:331:A:VAL:HB	1:332:A:ASN:H	12	0.4
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	13	0.4
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	15	0.4
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	1	0.4
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	5	0.4
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	20	0.4
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG21	11	0.4
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG22	11	0.4
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG23	11	0.4
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG21	13	0.4
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG22	13	0.4
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG23	13	0.4
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	7	0.4
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD11	19	0.39
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD12	19	0.39
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD13	19	0.39
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD11	19	0.39
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD12	19	0.39
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD13	19	0.39
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	14	0.39
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	14	0.39
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	14	0.39
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	14	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	14	0.39
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	14	0.39
(1,1175)	1:293:A:VAL:HG11	1:302:A:PHE:H	3	0.39
(1,1175)	1:293:A:VAL:HG12	1:302:A:PHE:H	3	0.39
(1,1175)	1:293:A:VAL:HG13	1:302:A:PHE:H	3	0.39
(1,1175)	1:293:A:VAL:HG21	1:302:A:PHE:H	3	0.39
(1,1175)	1:293:A:VAL:HG22	1:302:A:PHE:H	3	0.39
(1,1175)	1:293:A:VAL:HG23	1:302:A:PHE:H	3	0.39
(1,1155)	1:285:A:LEU:HD11	1:315:A:ILE:HD11	18	0.39
(1,1155)	1:285:A:LEU:HD11	1:315:A:ILE:HD12	18	0.39
(1,1155)	1:285:A:LEU:HD11	1:315:A:ILE:HD13	18	0.39
(1,1155)	1:285:A:LEU:HD12	1:315:A:ILE:HD11	18	0.39
(1,1155)	1:285:A:LEU:HD12	1:315:A:ILE:HD12	18	0.39
(1,1155)	1:285:A:LEU:HD12	1:315:A:ILE:HD13	18	0.39
(1,1155)	1:285:A:LEU:HD13	1:315:A:ILE:HD11	18	0.39
(1,1155)	1:285:A:LEU:HD13	1:315:A:ILE:HD12	18	0.39
(1,1155)	1:285:A:LEU:HD13	1:315:A:ILE:HD13	18	0.39
(1,1155)	1:285:A:LEU:HD21	1:315:A:ILE:HD11	18	0.39
(1,1155)	1:285:A:LEU:HD21	1:315:A:ILE:HD12	18	0.39
(1,1155)	1:285:A:LEU:HD21	1:315:A:ILE:HD13	18	0.39
(1,1155)	1:285:A:LEU:HD22	1:315:A:ILE:HD11	18	0.39
(1,1155)	1:285:A:LEU:HD22	1:315:A:ILE:HD12	18	0.39
(1,1155)	1:285:A:LEU:HD22	1:315:A:ILE:HD13	18	0.39
(1,1155)	1:285:A:LEU:HD23	1:315:A:ILE:HD11	18	0.39
(1,1155)	1:285:A:LEU:HD23	1:315:A:ILE:HD12	18	0.39
(1,1155)	1:285:A:LEU:HD23	1:315:A:ILE:HD13	18	0.39
(1,1048)	1:252:A:GLU:HB2	1:270:A:LYS:HD2	3	0.39
(1,1048)	1:252:A:GLU:HB2	1:270:A:LYS:HD3	3	0.39
(1,1048)	1:252:A:GLU:HB3	1:270:A:LYS:HD2	3	0.39
(1,1048)	1:252:A:GLU:HB3	1:270:A:LYS:HD3	3	0.39
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	17	0.39
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	17	0.39
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	17	0.39
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	17	0.39
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	17	0.39
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	17	0.39
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD11	5	0.39
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD12	5	0.39
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD13	5	0.39
(1,939)	1:327:A:GLY:HA3	1:328:A:GLN:HG2	4	0.39
(1,939)	1:327:A:GLY:HA3	1:328:A:GLN:HG3	4	0.39
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD11	8	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD12	8	0.39
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD13	8	0.39
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD11	8	0.39
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD12	8	0.39
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD13	8	0.39
(1,900)	1:244:A:GLN:HB3	1:322:A:ILE:HA	10	0.39
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	2	0.39
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	2	0.39
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	2	0.39
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG21	10	0.39
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG22	10	0.39
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG23	10	0.39
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG21	10	0.39
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG22	10	0.39
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG23	10	0.39
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	20	0.39
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	8	0.39
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	8	0.39
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	8	0.39
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	6	0.39
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	6	0.39
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	6	0.39
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	9	0.39
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	9	0.39
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	9	0.39
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	7	0.39
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	7	0.39
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	7	0.39
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	10	0.39
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	10	0.39
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	10	0.39
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	13	0.39
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	13	0.39
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	13	0.39
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	15	0.39
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	15	0.39
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	15	0.39
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	19	0.39
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	19	0.39
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	19	0.39
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	20	0.39
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	20	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	20	0.39
(1,612)	1:250:A:THR:HB	1:270:A:LYS:HB2	17	0.39
(1,544)	1:258:A:TRP:HA	1:259:A:TYR:HD1	2	0.39
(1,511)	1:259:A:TYR:HB3	1:334:A:THR:H	1	0.39
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	19	0.39
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	19	0.39
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	19	0.39
(1,397)	1:318:A:ALA:H	1:326:A:SER:HB3	17	0.39
(1,397)	1:318:A:ALA:H	1:326:A:SER:HB3	19	0.39
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	18	0.39
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	3	0.39
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	7	0.39
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	17	0.39
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	18	0.39
(1,270)	1:296:A:GLN:HG2	1:299:A:THR:H	2	0.39
(1,270)	1:296:A:GLN:HG3	1:299:A:THR:H	2	0.39
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	15	0.39
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	15	0.39
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	7	0.39
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	7	0.39
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	7	0.39
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	8	0.39
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	8	0.39
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	8	0.39
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	11	0.39
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	11	0.39
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	11	0.39
(1,21)	1:244:A:GLN:HB3	1:245:A:TYR:H	20	0.39
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB2	1	0.38
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB3	1	0.38
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB2	1	0.38
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB3	1	0.38
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB2	1	0.38
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB3	1	0.38
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	7	0.38
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	7	0.38
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	7	0.38
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	7	0.38
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	7	0.38
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	7	0.38
(1,1010)	1:246:A:GLU:HB2	1:325:A:ARG:HD2	11	0.38
(1,1010)	1:246:A:GLU:HB2	1:325:A:ARG:HD3	11	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1010)	1:246:A:GLU:HB3	1:325:A:ARG:HD2	11	0.38
(1,1010)	1:246:A:GLU:HB3	1:325:A:ARG:HD3	11	0.38
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD11	6	0.38
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD12	6	0.38
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD13	6	0.38
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD11	6	0.38
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD12	6	0.38
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD13	6	0.38
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	16	0.38
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	16	0.38
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	16	0.38
(1,810)	1:296:A:GLN:HG2	1:299:A:THR:HB	13	0.38
(1,810)	1:296:A:GLN:HG3	1:299:A:THR:HB	13	0.38
(1,683)	1:247:A:PRO:HB2	1:325:A:ARG:HB2	2	0.38
(1,644)	1:251:A:ILE:HD11	1:328:A:GLN:HA	19	0.38
(1,644)	1:251:A:ILE:HD12	1:328:A:GLN:HA	19	0.38
(1,644)	1:251:A:ILE:HD13	1:328:A:GLN:HA	19	0.38
(1,639)	1:251:A:ILE:HD11	1:314:A:TYR:HB3	17	0.38
(1,639)	1:251:A:ILE:HD12	1:314:A:TYR:HB3	17	0.38
(1,639)	1:251:A:ILE:HD13	1:314:A:TYR:HB3	17	0.38
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	4	0.38
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	4	0.38
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	4	0.38
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	12	0.38
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	12	0.38
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	12	0.38
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	2	0.38
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	2	0.38
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	2	0.38
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	3	0.38
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	3	0.38
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	3	0.38
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	4	0.38
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	4	0.38
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	4	0.38
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	6	0.38
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	6	0.38
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	6	0.38
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	8	0.38
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	8	0.38
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	8	0.38
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	11	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	11	0.38
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	11	0.38
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	14	0.38
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	14	0.38
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	14	0.38
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	16	0.38
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	16	0.38
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	16	0.38
(1,626)	1:251:A:ILE:HG21	1:251:A:ILE:HG12	18	0.38
(1,626)	1:251:A:ILE:HG22	1:251:A:ILE:HG12	18	0.38
(1,626)	1:251:A:ILE:HG23	1:251:A:ILE:HG12	18	0.38
(1,573)	1:244:A:GLN:HA	1:245:A:TYR:HD1	18	0.38
(1,573)	1:244:A:GLN:HA	1:245:A:TYR:HD1	19	0.38
(1,528)	1:324:A:THR:H	1:325:A:ARG:HG2	8	0.38
(1,523)	1:258:A:TRP:H	1:259:A:TYR:HE1	15	0.38
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	11	0.38
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	11	0.38
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	7	0.38
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	19	0.38
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	16	0.38
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	16	0.38
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	20	0.38
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	20	0.38
(1,101)	1:261:A:GLN:H	1:305:A:PRO:HB2	6	0.38
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	14	0.38
(1,13)	1:244:A:GLN:H	1:244:A:GLN:HB2	12	0.38
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG2	4	0.37
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG3	4	0.37
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG2	4	0.37
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG3	4	0.37
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG2	4	0.37
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG3	4	0.37
(1,1168)	1:291:A:LYS:HA	1:291:A:LYS:HG2	10	0.37
(1,1168)	1:291:A:LYS:HA	1:291:A:LYS:HG3	10	0.37
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	19	0.37
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	19	0.37
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	20	0.37
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	20	0.37
(1,1142)	1:280:A:TYR:H	1:281:A:HIS:HB2	14	0.37
(1,1142)	1:280:A:TYR:H	1:281:A:HIS:HB3	14	0.37
(1,1095)	1:262:A:ARG:HG2	1:264:A:ASP:HB3	15	0.37
(1,1095)	1:262:A:ARG:HG3	1:264:A:ASP:HB3	15	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	13	0.37
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	13	0.37
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	13	0.37
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	13	0.37
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	13	0.37
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	13	0.37
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG21	4	0.37
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG22	4	0.37
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG23	4	0.37
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG21	13	0.37
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG22	13	0.37
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG23	13	0.37
(1,939)	1:327:A:GLY:HA3	1:328:A:GLN:HG2	6	0.37
(1,939)	1:327:A:GLY:HA3	1:328:A:GLN:HG3	6	0.37
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	17	0.37
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	17	0.37
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	17	0.37
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	6	0.37
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	6	0.37
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	6	0.37
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	9	0.37
(1,757)	1:245:A:TYR:HD1	1:273:A:ALA:HA	16	0.37
(1,727)	1:266:A:LYS:HG3	1:267:A:LEU:H	5	0.37
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	18	0.37
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	18	0.37
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	18	0.37
(1,682)	1:262:A:ARG:HA	1:262:A:ARG:HD2	4	0.37
(1,682)	1:262:A:ARG:HA	1:262:A:ARG:HD3	4	0.37
(1,645)	1:251:A:ILE:HD11	1:314:A:TYR:H	17	0.37
(1,645)	1:251:A:ILE:HD12	1:314:A:TYR:H	17	0.37
(1,645)	1:251:A:ILE:HD13	1:314:A:TYR:H	17	0.37
(1,644)	1:251:A:ILE:HD11	1:328:A:GLN:HA	6	0.37
(1,644)	1:251:A:ILE:HD12	1:328:A:GLN:HA	6	0.37
(1,644)	1:251:A:ILE:HD13	1:328:A:GLN:HA	6	0.37
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	1	0.37
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	1	0.37
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	1	0.37
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	2	0.37
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	2	0.37
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	2	0.37
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	12	0.37
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	12	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	12	0.37
(1,557)	1:300:A:LEU:HB2	1:302:A:PHE:HZ	18	0.37
(1,557)	1:300:A:LEU:HB3	1:302:A:PHE:HZ	18	0.37
(1,544)	1:258:A:TRP:HA	1:259:A:TYR:HD1	17	0.37
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	14	0.37
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	14	0.37
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	14	0.37
(1,397)	1:318:A:ALA:H	1:326:A:SER:HB3	10	0.37
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	5	0.37
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	6	0.37
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	18	0.37
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	9	0.37
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	17	0.37
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	9	0.37
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	15	0.37
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	14	0.37
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	5	0.37
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	5	0.37
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	13	0.37
(1,111)	1:263:A:THR:H	1:264:A:ASP:HB3	15	0.37
(1,111)	1:263:A:THR:H	1:264:A:ASP:HB2	15	0.37
(1,101)	1:261:A:GLN:H	1:305:A:PRO:HB2	3	0.37
(1,72)	1:258:A:TRP:H	1:334:A:THR:H	15	0.37
(1,72)	1:258:A:TRP:H	1:334:A:THR:H	17	0.37
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	1	0.37
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD11	4	0.36
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD12	4	0.36
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD13	4	0.36
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD11	4	0.36
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD12	4	0.36
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD13	4	0.36
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD11	6	0.36
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD12	6	0.36
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD13	6	0.36
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD11	6	0.36
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD12	6	0.36
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD13	6	0.36
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	5	0.36
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	5	0.36
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	5	0.36
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	5	0.36
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	5	0.36
(1,1168)	1:291:A:LYS:HA	1:291:A:LYS:HG2	16	0.36
(1,1168)	1:291:A:LYS:HA	1:291:A:LYS:HG3	16	0.36
(1,1168)	1:291:A:LYS:HA	1:291:A:LYS:HG2	18	0.36
(1,1168)	1:291:A:LYS:HA	1:291:A:LYS:HG3	18	0.36
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	1	0.36
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	1	0.36
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	12	0.36
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	12	0.36
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	12	0.36
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	12	0.36
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	12	0.36
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	12	0.36
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG2	11	0.36
(1,1045)	1:251:A:ILE:HD11	1:328:A:GLN:HG3	11	0.36
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG2	11	0.36
(1,1045)	1:251:A:ILE:HD12	1:328:A:GLN:HG3	11	0.36
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG2	11	0.36
(1,1045)	1:251:A:ILE:HD13	1:328:A:GLN:HG3	11	0.36
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG21	5	0.36
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG22	5	0.36
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG23	5	0.36
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG21	8	0.36
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG22	8	0.36
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG23	8	0.36
(1,940)	1:251:A:ILE:HD11	1:327:A:GLY:HA2	3	0.36
(1,940)	1:251:A:ILE:HD12	1:327:A:GLY:HA2	3	0.36
(1,940)	1:251:A:ILE:HD13	1:327:A:GLY:HA2	3	0.36
(1,905)	1:247:A:PRO:HD2	1:322:A:ILE:HG12	1	0.36
(1,905)	1:247:A:PRO:HD3	1:322:A:ILE:HG12	1	0.36
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	1	0.36
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	1	0.36
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	1	0.36
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	11	0.36
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	11	0.36
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	11	0.36
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	19	0.36
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	19	0.36
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	19	0.36
(1,827)	1:261:A:GLN:HA	1:305:A:PRO:HB2	19	0.36
(1,816)	1:299:A:THR:HG21	1:301:A:PHE:HZ	14	0.36
(1,816)	1:299:A:THR:HG22	1:301:A:PHE:HZ	14	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,816)	1:299:A:THR:HG23	1:301:A:PHE:HZ	14	0.36
(1,768)	1:244:A:GLN:HB2	1:274:A:ASN:HB3	3	0.36
(1,731)	1:267:A:LEU:HB2	1:314:A:TYR:HE2	8	0.36
(1,731)	1:267:A:LEU:HB3	1:314:A:TYR:HE2	8	0.36
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	4	0.36
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	8	0.36
(1,685)	1:324:A:THR:HB	1:325:A:ARG:HG2	13	0.36
(1,644)	1:251:A:ILE:HD11	1:328:A:GLN:HA	3	0.36
(1,644)	1:251:A:ILE:HD12	1:328:A:GLN:HA	3	0.36
(1,644)	1:251:A:ILE:HD13	1:328:A:GLN:HA	3	0.36
(1,644)	1:251:A:ILE:HD11	1:328:A:GLN:HA	4	0.36
(1,644)	1:251:A:ILE:HD12	1:328:A:GLN:HA	4	0.36
(1,644)	1:251:A:ILE:HD13	1:328:A:GLN:HA	4	0.36
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	15	0.36
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	15	0.36
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	15	0.36
(1,573)	1:244:A:GLN:HA	1:245:A:TYR:HD1	20	0.36
(1,544)	1:258:A:TRP:HA	1:259:A:TYR:HD1	16	0.36
(1,537)	1:251:A:ILE:HD11	1:316:A:CYS:HB2	16	0.36
(1,537)	1:251:A:ILE:HD12	1:316:A:CYS:HB2	16	0.36
(1,537)	1:251:A:ILE:HD13	1:316:A:CYS:HB2	16	0.36
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	6	0.36
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	6	0.36
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	6	0.36
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	14	0.36
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	12	0.36
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	20	0.36
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	4	0.36
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	4	0.36
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	1	0.36
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	1	0.36
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	1	0.36
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	1	0.36
(1,70)	1:257:A:ASN:H	1:258:A:TRP:HA	4	0.36
(1,18)	1:245:A:TYR:H	1:273:A:ALA:HA	2	0.36
(1,1192)	1:303:A:ARG:HG2	1:304:A:GLY:H	4	0.35
(1,1192)	1:303:A:ARG:HG3	1:304:A:GLY:H	4	0.35
(1,1168)	1:291:A:LYS:HA	1:291:A:LYS:HG2	1	0.35
(1,1168)	1:291:A:LYS:HA	1:291:A:LYS:HG3	1	0.35
(1,1168)	1:291:A:LYS:HA	1:291:A:LYS:HG2	6	0.35
(1,1168)	1:291:A:LYS:HA	1:291:A:LYS:HG3	6	0.35
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	3	0.35
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	5	0.35
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	5	0.35
(1,1142)	1:280:A:TYR:H	1:281:A:HIS:HB2	10	0.35
(1,1142)	1:280:A:TYR:H	1:281:A:HIS:HB3	10	0.35
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB2	16	0.35
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB3	16	0.35
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB2	16	0.35
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB3	16	0.35
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB2	16	0.35
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB3	16	0.35
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	1	0.35
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	1	0.35
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	1	0.35
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	1	0.35
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	1	0.35
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	1	0.35
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	4	0.35
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	4	0.35
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	4	0.35
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	4	0.35
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	4	0.35
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	4	0.35
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	7	0.35
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	7	0.35
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	7	0.35
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	7	0.35
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	7	0.35
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	7	0.35
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	4	0.35
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	4	0.35
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	4	0.35
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	4	0.35
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	4	0.35
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	4	0.35
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	4	0.35
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	4	0.35
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	4	0.35
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	4	0.35
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	4	0.35
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	4	0.35
(1,1048)	1:252:A:GLU:HB2	1:270:A:LYS:HD2	16	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1048)	1:252:A:GLU:HB2	1:270:A:LYS:HD3	16	0.35
(1,1048)	1:252:A:GLU:HB3	1:270:A:LYS:HD2	16	0.35
(1,1048)	1:252:A:GLU:HB3	1:270:A:LYS:HD3	16	0.35
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD11	16	0.35
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD12	16	0.35
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD13	16	0.35
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD11	19	0.35
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD12	19	0.35
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD13	19	0.35
(1,905)	1:247:A:PRO:HD2	1:322:A:ILE:HG12	8	0.35
(1,905)	1:247:A:PRO:HD3	1:322:A:ILE:HG12	8	0.35
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	14	0.35
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	14	0.35
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	14	0.35
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	19	0.35
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	19	0.35
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	19	0.35
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	10	0.35
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	10	0.35
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	10	0.35
(1,740)	1:268:A:THR:HA	1:269:A:CYS:HB3	5	0.35
(1,726)	1:266:A:LYS:HG3	1:301:A:PHE:HD1	1	0.35
(1,657)	1:308:A:TYR:HE1	1:333:A:ILE:HB	4	0.35
(1,644)	1:251:A:ILE:HD11	1:328:A:GLN:HA	8	0.35
(1,644)	1:251:A:ILE:HD12	1:328:A:GLN:HA	8	0.35
(1,644)	1:251:A:ILE:HD13	1:328:A:GLN:HA	8	0.35
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	8	0.35
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	8	0.35
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	8	0.35
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	10	0.35
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	10	0.35
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	10	0.35
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	11	0.35
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	11	0.35
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	11	0.35
(1,564)	1:243:A:VAL:HA	1:244:A:GLN:HG3	5	0.35
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	10	0.35
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	14	0.35
(1,283)	1:296:A:GLN:HG2	1:301:A:PHE:H	6	0.35
(1,283)	1:296:A:GLN:HG3	1:301:A:PHE:H	6	0.35
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	7	0.35
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	9	0.35
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	9	0.35
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	17	0.35
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	17	0.35
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	4	0.35
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	9	0.35
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	9	0.35
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	9	0.35
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	17	0.35
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	17	0.35
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	17	0.35
(1,13)	1:244:A:GLN:H	1:244:A:GLN:HB2	1	0.35
(1,1250)	1:330:A:GLU:HB2	1:331:A:VAL:H	4	0.34
(1,1250)	1:330:A:GLU:HB3	1:331:A:VAL:H	4	0.34
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD11	5	0.34
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD12	5	0.34
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD13	5	0.34
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD11	5	0.34
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD12	5	0.34
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD13	5	0.34
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG2	7	0.34
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG3	7	0.34
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG2	7	0.34
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG3	7	0.34
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG2	7	0.34
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG3	7	0.34
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	8	0.34
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	8	0.34
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	8	0.34
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	8	0.34
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	8	0.34
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	8	0.34
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	17	0.34
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	17	0.34
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB1	9	0.34
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB2	9	0.34
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB3	9	0.34
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB1	9	0.34
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB2	9	0.34
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB3	9	0.34
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB2	18	0.34
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB3	18	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB2	18	0.34
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB3	18	0.34
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB2	18	0.34
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB3	18	0.34
(1,1116)	1:267:A:LEU:HD11	1:329:A:VAL:HG21	9	0.34
(1,1116)	1:267:A:LEU:HD11	1:329:A:VAL:HG22	9	0.34
(1,1116)	1:267:A:LEU:HD11	1:329:A:VAL:HG23	9	0.34
(1,1116)	1:267:A:LEU:HD12	1:329:A:VAL:HG21	9	0.34
(1,1116)	1:267:A:LEU:HD12	1:329:A:VAL:HG22	9	0.34
(1,1116)	1:267:A:LEU:HD12	1:329:A:VAL:HG23	9	0.34
(1,1116)	1:267:A:LEU:HD13	1:329:A:VAL:HG21	9	0.34
(1,1116)	1:267:A:LEU:HD13	1:329:A:VAL:HG22	9	0.34
(1,1116)	1:267:A:LEU:HD13	1:329:A:VAL:HG23	9	0.34
(1,1116)	1:267:A:LEU:HD21	1:329:A:VAL:HG21	9	0.34
(1,1116)	1:267:A:LEU:HD21	1:329:A:VAL:HG22	9	0.34
(1,1116)	1:267:A:LEU:HD21	1:329:A:VAL:HG23	9	0.34
(1,1116)	1:267:A:LEU:HD22	1:329:A:VAL:HG21	9	0.34
(1,1116)	1:267:A:LEU:HD22	1:329:A:VAL:HG22	9	0.34
(1,1116)	1:267:A:LEU:HD22	1:329:A:VAL:HG23	9	0.34
(1,1116)	1:267:A:LEU:HD23	1:329:A:VAL:HG21	9	0.34
(1,1116)	1:267:A:LEU:HD23	1:329:A:VAL:HG22	9	0.34
(1,1116)	1:267:A:LEU:HD23	1:329:A:VAL:HG23	9	0.34
(1,1109)	1:267:A:LEU:HD11	1:268:A:THR:H	4	0.34
(1,1109)	1:267:A:LEU:HD12	1:268:A:THR:H	4	0.34
(1,1109)	1:267:A:LEU:HD13	1:268:A:THR:H	4	0.34
(1,1109)	1:267:A:LEU:HD21	1:268:A:THR:H	4	0.34
(1,1109)	1:267:A:LEU:HD22	1:268:A:THR:H	4	0.34
(1,1109)	1:267:A:LEU:HD23	1:268:A:THR:H	4	0.34
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	2	0.34
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	2	0.34
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	2	0.34
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	2	0.34
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	2	0.34
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	2	0.34
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	16	0.34
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	16	0.34
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	16	0.34
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	16	0.34
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	16	0.34
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	16	0.34
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	4	0.34
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	4	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	4	0.34
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	4	0.34
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	4	0.34
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	4	0.34
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD11	10	0.34
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD12	10	0.34
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD13	10	0.34
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD21	10	0.34
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD22	10	0.34
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD23	10	0.34
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	2	0.34
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	2	0.34
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	2	0.34
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	2	0.34
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	2	0.34
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	2	0.34
(1,905)	1:247:A:PRO:HD2	1:322:A:ILE:HG12	2	0.34
(1,905)	1:247:A:PRO:HD3	1:322:A:ILE:HG12	2	0.34
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	8	0.34
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	8	0.34
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	8	0.34
(1,871)	1:315:A:ILE:HD11	1:328:A:GLN:HB3	1	0.34
(1,871)	1:315:A:ILE:HD12	1:328:A:GLN:HB3	1	0.34
(1,871)	1:315:A:ILE:HD13	1:328:A:GLN:HB3	1	0.34
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	12	0.34
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	12	0.34
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	12	0.34
(1,757)	1:245:A:TYR:HD1	1:273:A:ALA:HA	1	0.34
(1,740)	1:268:A:THR:HA	1:269:A:CYS:HB3	4	0.34
(1,740)	1:268:A:THR:HA	1:269:A:CYS:HB3	11	0.34
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG21	3	0.34
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG22	3	0.34
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG23	3	0.34
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG21	3	0.34
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG22	3	0.34
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG23	3	0.34
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG21	9	0.34
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG22	9	0.34
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG23	9	0.34
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG21	9	0.34
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG22	9	0.34
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG23	9	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG21	14	0.34
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG22	14	0.34
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG23	14	0.34
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG21	14	0.34
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG22	14	0.34
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG23	14	0.34
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	8	0.34
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	8	0.34
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	8	0.34
(1,658)	1:308:A:TYR:HD1	1:333:A:ILE:HB	6	0.34
(1,655)	1:301:A:PHE:HA	1:302:A:PHE:HE1	10	0.34
(1,645)	1:251:A:ILE:HD11	1:314:A:TYR:H	1	0.34
(1,645)	1:251:A:ILE:HD12	1:314:A:TYR:H	1	0.34
(1,645)	1:251:A:ILE:HD13	1:314:A:TYR:H	1	0.34
(1,644)	1:251:A:ILE:HD11	1:328:A:GLN:HA	12	0.34
(1,644)	1:251:A:ILE:HD12	1:328:A:GLN:HA	12	0.34
(1,644)	1:251:A:ILE:HD13	1:328:A:GLN:HA	12	0.34
(1,641)	1:251:A:ILE:HD11	1:316:A:CYS:HA	11	0.34
(1,641)	1:251:A:ILE:HD12	1:316:A:CYS:HA	11	0.34
(1,641)	1:251:A:ILE:HD13	1:316:A:CYS:HA	11	0.34
(1,639)	1:251:A:ILE:HD11	1:314:A:TYR:HB3	8	0.34
(1,639)	1:251:A:ILE:HD12	1:314:A:TYR:HB3	8	0.34
(1,639)	1:251:A:ILE:HD13	1:314:A:TYR:HB3	8	0.34
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	13	0.34
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	13	0.34
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	13	0.34
(1,555)	1:300:A:LEU:HB2	1:314:A:TYR:HB2	18	0.34
(1,555)	1:300:A:LEU:HB3	1:314:A:TYR:HB2	18	0.34
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	13	0.34
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	13	0.34
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	13	0.34
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	1	0.34
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	1	0.34
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	1	0.34
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	2	0.34
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	6	0.34
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	8	0.34
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	5	0.34
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	5	0.34
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	5	0.34
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	8	0.34
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	8	0.34
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	5	0.34
(1,1208)	1:310:A:LEU:HD11	1:314:A:TYR:HE1	5	0.33
(1,1208)	1:310:A:LEU:HD12	1:314:A:TYR:HE1	5	0.33
(1,1208)	1:310:A:LEU:HD13	1:314:A:TYR:HE1	5	0.33
(1,1208)	1:310:A:LEU:HD21	1:314:A:TYR:HE1	5	0.33
(1,1208)	1:310:A:LEU:HD22	1:314:A:TYR:HE1	5	0.33
(1,1208)	1:310:A:LEU:HD23	1:314:A:TYR:HE1	5	0.33
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	13	0.33
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	13	0.33
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	13	0.33
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	13	0.33
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	13	0.33
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	13	0.33
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	7	0.33
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	7	0.33
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	8	0.33
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	8	0.33
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	13	0.33
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	13	0.33
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB1	17	0.33
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB2	17	0.33
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB3	17	0.33
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB1	17	0.33
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB2	17	0.33
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB3	17	0.33
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB2	15	0.33
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB3	15	0.33
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB2	15	0.33
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB3	15	0.33
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB2	15	0.33
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB3	15	0.33
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	14	0.33
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	14	0.33
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	14	0.33
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	14	0.33
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	14	0.33
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	14	0.33
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD11	7	0.33
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD12	7	0.33
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD13	7	0.33
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD21	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD22	7	0.33
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD23	7	0.33
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	14	0.33
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	14	0.33
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	14	0.33
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	14	0.33
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	14	0.33
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	14	0.33
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG21	14	0.33
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG22	14	0.33
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG23	14	0.33
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	15	0.33
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	15	0.33
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	15	0.33
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	7	0.33
(1,731)	1:267:A:LEU:HB2	1:314:A:TYR:HE2	5	0.33
(1,731)	1:267:A:LEU:HB3	1:314:A:TYR:HE2	5	0.33
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	19	0.33
(1,655)	1:301:A:PHE:HA	1:302:A:PHE:HE1	4	0.33
(1,641)	1:251:A:ILE:HD11	1:316:A:CYS:HA	4	0.33
(1,641)	1:251:A:ILE:HD12	1:316:A:CYS:HA	4	0.33
(1,641)	1:251:A:ILE:HD13	1:316:A:CYS:HA	4	0.33
(1,641)	1:251:A:ILE:HD11	1:316:A:CYS:HA	7	0.33
(1,641)	1:251:A:ILE:HD12	1:316:A:CYS:HA	7	0.33
(1,641)	1:251:A:ILE:HD13	1:316:A:CYS:HA	7	0.33
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	17	0.33
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	17	0.33
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	17	0.33
(1,573)	1:244:A:GLN:HA	1:245:A:TYR:HD1	7	0.33
(1,544)	1:258:A:TRP:HA	1:259:A:TYR:HD1	5	0.33
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	11	0.33
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	11	0.33
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	11	0.33
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	20	0.33
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	4	0.33
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	17	0.33
(1,285)	1:295:A:ALA:HB1	1:301:A:PHE:H	20	0.33
(1,285)	1:295:A:ALA:HB2	1:301:A:PHE:H	20	0.33
(1,285)	1:295:A:ALA:HB3	1:301:A:PHE:H	20	0.33
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	2	0.33
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	2	0.33
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	10	0.33
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	15	0.33
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	15	0.33
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	15	0.33
(1,70)	1:257:A:ASN:H	1:258:A:TRP:HA	8	0.33
(1,14)	1:244:A:GLN:H	1:244:A:GLN:HG2	6	0.33
(1,13)	1:244:A:GLN:H	1:244:A:GLN:HB2	4	0.33
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	18	0.33
(1,1208)	1:310:A:LEU:HD11	1:314:A:TYR:HE1	9	0.32
(1,1208)	1:310:A:LEU:HD12	1:314:A:TYR:HE1	9	0.32
(1,1208)	1:310:A:LEU:HD13	1:314:A:TYR:HE1	9	0.32
(1,1208)	1:310:A:LEU:HD21	1:314:A:TYR:HE1	9	0.32
(1,1208)	1:310:A:LEU:HD22	1:314:A:TYR:HE1	9	0.32
(1,1208)	1:310:A:LEU:HD23	1:314:A:TYR:HE1	9	0.32
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB2	10	0.32
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB3	10	0.32
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB2	10	0.32
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB3	10	0.32
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB2	10	0.32
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB3	10	0.32
(1,1116)	1:267:A:LEU:HD11	1:329:A:VAL:HG21	14	0.32
(1,1116)	1:267:A:LEU:HD11	1:329:A:VAL:HG22	14	0.32
(1,1116)	1:267:A:LEU:HD11	1:329:A:VAL:HG23	14	0.32
(1,1116)	1:267:A:LEU:HD12	1:329:A:VAL:HG21	14	0.32
(1,1116)	1:267:A:LEU:HD12	1:329:A:VAL:HG22	14	0.32
(1,1116)	1:267:A:LEU:HD12	1:329:A:VAL:HG23	14	0.32
(1,1116)	1:267:A:LEU:HD13	1:329:A:VAL:HG21	14	0.32
(1,1116)	1:267:A:LEU:HD13	1:329:A:VAL:HG22	14	0.32
(1,1116)	1:267:A:LEU:HD13	1:329:A:VAL:HG23	14	0.32
(1,1116)	1:267:A:LEU:HD21	1:329:A:VAL:HG21	14	0.32
(1,1116)	1:267:A:LEU:HD21	1:329:A:VAL:HG22	14	0.32
(1,1116)	1:267:A:LEU:HD21	1:329:A:VAL:HG23	14	0.32
(1,1116)	1:267:A:LEU:HD22	1:329:A:VAL:HG21	14	0.32
(1,1116)	1:267:A:LEU:HD22	1:329:A:VAL:HG22	14	0.32
(1,1116)	1:267:A:LEU:HD22	1:329:A:VAL:HG23	14	0.32
(1,1116)	1:267:A:LEU:HD23	1:329:A:VAL:HG21	14	0.32
(1,1116)	1:267:A:LEU:HD23	1:329:A:VAL:HG22	14	0.32
(1,1116)	1:267:A:LEU:HD23	1:329:A:VAL:HG23	14	0.32
(1,1103)	1:266:A:LYS:HE2	1:301:A:PHE:HD1	17	0.32
(1,1103)	1:266:A:LYS:HE3	1:301:A:PHE:HD1	17	0.32
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	5	0.32
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	5	0.32
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	5	0.32
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	5	0.32
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	5	0.32
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	13	0.32
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	13	0.32
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	13	0.32
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	13	0.32
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	13	0.32
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	13	0.32
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG21	19	0.32
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG22	19	0.32
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG23	19	0.32
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	13	0.32
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	13	0.32
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	13	0.32
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	19	0.32
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	19	0.32
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	19	0.32
(1,740)	1:268:A:THR:HA	1:269:A:CYS:HB3	6	0.32
(1,740)	1:268:A:THR:HA	1:269:A:CYS:HB3	14	0.32
(1,740)	1:268:A:THR:HA	1:269:A:CYS:HB3	16	0.32
(1,731)	1:267:A:LEU:HB2	1:314:A:TYR:HE2	15	0.32
(1,731)	1:267:A:LEU:HB3	1:314:A:TYR:HE2	15	0.32
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	17	0.32
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	17	0.32
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	17	0.32
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	13	0.32
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	9	0.32
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	13	0.32
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	16	0.32
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	3	0.32
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	3	0.32
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	3	0.32
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	14	0.32
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	14	0.32
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	14	0.32
(1,645)	1:251:A:ILE:HD11	1:314:A:TYR:H	13	0.32
(1,645)	1:251:A:ILE:HD12	1:314:A:TYR:H	13	0.32
(1,645)	1:251:A:ILE:HD13	1:314:A:TYR:H	13	0.32
(1,645)	1:251:A:ILE:HD11	1:314:A:TYR:H	18	0.32
(1,645)	1:251:A:ILE:HD12	1:314:A:TYR:H	18	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,645)	1:251:A:ILE:HD13	1:314:A:TYR:H	18	0.32
(1,641)	1:251:A:ILE:HD11	1:316:A:CYS:HA	12	0.32
(1,641)	1:251:A:ILE:HD12	1:316:A:CYS:HA	12	0.32
(1,641)	1:251:A:ILE:HD13	1:316:A:CYS:HA	12	0.32
(1,511)	1:259:A:TYR:HB3	1:334:A:THR:H	8	0.32
(1,511)	1:259:A:TYR:HB3	1:334:A:THR:H	20	0.32
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	7	0.32
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	7	0.32
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	7	0.32
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	10	0.32
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	13	0.32
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	4	0.32
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	18	0.32
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	10	0.32
(1,270)	1:296:A:GLN:HG2	1:299:A:THR:H	14	0.32
(1,270)	1:296:A:GLN:HG3	1:299:A:THR:H	14	0.32
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	12	0.32
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	12	0.32
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	14	0.32
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	14	0.32
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	19	0.32
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	19	0.32
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	17	0.32
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	4	0.32
(1,21)	1:244:A:GLN:HB3	1:245:A:TYR:H	18	0.32
(1,1250)	1:330:A:GLU:HB2	1:331:A:VAL:H	5	0.31
(1,1250)	1:330:A:GLU:HB3	1:331:A:VAL:H	5	0.31
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	12	0.31
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	12	0.31
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB1	13	0.31
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB2	13	0.31
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB3	13	0.31
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB1	13	0.31
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB2	13	0.31
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB3	13	0.31
(1,1142)	1:280:A:TYR:H	1:281:A:HIS:HB2	19	0.31
(1,1142)	1:280:A:TYR:H	1:281:A:HIS:HB3	19	0.31
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	4	0.31
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	4	0.31
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	4	0.31
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	4	0.31
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	4	0.31
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	8	0.31
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	8	0.31
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	8	0.31
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	8	0.31
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	8	0.31
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	8	0.31
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	9	0.31
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	9	0.31
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	9	0.31
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	9	0.31
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	9	0.31
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	9	0.31
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	10	0.31
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	10	0.31
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	10	0.31
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	10	0.31
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	10	0.31
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	10	0.31
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	11	0.31
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	11	0.31
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	11	0.31
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	11	0.31
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	11	0.31
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	11	0.31
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	9	0.31
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	9	0.31
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	9	0.31
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	9	0.31
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	9	0.31
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	9	0.31
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	18	0.31
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	18	0.31
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	18	0.31
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	18	0.31
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	18	0.31
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	18	0.31
(1,1047)	1:252:A:GLU:H	1:270:A:LYS:HD2	16	0.31
(1,1047)	1:252:A:GLU:H	1:270:A:LYS:HD3	16	0.31
(1,982)	1:308:A:TYR:HA	1:308:A:TYR:HD1	6	0.31
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	13	0.31
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	13	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	13	0.31
(1,740)	1:268:A:THR:HA	1:269:A:CYS:HB3	15	0.31
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	16	0.31
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	16	0.31
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	16	0.31
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	20	0.31
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	20	0.31
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	20	0.31
(1,691)	1:264:A:ASP:HB3	1:265:A:VAL:HA	14	0.31
(1,655)	1:301:A:PHE:HA	1:302:A:PHE:HE1	19	0.31
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	6	0.31
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	6	0.31
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	6	0.31
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	9	0.31
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	9	0.31
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	9	0.31
(1,645)	1:251:A:ILE:HD11	1:314:A:TYR:H	5	0.31
(1,645)	1:251:A:ILE:HD12	1:314:A:TYR:H	5	0.31
(1,645)	1:251:A:ILE:HD13	1:314:A:TYR:H	5	0.31
(1,641)	1:251:A:ILE:HD11	1:316:A:CYS:HA	16	0.31
(1,641)	1:251:A:ILE:HD12	1:316:A:CYS:HA	16	0.31
(1,641)	1:251:A:ILE:HD13	1:316:A:CYS:HA	16	0.31
(1,641)	1:251:A:ILE:HD11	1:316:A:CYS:HA	18	0.31
(1,641)	1:251:A:ILE:HD12	1:316:A:CYS:HA	18	0.31
(1,641)	1:251:A:ILE:HD13	1:316:A:CYS:HA	18	0.31
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	15	0.31
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	15	0.31
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	15	0.31
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	18	0.31
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	18	0.31
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	18	0.31
(1,627)	1:251:A:ILE:HG21	1:267:A:LEU:HG	5	0.31
(1,627)	1:251:A:ILE:HG22	1:267:A:LEU:HG	5	0.31
(1,627)	1:251:A:ILE:HG23	1:267:A:LEU:HG	5	0.31
(1,495)	1:331:A:VAL:HB	1:332:A:ASN:H	2	0.31
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	9	0.31
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	9	0.31
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	9	0.31
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	5	0.31
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	2	0.31
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	5	0.31
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	16	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	18	0.31
(1,259)	1:294:A:GLU:H	1:294:A:GLU:HG3	3	0.31
(1,259)	1:294:A:GLU:H	1:294:A:GLU:HG2	3	0.31
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	9	0.31
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	9	0.31
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	9	0.31
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	7	0.31
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD11	12	0.3
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD12	12	0.3
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD13	12	0.3
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD11	12	0.3
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD12	12	0.3
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD13	12	0.3
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	9	0.3
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	9	0.3
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	9	0.3
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	9	0.3
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	9	0.3
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	9	0.3
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	10	0.3
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	10	0.3
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	10	0.3
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	10	0.3
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	10	0.3
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	10	0.3
(1,1192)	1:303:A:ARG:HG2	1:304:A:GLY:H	15	0.3
(1,1192)	1:303:A:ARG:HG3	1:304:A:GLY:H	15	0.3
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB2	17	0.3
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB3	17	0.3
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB2	17	0.3
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB3	17	0.3
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB2	17	0.3
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB3	17	0.3
(1,1122)	1:270:A:LYS:HB2	1:270:A:LYS:HD2	10	0.3
(1,1122)	1:270:A:LYS:HB2	1:270:A:LYS:HD3	10	0.3
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	7	0.3
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	7	0.3
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	7	0.3
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	7	0.3
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	7	0.3
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	7	0.3
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	20	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	20	0.3
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	20	0.3
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	20	0.3
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	20	0.3
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	20	0.3
(1,1015)	1:246:A:GLU:HG2	1:325:A:ARG:HG2	20	0.3
(1,1015)	1:246:A:GLU:HG3	1:325:A:ARG:HG2	20	0.3
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	17	0.3
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	17	0.3
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	17	0.3
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG21	15	0.3
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG22	15	0.3
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG23	15	0.3
(1,905)	1:247:A:PRO:HD2	1:322:A:ILE:HG12	5	0.3
(1,905)	1:247:A:PRO:HD3	1:322:A:ILE:HG12	5	0.3
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	4	0.3
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	4	0.3
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	4	0.3
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	9	0.3
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	9	0.3
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	9	0.3
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	3	0.3
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	3	0.3
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	3	0.3
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	1	0.3
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	12	0.3
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	17	0.3
(1,805)	1:290:A:PRO:HD3	1:314:A:TYR:HE1	18	0.3
(1,805)	1:290:A:PRO:HD2	1:314:A:TYR:HE1	18	0.3
(1,740)	1:268:A:THR:HA	1:269:A:CYS:HB3	2	0.3
(1,727)	1:266:A:LYS:HG3	1:267:A:LEU:H	13	0.3
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG21	2	0.3
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG22	2	0.3
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG23	2	0.3
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG21	2	0.3
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG22	2	0.3
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG23	2	0.3
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	6	0.3
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	6	0.3
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	6	0.3
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	13	0.3
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	13	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	13	0.3
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	10	0.3
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	10	0.3
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	10	0.3
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	10	0.3
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	10	0.3
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	10	0.3
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	10	0.3
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	10	0.3
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	10	0.3
(1,612)	1:250:A:THR:HB	1:270:A:LYS:HB2	16	0.3
(1,544)	1:258:A:TRP:HA	1:259:A:TYR:HD1	20	0.3
(1,511)	1:259:A:TYR:HB3	1:334:A:THR:H	15	0.3
(1,495)	1:331:A:VAL:HB	1:332:A:ASN:H	1	0.3
(1,386)	1:316:A:CYS:H	1:316:A:CYS:HB3	8	0.3
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	3	0.3
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	11	0.3
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	19	0.3
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	9	0.3
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	3	0.3
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	4	0.3
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	4	0.3
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	4	0.3
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	12	0.3
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	12	0.3
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	12	0.3
(1,70)	1:257:A:ASN:H	1:258:A:TRP:HA	13	0.3
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	1	0.3
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	8	0.3
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	2	0.3
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG2	1	0.29
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG3	1	0.29
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG2	1	0.29
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG3	1	0.29
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG2	1	0.29
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG3	1	0.29
(1,1192)	1:303:A:ARG:HG2	1:304:A:GLY:H	2	0.29
(1,1192)	1:303:A:ARG:HG3	1:304:A:GLY:H	2	0.29
(1,1175)	1:293:A:VAL:HG11	1:302:A:PHE:H	11	0.29
(1,1175)	1:293:A:VAL:HG12	1:302:A:PHE:H	11	0.29
(1,1175)	1:293:A:VAL:HG13	1:302:A:PHE:H	11	0.29
(1,1175)	1:293:A:VAL:HG21	1:302:A:PHE:H	11	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1175)	1:293:A:VAL:HG22	1:302:A:PHE:H	11	0.29
(1,1175)	1:293:A:VAL:HG23	1:302:A:PHE:H	11	0.29
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB2	14	0.29
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB3	14	0.29
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB2	14	0.29
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB3	14	0.29
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB2	14	0.29
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB3	14	0.29
(1,1097)	1:266:A:LYS:HB2	1:266:A:LYS:HE2	3	0.29
(1,1097)	1:266:A:LYS:HB2	1:266:A:LYS:HE3	3	0.29
(1,1097)	1:266:A:LYS:HB3	1:266:A:LYS:HE2	3	0.29
(1,1097)	1:266:A:LYS:HB3	1:266:A:LYS:HE3	3	0.29
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	3	0.29
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	3	0.29
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	3	0.29
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	3	0.29
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	3	0.29
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	3	0.29
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	15	0.29
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	15	0.29
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	15	0.29
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	15	0.29
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	15	0.29
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	15	0.29
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	18	0.29
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	18	0.29
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	18	0.29
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	18	0.29
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	18	0.29
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	18	0.29
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	6	0.29
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	6	0.29
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	6	0.29
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	6	0.29
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	6	0.29
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	6	0.29
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD11	7	0.29
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD12	7	0.29
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD13	7	0.29
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD21	7	0.29
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD22	7	0.29
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD23	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD11	1	0.29
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD12	1	0.29
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD13	1	0.29
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD21	1	0.29
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD22	1	0.29
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD23	1	0.29
(1,1010)	1:246:A:GLU:HB2	1:325:A:ARG:HD2	20	0.29
(1,1010)	1:246:A:GLU:HB2	1:325:A:ARG:HD3	20	0.29
(1,1010)	1:246:A:GLU:HB3	1:325:A:ARG:HD2	20	0.29
(1,1010)	1:246:A:GLU:HB3	1:325:A:ARG:HD3	20	0.29
(1,940)	1:251:A:ILE:HD11	1:327:A:GLY:HA2	16	0.29
(1,940)	1:251:A:ILE:HD12	1:327:A:GLY:HA2	16	0.29
(1,940)	1:251:A:ILE:HD13	1:327:A:GLY:HA2	16	0.29
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	13	0.29
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	13	0.29
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	13	0.29
(1,851)	1:313:A:THR:HG21	1:328:A:GLN:HB3	6	0.29
(1,851)	1:313:A:THR:HG22	1:328:A:GLN:HB3	6	0.29
(1,851)	1:313:A:THR:HG23	1:328:A:GLN:HB3	6	0.29
(1,757)	1:245:A:TYR:HD1	1:273:A:ALA:HA	5	0.29
(1,740)	1:268:A:THR:HA	1:269:A:CYS:HB3	20	0.29
(1,727)	1:266:A:LYS:HG3	1:267:A:LEU:H	6	0.29
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	4	0.29
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	4	0.29
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	4	0.29
(1,692)	1:265:A:VAL:HA	1:266:A:LYS:HG2	5	0.29
(1,645)	1:251:A:ILE:HD11	1:314:A:TYR:H	19	0.29
(1,645)	1:251:A:ILE:HD12	1:314:A:TYR:H	19	0.29
(1,645)	1:251:A:ILE:HD13	1:314:A:TYR:H	19	0.29
(1,644)	1:251:A:ILE:HD11	1:328:A:GLN:HA	14	0.29
(1,644)	1:251:A:ILE:HD12	1:328:A:GLN:HA	14	0.29
(1,644)	1:251:A:ILE:HD13	1:328:A:GLN:HA	14	0.29
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	20	0.29
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	20	0.29
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	20	0.29
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	9	0.29
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	9	0.29
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	9	0.29
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	5	0.29
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	5	0.29
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	5	0.29
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	5	0.29
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	5	0.29
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	5	0.29
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	5	0.29
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	5	0.29
(1,535)	1:249:A:VAL:HG11	1:316:A:CYS:HB3	8	0.29
(1,535)	1:249:A:VAL:HG12	1:316:A:CYS:HB3	8	0.29
(1,535)	1:249:A:VAL:HG13	1:316:A:CYS:HB3	8	0.29
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	20	0.29
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	20	0.29
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	20	0.29
(1,441)	1:246:A:GLU:HB2	1:324:A:THR:H	6	0.29
(1,441)	1:246:A:GLU:HB3	1:324:A:THR:H	6	0.29
(1,397)	1:318:A:ALA:H	1:326:A:SER:HB3	3	0.29
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	15	0.29
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	15	0.29
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	15	0.29
(1,323)	1:302:A:PHE:HB3	1:306:A:ILE:H	18	0.29
(1,307)	1:303:A:ARG:H	1:303:A:ARG:HD2	6	0.29
(1,307)	1:303:A:ARG:H	1:303:A:ARG:HD3	6	0.29
(1,270)	1:296:A:GLN:HG2	1:299:A:THR:H	16	0.29
(1,270)	1:296:A:GLN:HG3	1:299:A:THR:H	16	0.29
(1,259)	1:294:A:GLU:H	1:294:A:GLU:HG3	12	0.29
(1,259)	1:294:A:GLU:H	1:294:A:GLU:HG2	12	0.29
(1,259)	1:294:A:GLU:H	1:294:A:GLU:HG3	13	0.29
(1,259)	1:294:A:GLU:H	1:294:A:GLU:HG2	13	0.29
(1,259)	1:294:A:GLU:H	1:294:A:GLU:HG3	17	0.29
(1,259)	1:294:A:GLU:H	1:294:A:GLU:HG2	17	0.29
(1,157)	1:268:A:THR:H	1:269:A:CYS:HB2	12	0.29
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG21	17	0.29
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG22	17	0.29
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG23	17	0.29
(1,70)	1:257:A:ASN:H	1:258:A:TRP:HA	7	0.29
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD11	17	0.28
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD12	17	0.28
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD13	17	0.28
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD11	17	0.28
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD12	17	0.28
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD13	17	0.28
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG21	9	0.28
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG22	9	0.28
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG23	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	9	0.28
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	9	0.28
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	9	0.28
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	6	0.28
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	6	0.28
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	6	0.28
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	6	0.28
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	6	0.28
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	6	0.28
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	16	0.28
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	16	0.28
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	16	0.28
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	16	0.28
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	16	0.28
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	16	0.28
(1,1175)	1:293:A:VAL:HG11	1:302:A:PHE:H	7	0.28
(1,1175)	1:293:A:VAL:HG12	1:302:A:PHE:H	7	0.28
(1,1175)	1:293:A:VAL:HG13	1:302:A:PHE:H	7	0.28
(1,1175)	1:293:A:VAL:HG21	1:302:A:PHE:H	7	0.28
(1,1175)	1:293:A:VAL:HG22	1:302:A:PHE:H	7	0.28
(1,1175)	1:293:A:VAL:HG23	1:302:A:PHE:H	7	0.28
(1,1173)	1:293:A:VAL:HG11	1:294:A:GLU:H	11	0.28
(1,1173)	1:293:A:VAL:HG12	1:294:A:GLU:H	11	0.28
(1,1173)	1:293:A:VAL:HG13	1:294:A:GLU:H	11	0.28
(1,1173)	1:293:A:VAL:HG21	1:294:A:GLU:H	11	0.28
(1,1173)	1:293:A:VAL:HG22	1:294:A:GLU:H	11	0.28
(1,1173)	1:293:A:VAL:HG23	1:294:A:GLU:H	11	0.28
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB1	5	0.28
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB2	5	0.28
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB3	5	0.28
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB1	5	0.28
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB2	5	0.28
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB3	5	0.28
(1,1142)	1:280:A:TYR:H	1:281:A:HIS:HB2	18	0.28
(1,1142)	1:280:A:TYR:H	1:281:A:HIS:HB3	18	0.28
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	5	0.28
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	5	0.28
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	5	0.28
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	5	0.28
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	5	0.28
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	5	0.28
(1,1010)	1:246:A:GLU:HB2	1:325:A:ARG:HD2	19	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1010)	1:246:A:GLU:HB2	1:325:A:ARG:HD3	19	0.28
(1,1010)	1:246:A:GLU:HB3	1:325:A:ARG:HD2	19	0.28
(1,1010)	1:246:A:GLU:HB3	1:325:A:ARG:HD3	19	0.28
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD11	10	0.28
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD12	10	0.28
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD13	10	0.28
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG21	9	0.28
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG22	9	0.28
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG23	9	0.28
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	5	0.28
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	5	0.28
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	5	0.28
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD11	14	0.28
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD12	14	0.28
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD13	14	0.28
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD11	14	0.28
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD12	14	0.28
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD13	14	0.28
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	16	0.28
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	16	0.28
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	16	0.28
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	18	0.28
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	18	0.28
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	18	0.28
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	10	0.28
(1,803)	1:290:A:PRO:HG2	1:314:A:TYR:HE1	12	0.28
(1,803)	1:290:A:PRO:HG3	1:314:A:TYR:HE1	12	0.28
(1,776)	1:273:A:ALA:HB1	1:277:A:ALA:HA	15	0.28
(1,776)	1:273:A:ALA:HB2	1:277:A:ALA:HA	15	0.28
(1,776)	1:273:A:ALA:HB3	1:277:A:ALA:HA	15	0.28
(1,776)	1:273:A:ALA:HB1	1:277:A:ALA:HA	20	0.28
(1,776)	1:273:A:ALA:HB2	1:277:A:ALA:HA	20	0.28
(1,776)	1:273:A:ALA:HB3	1:277:A:ALA:HA	20	0.28
(1,770)	1:274:A:ASN:HB2	1:322:A:ILE:HG13	4	0.28
(1,770)	1:274:A:ASN:HB3	1:322:A:ILE:HG13	4	0.28
(1,757)	1:245:A:TYR:HD1	1:273:A:ALA:HA	4	0.28
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG21	5	0.28
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG22	5	0.28
(1,710)	1:266:A:LYS:HA	1:299:A:THR:HG23	5	0.28
(1,682)	1:262:A:ARG:HA	1:262:A:ARG:HD2	20	0.28
(1,682)	1:262:A:ARG:HA	1:262:A:ARG:HD3	20	0.28
(1,665)	1:259:A:TYR:HA	1:333:A:ILE:HG21	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,665)	1:259:A:TYR:HA	1:333:A:ILE:HG22	1	0.28
(1,665)	1:259:A:TYR:HA	1:333:A:ILE:HG23	1	0.28
(1,644)	1:251:A:ILE:HD11	1:328:A:GLN:HA	17	0.28
(1,644)	1:251:A:ILE:HD12	1:328:A:GLN:HA	17	0.28
(1,644)	1:251:A:ILE:HD13	1:328:A:GLN:HA	17	0.28
(1,639)	1:251:A:ILE:HD11	1:314:A:TYR:HB3	14	0.28
(1,639)	1:251:A:ILE:HD12	1:314:A:TYR:HB3	14	0.28
(1,639)	1:251:A:ILE:HD13	1:314:A:TYR:HB3	14	0.28
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	20	0.28
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	20	0.28
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	20	0.28
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	20	0.28
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	20	0.28
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	20	0.28
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	20	0.28
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	20	0.28
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	20	0.28
(1,608)	1:250:A:THR:HA	1:251:A:ILE:HG13	1	0.28
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	13	0.28
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	13	0.28
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	13	0.28
(1,511)	1:259:A:TYR:HB3	1:334:A:THR:H	14	0.28
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	4	0.28
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	4	0.28
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	4	0.28
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	10	0.28
(1,290)	1:265:A:VAL:H	1:302:A:PHE:H	14	0.28
(1,190)	1:245:A:TYR:H	1:274:A:ASN:H	2	0.28
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	14	0.28
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	12	0.28
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG21	1	0.28
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG22	1	0.28
(1,78)	1:258:A:TRP:H	1:333:A:ILE:HG23	1	0.28
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	6	0.28
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	13	0.28
(1,46)	1:250:A:THR:H	1:270:A:LYS:HB2	20	0.28
(1,13)	1:244:A:GLN:H	1:244:A:GLN:HB2	11	0.28
(1,1245)	1:325:A:ARG:HD2	1:326:A:SER:H	8	0.27
(1,1245)	1:325:A:ARG:HD3	1:326:A:SER:H	8	0.27
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG2	13	0.27
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG3	13	0.27
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG2	13	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG3	13	0.27
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG2	13	0.27
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG3	13	0.27
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG2	16	0.27
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG3	16	0.27
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG2	16	0.27
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG3	16	0.27
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG2	16	0.27
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG3	16	0.27
(1,1208)	1:310:A:LEU:HD11	1:314:A:TYR:HE1	17	0.27
(1,1208)	1:310:A:LEU:HD12	1:314:A:TYR:HE1	17	0.27
(1,1208)	1:310:A:LEU:HD13	1:314:A:TYR:HE1	17	0.27
(1,1208)	1:310:A:LEU:HD21	1:314:A:TYR:HE1	17	0.27
(1,1208)	1:310:A:LEU:HD22	1:314:A:TYR:HE1	17	0.27
(1,1208)	1:310:A:LEU:HD23	1:314:A:TYR:HE1	17	0.27
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG21	19	0.27
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG22	19	0.27
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG23	19	0.27
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	19	0.27
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	19	0.27
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	19	0.27
(1,1192)	1:303:A:ARG:HG2	1:304:A:GLY:H	20	0.27
(1,1192)	1:303:A:ARG:HG3	1:304:A:GLY:H	20	0.27
(1,1173)	1:293:A:VAL:HG11	1:294:A:GLU:H	5	0.27
(1,1173)	1:293:A:VAL:HG12	1:294:A:GLU:H	5	0.27
(1,1173)	1:293:A:VAL:HG13	1:294:A:GLU:H	5	0.27
(1,1173)	1:293:A:VAL:HG21	1:294:A:GLU:H	5	0.27
(1,1173)	1:293:A:VAL:HG22	1:294:A:GLU:H	5	0.27
(1,1173)	1:293:A:VAL:HG23	1:294:A:GLU:H	5	0.27
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB1	6	0.27
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB2	6	0.27
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB3	6	0.27
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB1	6	0.27
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB2	6	0.27
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB3	6	0.27
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	19	0.27
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	19	0.27
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	19	0.27
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	19	0.27
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	19	0.27
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	19	0.27
(1,999)	1:243:A:VAL:HG11	1:245:A:TYR:HB2	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,999)	1:243:A:VAL:HG11	1:245:A:TYR:HB3	17	0.27
(1,999)	1:243:A:VAL:HG12	1:245:A:TYR:HB2	17	0.27
(1,999)	1:243:A:VAL:HG12	1:245:A:TYR:HB3	17	0.27
(1,999)	1:243:A:VAL:HG13	1:245:A:TYR:HB2	17	0.27
(1,999)	1:243:A:VAL:HG13	1:245:A:TYR:HB3	17	0.27
(1,999)	1:243:A:VAL:HG21	1:245:A:TYR:HB2	17	0.27
(1,999)	1:243:A:VAL:HG21	1:245:A:TYR:HB3	17	0.27
(1,999)	1:243:A:VAL:HG22	1:245:A:TYR:HB2	17	0.27
(1,999)	1:243:A:VAL:HG22	1:245:A:TYR:HB3	17	0.27
(1,999)	1:243:A:VAL:HG23	1:245:A:TYR:HB2	17	0.27
(1,999)	1:243:A:VAL:HG23	1:245:A:TYR:HB3	17	0.27
(1,905)	1:247:A:PRO:HD2	1:322:A:ILE:HG12	14	0.27
(1,905)	1:247:A:PRO:HD3	1:322:A:ILE:HG12	14	0.27
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	15	0.27
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	15	0.27
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	15	0.27
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	8	0.27
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	8	0.27
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	8	0.27
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	14	0.27
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	14	0.27
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	14	0.27
(1,776)	1:273:A:ALA:HB1	1:277:A:ALA:HA	6	0.27
(1,776)	1:273:A:ALA:HB2	1:277:A:ALA:HA	6	0.27
(1,776)	1:273:A:ALA:HB3	1:277:A:ALA:HA	6	0.27
(1,770)	1:274:A:ASN:HB2	1:322:A:ILE:HG13	2	0.27
(1,770)	1:274:A:ASN:HB3	1:322:A:ILE:HG13	2	0.27
(1,724)	1:266:A:LYS:HD3	1:301:A:PHE:HD1	16	0.27
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	20	0.27
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	20	0.27
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	20	0.27
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG11	5	0.27
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG12	5	0.27
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG13	5	0.27
(1,655)	1:301:A:PHE:HA	1:302:A:PHE:HE1	6	0.27
(1,655)	1:301:A:PHE:HA	1:302:A:PHE:HE1	14	0.27
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	1	0.27
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	1	0.27
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	1	0.27
(1,645)	1:251:A:ILE:HD11	1:314:A:TYR:H	11	0.27
(1,645)	1:251:A:ILE:HD12	1:314:A:TYR:H	11	0.27
(1,645)	1:251:A:ILE:HD13	1:314:A:TYR:H	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,644)	1:251:A:ILE:HD11	1:328:A:GLN:HA	10	0.27
(1,644)	1:251:A:ILE:HD12	1:328:A:GLN:HA	10	0.27
(1,644)	1:251:A:ILE:HD13	1:328:A:GLN:HA	10	0.27
(1,641)	1:251:A:ILE:HD11	1:316:A:CYS:HA	8	0.27
(1,641)	1:251:A:ILE:HD12	1:316:A:CYS:HA	8	0.27
(1,641)	1:251:A:ILE:HD13	1:316:A:CYS:HA	8	0.27
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	5	0.27
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	5	0.27
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	5	0.27
(1,535)	1:249:A:VAL:HG11	1:316:A:CYS:HB3	18	0.27
(1,535)	1:249:A:VAL:HG12	1:316:A:CYS:HB3	18	0.27
(1,535)	1:249:A:VAL:HG13	1:316:A:CYS:HB3	18	0.27
(1,513)	1:333:A:ILE:HB	1:334:A:THR:H	2	0.27
(1,457)	1:250:A:THR:H	1:327:A:GLY:H	15	0.27
(1,290)	1:265:A:VAL:H	1:302:A:PHE:H	19	0.27
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	18	0.27
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	18	0.27
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	16	0.27
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	16	0.27
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	16	0.27
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	16	0.27
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD11	6	0.27
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD12	6	0.27
(1,124)	1:265:A:VAL:H	1:306:A:ILE:HD13	6	0.27
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	18	0.27
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	18	0.27
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	18	0.27
(1,77)	1:258:A:TRP:H	1:333:A:ILE:HD11	15	0.27
(1,77)	1:258:A:TRP:H	1:333:A:ILE:HD12	15	0.27
(1,77)	1:258:A:TRP:H	1:333:A:ILE:HD13	15	0.27
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD11	13	0.26
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD12	13	0.26
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD13	13	0.26
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD11	13	0.26
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD12	13	0.26
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD13	13	0.26
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG2	14	0.26
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG3	14	0.26
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG2	14	0.26
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG3	14	0.26
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG2	14	0.26
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG3	14	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	4	0.26
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	4	0.26
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	4	0.26
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	4	0.26
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	4	0.26
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	4	0.26
(1,1192)	1:303:A:ARG:HG2	1:304:A:GLY:H	1	0.26
(1,1192)	1:303:A:ARG:HG3	1:304:A:GLY:H	1	0.26
(1,1173)	1:293:A:VAL:HG11	1:294:A:GLU:H	9	0.26
(1,1173)	1:293:A:VAL:HG12	1:294:A:GLU:H	9	0.26
(1,1173)	1:293:A:VAL:HG13	1:294:A:GLU:H	9	0.26
(1,1173)	1:293:A:VAL:HG21	1:294:A:GLU:H	9	0.26
(1,1173)	1:293:A:VAL:HG22	1:294:A:GLU:H	9	0.26
(1,1173)	1:293:A:VAL:HG23	1:294:A:GLU:H	9	0.26
(1,1173)	1:293:A:VAL:HG11	1:294:A:GLU:H	13	0.26
(1,1173)	1:293:A:VAL:HG12	1:294:A:GLU:H	13	0.26
(1,1173)	1:293:A:VAL:HG13	1:294:A:GLU:H	13	0.26
(1,1173)	1:293:A:VAL:HG21	1:294:A:GLU:H	13	0.26
(1,1173)	1:293:A:VAL:HG22	1:294:A:GLU:H	13	0.26
(1,1173)	1:293:A:VAL:HG23	1:294:A:GLU:H	13	0.26
(1,1155)	1:285:A:LEU:HD11	1:315:A:ILE:HD11	2	0.26
(1,1155)	1:285:A:LEU:HD11	1:315:A:ILE:HD12	2	0.26
(1,1155)	1:285:A:LEU:HD11	1:315:A:ILE:HD13	2	0.26
(1,1155)	1:285:A:LEU:HD12	1:315:A:ILE:HD11	2	0.26
(1,1155)	1:285:A:LEU:HD12	1:315:A:ILE:HD12	2	0.26
(1,1155)	1:285:A:LEU:HD12	1:315:A:ILE:HD13	2	0.26
(1,1155)	1:285:A:LEU:HD13	1:315:A:ILE:HD11	2	0.26
(1,1155)	1:285:A:LEU:HD13	1:315:A:ILE:HD12	2	0.26
(1,1155)	1:285:A:LEU:HD13	1:315:A:ILE:HD13	2	0.26
(1,1155)	1:285:A:LEU:HD21	1:315:A:ILE:HD11	2	0.26
(1,1155)	1:285:A:LEU:HD21	1:315:A:ILE:HD12	2	0.26
(1,1155)	1:285:A:LEU:HD21	1:315:A:ILE:HD13	2	0.26
(1,1155)	1:285:A:LEU:HD22	1:315:A:ILE:HD11	2	0.26
(1,1155)	1:285:A:LEU:HD22	1:315:A:ILE:HD12	2	0.26
(1,1155)	1:285:A:LEU:HD22	1:315:A:ILE:HD13	2	0.26
(1,1155)	1:285:A:LEU:HD23	1:315:A:ILE:HD11	2	0.26
(1,1155)	1:285:A:LEU:HD23	1:315:A:ILE:HD12	2	0.26
(1,1155)	1:285:A:LEU:HD23	1:315:A:ILE:HD13	2	0.26
(1,1146)	1:281:A:HIS:HB2	1:317:A:GLU:HB3	2	0.26
(1,1146)	1:281:A:HIS:HB3	1:317:A:GLU:HB3	2	0.26
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	9	0.26
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB2	2	0.26
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB3	2	0.26
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB2	2	0.26
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB3	2	0.26
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB2	2	0.26
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB3	2	0.26
(1,1122)	1:270:A:LYS:HB2	1:270:A:LYS:HD2	20	0.26
(1,1122)	1:270:A:LYS:HB2	1:270:A:LYS:HD3	20	0.26
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	17	0.26
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	17	0.26
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG21	6	0.26
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG22	6	0.26
(1,970)	1:259:A:TYR:HD1	1:333:A:ILE:HG23	6	0.26
(1,939)	1:327:A:GLY:HA3	1:328:A:GLN:HG2	13	0.26
(1,939)	1:327:A:GLY:HA3	1:328:A:GLN:HG3	13	0.26
(1,939)	1:327:A:GLY:HA3	1:328:A:GLN:HG2	15	0.26
(1,939)	1:327:A:GLY:HA3	1:328:A:GLN:HG3	15	0.26
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD11	2	0.26
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD12	2	0.26
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD13	2	0.26
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD11	2	0.26
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD12	2	0.26
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD13	2	0.26
(1,905)	1:247:A:PRO:HD2	1:322:A:ILE:HG12	17	0.26
(1,905)	1:247:A:PRO:HD3	1:322:A:ILE:HG12	17	0.26
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	2	0.26
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	2	0.26
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	2	0.26
(1,820)	1:300:A:LEU:HG	1:314:A:TYR:HE2	17	0.26
(1,810)	1:296:A:GLN:HG2	1:299:A:THR:HB	2	0.26
(1,810)	1:296:A:GLN:HG3	1:299:A:THR:HB	2	0.26
(1,790)	1:284:A:THR:HG21	1:314:A:TYR:HD2	11	0.26
(1,790)	1:284:A:THR:HG22	1:314:A:TYR:HD2	11	0.26
(1,790)	1:284:A:THR:HG23	1:314:A:TYR:HD2	11	0.26
(1,727)	1:266:A:LYS:HG3	1:267:A:LEU:H	10	0.26
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	12	0.26
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	14	0.26
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	14	0.26
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	14	0.26
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	5	0.26
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	5	0.26
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	13	0.26
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	13	0.26
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	13	0.26
(1,644)	1:251:A:ILE:HD11	1:328:A:GLN:HA	5	0.26
(1,644)	1:251:A:ILE:HD12	1:328:A:GLN:HA	5	0.26
(1,644)	1:251:A:ILE:HD13	1:328:A:GLN:HA	5	0.26
(1,639)	1:251:A:ILE:HD11	1:314:A:TYR:HB3	19	0.26
(1,639)	1:251:A:ILE:HD12	1:314:A:TYR:HB3	19	0.26
(1,639)	1:251:A:ILE:HD13	1:314:A:TYR:HB3	19	0.26
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	1	0.26
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	1	0.26
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	1	0.26
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	1	0.26
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	1	0.26
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	1	0.26
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	1	0.26
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	1	0.26
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	1	0.26
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	20	0.26
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	20	0.26
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	20	0.26
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	20	0.26
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	20	0.26
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	20	0.26
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	20	0.26
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	20	0.26
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	20	0.26
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	7	0.26
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	7	0.26
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	7	0.26
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	3	0.26
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	3	0.26
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	3	0.26
(1,555)	1:300:A:LEU:HB2	1:314:A:TYR:HB2	9	0.26
(1,555)	1:300:A:LEU:HB3	1:314:A:TYR:HB2	9	0.26
(1,470)	1:251:A:ILE:HD11	1:328:A:GLN:H	17	0.26
(1,470)	1:251:A:ILE:HD12	1:328:A:GLN:H	17	0.26
(1,470)	1:251:A:ILE:HD13	1:328:A:GLN:H	17	0.26
(1,420)	1:318:A:ALA:HB1	1:320:A:ASN:H	14	0.26
(1,420)	1:318:A:ALA:HB2	1:320:A:ASN:H	14	0.26
(1,420)	1:318:A:ALA:HB3	1:320:A:ASN:H	14	0.26
(1,397)	1:318:A:ALA:H	1:326:A:SER:HB3	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	1	0.26
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	2	0.26
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	2	0.26
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	2	0.26
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	3	0.26
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	3	0.26
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	3	0.26
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	9	0.26
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	9	0.26
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	9	0.26
(1,295)	1:302:A:PHE:H	1:303:A:ARG:HA	10	0.26
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	6	0.26
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	6	0.26
(1,70)	1:257:A:ASN:H	1:258:A:TRP:HA	1	0.26
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	13	0.26
(1,13)	1:244:A:GLN:H	1:244:A:GLN:HB2	20	0.26
(1,1250)	1:330:A:GLU:HB2	1:331:A:VAL:H	8	0.25
(1,1250)	1:330:A:GLU:HB3	1:331:A:VAL:H	8	0.25
(1,1250)	1:330:A:GLU:HB2	1:331:A:VAL:H	9	0.25
(1,1250)	1:330:A:GLU:HB3	1:331:A:VAL:H	9	0.25
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG11	6	0.25
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG12	6	0.25
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG13	6	0.25
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG21	6	0.25
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG22	6	0.25
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG23	6	0.25
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD11	3	0.25
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD12	3	0.25
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD13	3	0.25
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD11	3	0.25
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD12	3	0.25
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD13	3	0.25
(1,1208)	1:310:A:LEU:HD11	1:314:A:TYR:HE1	14	0.25
(1,1208)	1:310:A:LEU:HD12	1:314:A:TYR:HE1	14	0.25
(1,1208)	1:310:A:LEU:HD13	1:314:A:TYR:HE1	14	0.25
(1,1208)	1:310:A:LEU:HD21	1:314:A:TYR:HE1	14	0.25
(1,1208)	1:310:A:LEU:HD22	1:314:A:TYR:HE1	14	0.25
(1,1208)	1:310:A:LEU:HD23	1:314:A:TYR:HE1	14	0.25
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	1	0.25
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	1	0.25
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	1	0.25
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	1	0.25
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	1	0.25
(1,1175)	1:293:A:VAL:HG11	1:302:A:PHE:H	8	0.25
(1,1175)	1:293:A:VAL:HG12	1:302:A:PHE:H	8	0.25
(1,1175)	1:293:A:VAL:HG13	1:302:A:PHE:H	8	0.25
(1,1175)	1:293:A:VAL:HG21	1:302:A:PHE:H	8	0.25
(1,1175)	1:293:A:VAL:HG22	1:302:A:PHE:H	8	0.25
(1,1175)	1:293:A:VAL:HG23	1:302:A:PHE:H	8	0.25
(1,1173)	1:293:A:VAL:HG11	1:294:A:GLU:H	12	0.25
(1,1173)	1:293:A:VAL:HG12	1:294:A:GLU:H	12	0.25
(1,1173)	1:293:A:VAL:HG13	1:294:A:GLU:H	12	0.25
(1,1173)	1:293:A:VAL:HG21	1:294:A:GLU:H	12	0.25
(1,1173)	1:293:A:VAL:HG22	1:294:A:GLU:H	12	0.25
(1,1173)	1:293:A:VAL:HG23	1:294:A:GLU:H	12	0.25
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD11	10	0.25
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD12	10	0.25
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD13	10	0.25
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD21	10	0.25
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD22	10	0.25
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD23	10	0.25
(1,1146)	1:281:A:HIS:HB2	1:317:A:GLU:HB3	18	0.25
(1,1146)	1:281:A:HIS:HB3	1:317:A:GLU:HB3	18	0.25
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB2	4	0.25
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB3	4	0.25
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB2	4	0.25
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB3	4	0.25
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB2	4	0.25
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB3	4	0.25
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB2	8	0.25
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB3	8	0.25
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB2	8	0.25
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB3	8	0.25
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB2	8	0.25
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB3	8	0.25
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	1	0.25
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	1	0.25
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	1	0.25
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	1	0.25
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	1	0.25
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	1	0.25
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	17	0.25
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	17	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	17	0.25
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	17	0.25
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	17	0.25
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	17	0.25
(1,1010)	1:246:A:GLU:HB2	1:325:A:ARG:HD2	7	0.25
(1,1010)	1:246:A:GLU:HB2	1:325:A:ARG:HD3	7	0.25
(1,1010)	1:246:A:GLU:HB3	1:325:A:ARG:HD2	7	0.25
(1,1010)	1:246:A:GLU:HB3	1:325:A:ARG:HD3	7	0.25
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG21	6	0.25
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG22	6	0.25
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG23	6	0.25
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD11	4	0.25
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD12	4	0.25
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD13	4	0.25
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD11	4	0.25
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD12	4	0.25
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD13	4	0.25
(1,900)	1:244:A:GLN:HB3	1:322:A:ILE:HA	16	0.25
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	4	0.25
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	4	0.25
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	4	0.25
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	6	0.25
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	6	0.25
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	6	0.25
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	12	0.25
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	12	0.25
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	12	0.25
(1,876)	1:315:A:ILE:HD11	1:328:A:GLN:HA	2	0.25
(1,876)	1:315:A:ILE:HD12	1:328:A:GLN:HA	2	0.25
(1,876)	1:315:A:ILE:HD13	1:328:A:GLN:HA	2	0.25
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	3	0.25
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	3	0.25
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	3	0.25
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	2	0.25
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	18	0.25
(1,765)	1:245:A:TYR:HD1	1:273:A:ALA:HB1	8	0.25
(1,765)	1:245:A:TYR:HD1	1:273:A:ALA:HB2	8	0.25
(1,765)	1:245:A:TYR:HD1	1:273:A:ALA:HB3	8	0.25
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	15	0.25
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	15	0.25
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	15	0.25
(1,645)	1:251:A:ILE:HD11	1:314:A:TYR:H	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,645)	1:251:A:ILE:HD12	1:314:A:TYR:H	14	0.25
(1,645)	1:251:A:ILE:HD13	1:314:A:TYR:H	14	0.25
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	14	0.25
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	14	0.25
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	14	0.25
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	11	0.25
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	11	0.25
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	11	0.25
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	11	0.25
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	11	0.25
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	11	0.25
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	11	0.25
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	11	0.25
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	11	0.25
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	12	0.25
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	12	0.25
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	12	0.25
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	12	0.25
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	12	0.25
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	12	0.25
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	12	0.25
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	12	0.25
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	12	0.25
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	19	0.25
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	19	0.25
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	19	0.25
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	19	0.25
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	19	0.25
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	19	0.25
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	19	0.25
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	19	0.25
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	19	0.25
(1,630)	1:251:A:ILE:HG21	1:268:A:THR:HB	2	0.25
(1,630)	1:251:A:ILE:HG22	1:268:A:THR:HB	2	0.25
(1,630)	1:251:A:ILE:HG23	1:268:A:THR:HB	2	0.25
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	13	0.25
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	13	0.25
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	13	0.25
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	13	0.25
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	13	0.25
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	13	0.25
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	13	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	13	0.25
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	13	0.25
(1,614)	1:251:A:ILE:HA	1:268:A:THR:H	4	0.25
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB1	18	0.25
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB2	18	0.25
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB3	18	0.25
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB1	18	0.25
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB2	18	0.25
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB3	18	0.25
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	11	0.25
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	12	0.25
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	4	0.25
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	4	0.25
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	4	0.25
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	8	0.25
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	8	0.25
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	8	0.25
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	11	0.25
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	11	0.25
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	11	0.25
(1,276)	1:300:A:LEU:H	1:300:A:LEU:HG	11	0.25
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	11	0.25
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	11	0.25
(1,190)	1:245:A:TYR:H	1:274:A:ASN:H	3	0.25
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	6	0.25
(1,101)	1:261:A:GLN:H	1:305:A:PRO:HB2	12	0.25
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD11	1	0.24
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD12	1	0.24
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD13	1	0.24
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD11	1	0.24
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD12	1	0.24
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD13	1	0.24
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG2	15	0.24
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG3	15	0.24
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG2	15	0.24
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG3	15	0.24
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG2	15	0.24
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG3	15	0.24
(1,1208)	1:310:A:LEU:HD11	1:314:A:TYR:HE1	19	0.24
(1,1208)	1:310:A:LEU:HD12	1:314:A:TYR:HE1	19	0.24
(1,1208)	1:310:A:LEU:HD13	1:314:A:TYR:HE1	19	0.24
(1,1208)	1:310:A:LEU:HD21	1:314:A:TYR:HE1	19	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1208)	1:310:A:LEU:HD22	1:314:A:TYR:HE1	19	0.24
(1,1208)	1:310:A:LEU:HD23	1:314:A:TYR:HE1	19	0.24
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG21	5	0.24
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG22	5	0.24
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG23	5	0.24
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	5	0.24
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	5	0.24
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	5	0.24
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	7	0.24
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	7	0.24
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	7	0.24
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	7	0.24
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	7	0.24
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	7	0.24
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	19	0.24
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	19	0.24
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	19	0.24
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	19	0.24
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	19	0.24
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	19	0.24
(1,1192)	1:303:A:ARG:HG2	1:304:A:GLY:H	13	0.24
(1,1192)	1:303:A:ARG:HG3	1:304:A:GLY:H	13	0.24
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	12	0.24
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	12	0.24
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	12	0.24
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	12	0.24
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	12	0.24
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	12	0.24
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD11	8	0.24
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD12	8	0.24
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD13	8	0.24
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD21	8	0.24
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD22	8	0.24
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD23	8	0.24
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG11	16	0.24
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG12	16	0.24
(1,1053)	1:254:A:PHE:HB2	1:329:A:VAL:HG13	16	0.24
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG11	16	0.24
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG12	16	0.24
(1,1053)	1:254:A:PHE:HB3	1:329:A:VAL:HG13	16	0.24
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD11	6	0.24
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD12	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD13	6	0.24
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD21	6	0.24
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD22	6	0.24
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD23	6	0.24
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD11	12	0.24
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD12	12	0.24
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD13	12	0.24
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD21	12	0.24
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD22	12	0.24
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD23	12	0.24
(1,940)	1:251:A:ILE:HD11	1:327:A:GLY:HA2	19	0.24
(1,940)	1:251:A:ILE:HD12	1:327:A:GLY:HA2	19	0.24
(1,940)	1:251:A:ILE:HD13	1:327:A:GLY:HA2	19	0.24
(1,853)	1:313:A:THR:HG21	1:328:A:GLN:HA	16	0.24
(1,853)	1:313:A:THR:HG22	1:328:A:GLN:HA	16	0.24
(1,853)	1:313:A:THR:HG23	1:328:A:GLN:HA	16	0.24
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	4	0.24
(1,800)	1:285:A:LEU:HD21	1:313:A:THR:HB	1	0.24
(1,800)	1:285:A:LEU:HD22	1:313:A:THR:HB	1	0.24
(1,800)	1:285:A:LEU:HD23	1:313:A:THR:HB	1	0.24
(1,732)	1:267:A:LEU:HB2	1:302:A:PHE:HD1	13	0.24
(1,732)	1:267:A:LEU:HB3	1:302:A:PHE:HD1	13	0.24
(1,718)	1:266:A:LYS:HB2	1:301:A:PHE:HZ	11	0.24
(1,718)	1:266:A:LYS:HB3	1:301:A:PHE:HZ	11	0.24
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG11	11	0.24
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG12	11	0.24
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG13	11	0.24
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	3	0.24
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	3	0.24
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	3	0.24
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	8	0.24
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	8	0.24
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	8	0.24
(1,655)	1:301:A:PHE:HA	1:302:A:PHE:HE1	17	0.24
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	7	0.24
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	7	0.24
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	7	0.24
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	6	0.24
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	6	0.24
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	6	0.24
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	6	0.24
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	6	0.24
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	6	0.24
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	6	0.24
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	6	0.24
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	10	0.24
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	10	0.24
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	10	0.24
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	10	0.24
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	10	0.24
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	10	0.24
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	10	0.24
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	10	0.24
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	10	0.24
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	14	0.24
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	14	0.24
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	14	0.24
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	14	0.24
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	14	0.24
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	14	0.24
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	14	0.24
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	14	0.24
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	14	0.24
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	17	0.24
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	17	0.24
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	17	0.24
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	17	0.24
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	17	0.24
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	17	0.24
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	17	0.24
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	17	0.24
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	17	0.24
(1,630)	1:251:A:ILE:HG21	1:268:A:THR:HB	11	0.24
(1,630)	1:251:A:ILE:HG22	1:268:A:THR:HB	11	0.24
(1,630)	1:251:A:ILE:HG23	1:268:A:THR:HB	11	0.24
(1,627)	1:251:A:ILE:HG21	1:267:A:LEU:HG	1	0.24
(1,627)	1:251:A:ILE:HG22	1:267:A:LEU:HG	1	0.24
(1,627)	1:251:A:ILE:HG23	1:267:A:LEU:HG	1	0.24
(1,627)	1:251:A:ILE:HG21	1:267:A:LEU:HG	8	0.24
(1,627)	1:251:A:ILE:HG22	1:267:A:LEU:HG	8	0.24
(1,627)	1:251:A:ILE:HG23	1:267:A:LEU:HG	8	0.24
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	1	0.24
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	1	0.24
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	1	0.24
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	1	0.24
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	1	0.24
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	1	0.24
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	1	0.24
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	1	0.24
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG21	19	0.24
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG22	19	0.24
(1,624)	1:251:A:ILE:HG21	1:329:A:VAL:HG23	19	0.24
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG21	19	0.24
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG22	19	0.24
(1,624)	1:251:A:ILE:HG22	1:329:A:VAL:HG23	19	0.24
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG21	19	0.24
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG22	19	0.24
(1,624)	1:251:A:ILE:HG23	1:329:A:VAL:HG23	19	0.24
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB1	3	0.24
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB2	3	0.24
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB3	3	0.24
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB1	3	0.24
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB2	3	0.24
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB3	3	0.24
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB1	7	0.24
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB2	7	0.24
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB3	7	0.24
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB1	7	0.24
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB2	7	0.24
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB3	7	0.24
(1,511)	1:259:A:TYR:HB3	1:334:A:THR:H	19	0.24
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	3	0.24
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	3	0.24
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	3	0.24
(1,441)	1:246:A:GLU:HB2	1:324:A:THR:H	16	0.24
(1,441)	1:246:A:GLU:HB3	1:324:A:THR:H	16	0.24
(1,420)	1:318:A:ALA:HB1	1:320:A:ASN:H	17	0.24
(1,420)	1:318:A:ALA:HB2	1:320:A:ASN:H	17	0.24
(1,420)	1:318:A:ALA:HB3	1:320:A:ASN:H	17	0.24
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	3	0.24
(1,180)	1:247:A:PRO:HA	1:272:A:ASP:H	4	0.24
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	1	0.24
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	1	0.24
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	6	0.24
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	6	0.24
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	6	0.24
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	15	0.24
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	15	0.24
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	15	0.24
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	4	0.24
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	4	0.24
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	4	0.24
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD11	4	0.24
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD12	4	0.24
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD13	4	0.24
(1,1245)	1:325:A:ARG:HD2	1:326:A:SER:H	2	0.23
(1,1245)	1:325:A:ARG:HD3	1:326:A:SER:H	2	0.23
(1,1245)	1:325:A:ARG:HD2	1:326:A:SER:H	13	0.23
(1,1245)	1:325:A:ARG:HD3	1:326:A:SER:H	13	0.23
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	15	0.23
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	15	0.23
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	15	0.23
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	15	0.23
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	15	0.23
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	15	0.23
(1,1173)	1:293:A:VAL:HG11	1:294:A:GLU:H	1	0.23
(1,1173)	1:293:A:VAL:HG12	1:294:A:GLU:H	1	0.23
(1,1173)	1:293:A:VAL:HG13	1:294:A:GLU:H	1	0.23
(1,1173)	1:293:A:VAL:HG21	1:294:A:GLU:H	1	0.23
(1,1173)	1:293:A:VAL:HG22	1:294:A:GLU:H	1	0.23
(1,1173)	1:293:A:VAL:HG23	1:294:A:GLU:H	1	0.23
(1,1173)	1:293:A:VAL:HG11	1:294:A:GLU:H	6	0.23
(1,1173)	1:293:A:VAL:HG12	1:294:A:GLU:H	6	0.23
(1,1173)	1:293:A:VAL:HG13	1:294:A:GLU:H	6	0.23
(1,1173)	1:293:A:VAL:HG21	1:294:A:GLU:H	6	0.23
(1,1173)	1:293:A:VAL:HG22	1:294:A:GLU:H	6	0.23
(1,1173)	1:293:A:VAL:HG23	1:294:A:GLU:H	6	0.23
(1,1173)	1:293:A:VAL:HG11	1:294:A:GLU:H	14	0.23
(1,1173)	1:293:A:VAL:HG12	1:294:A:GLU:H	14	0.23
(1,1173)	1:293:A:VAL:HG13	1:294:A:GLU:H	14	0.23
(1,1173)	1:293:A:VAL:HG21	1:294:A:GLU:H	14	0.23
(1,1173)	1:293:A:VAL:HG22	1:294:A:GLU:H	14	0.23
(1,1173)	1:293:A:VAL:HG23	1:294:A:GLU:H	14	0.23
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	2	0.23
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	15	0.23
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	15	0.23
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	15	0.23
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	15	0.23
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	15	0.23
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	15	0.23
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	15	0.23
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	15	0.23
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	15	0.23
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	15	0.23
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	15	0.23
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	15	0.23
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD11	5	0.23
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD12	5	0.23
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD13	5	0.23
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD21	5	0.23
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD22	5	0.23
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD23	5	0.23
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	7	0.23
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	7	0.23
(1,1005)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	7	0.23
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD11	7	0.23
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD12	7	0.23
(1,1005)	1:244:A:GLN:HG3	1:322:A:ILE:HD13	7	0.23
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD11	1	0.23
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD12	1	0.23
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD13	1	0.23
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD11	1	0.23
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD12	1	0.23
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD13	1	0.23
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD11	12	0.23
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD12	12	0.23
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD13	12	0.23
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD11	12	0.23
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD12	12	0.23
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD13	12	0.23
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	20	0.23
(1,839)	1:302:A:PHE:HE1	1:306:A:ILE:HD11	3	0.23
(1,839)	1:302:A:PHE:HE1	1:306:A:ILE:HD12	3	0.23
(1,839)	1:302:A:PHE:HE1	1:306:A:ILE:HD13	3	0.23
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	3	0.23
(1,778)	1:277:A:ALA:HB1	1:320:A:ASN:HA	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,778)	1:277:A:ALA:HB2	1:320:A:ASN:HA	10	0.23
(1,778)	1:277:A:ALA:HB3	1:320:A:ASN:HA	10	0.23
(1,776)	1:273:A:ALA:HB1	1:277:A:ALA:HA	4	0.23
(1,776)	1:273:A:ALA:HB2	1:277:A:ALA:HA	4	0.23
(1,776)	1:273:A:ALA:HB3	1:277:A:ALA:HA	4	0.23
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	17	0.23
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	17	0.23
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	17	0.23
(1,683)	1:247:A:PRO:HB2	1:325:A:ARG:HB2	3	0.23
(1,641)	1:251:A:ILE:HD11	1:316:A:CYS:HA	15	0.23
(1,641)	1:251:A:ILE:HD12	1:316:A:CYS:HA	15	0.23
(1,641)	1:251:A:ILE:HD13	1:316:A:CYS:HA	15	0.23
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	9	0.23
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	9	0.23
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	9	0.23
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	9	0.23
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	9	0.23
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	9	0.23
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	9	0.23
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	9	0.23
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	9	0.23
(1,630)	1:251:A:ILE:HG21	1:268:A:THR:HB	14	0.23
(1,630)	1:251:A:ILE:HG22	1:268:A:THR:HB	14	0.23
(1,630)	1:251:A:ILE:HG23	1:268:A:THR:HB	14	0.23
(1,630)	1:251:A:ILE:HG21	1:268:A:THR:HB	15	0.23
(1,630)	1:251:A:ILE:HG22	1:268:A:THR:HB	15	0.23
(1,630)	1:251:A:ILE:HG23	1:268:A:THR:HB	15	0.23
(1,630)	1:251:A:ILE:HG21	1:268:A:THR:HB	19	0.23
(1,630)	1:251:A:ILE:HG22	1:268:A:THR:HB	19	0.23
(1,630)	1:251:A:ILE:HG23	1:268:A:THR:HB	19	0.23
(1,608)	1:250:A:THR:HA	1:251:A:ILE:HG13	11	0.23
(1,608)	1:250:A:THR:HA	1:251:A:ILE:HG13	12	0.23
(1,608)	1:250:A:THR:HA	1:251:A:ILE:HG13	20	0.23
(1,564)	1:243:A:VAL:HA	1:244:A:GLN:HG3	9	0.23
(1,541)	1:251:A:ILE:HG21	1:269:A:CYS:HB2	15	0.23
(1,541)	1:251:A:ILE:HG22	1:269:A:CYS:HB2	15	0.23
(1,541)	1:251:A:ILE:HG23	1:269:A:CYS:HB2	15	0.23
(1,511)	1:259:A:TYR:HB3	1:334:A:THR:H	17	0.23
(1,420)	1:318:A:ALA:HB1	1:320:A:ASN:H	8	0.23
(1,420)	1:318:A:ALA:HB2	1:320:A:ASN:H	8	0.23
(1,420)	1:318:A:ALA:HB3	1:320:A:ASN:H	8	0.23
(1,420)	1:318:A:ALA:HB1	1:320:A:ASN:H	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,420)	1:318:A:ALA:HB2	1:320:A:ASN:H	19	0.23
(1,420)	1:318:A:ALA:HB3	1:320:A:ASN:H	19	0.23
(1,397)	1:318:A:ALA:H	1:326:A:SER:HB3	2	0.23
(1,382)	1:315:A:ILE:H	1:328:A:GLN:HB3	8	0.23
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	15	0.23
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	14	0.23
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	14	0.23
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	14	0.23
(1,304)	1:302:A:PHE:H	1:303:A:ARG:H	4	0.23
(1,280)	1:301:A:PHE:H	1:301:A:PHE:HD1	17	0.23
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	1	0.23
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	2	0.23
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	2	0.23
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	2	0.23
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	5	0.23
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	5	0.23
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	5	0.23
(1,123)	1:265:A:VAL:H	1:266:A:LYS:HG2	1	0.23
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	1	0.23
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	17	0.23
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	13	0.23
(1,1250)	1:330:A:GLU:HB2	1:331:A:VAL:H	15	0.22
(1,1250)	1:330:A:GLU:HB3	1:331:A:VAL:H	15	0.22
(1,1173)	1:293:A:VAL:HG11	1:294:A:GLU:H	15	0.22
(1,1173)	1:293:A:VAL:HG12	1:294:A:GLU:H	15	0.22
(1,1173)	1:293:A:VAL:HG13	1:294:A:GLU:H	15	0.22
(1,1173)	1:293:A:VAL:HG21	1:294:A:GLU:H	15	0.22
(1,1173)	1:293:A:VAL:HG22	1:294:A:GLU:H	15	0.22
(1,1173)	1:293:A:VAL:HG23	1:294:A:GLU:H	15	0.22
(1,1160)	1:290:A:PRO:HB3	1:310:A:LEU:HD11	12	0.22
(1,1160)	1:290:A:PRO:HB3	1:310:A:LEU:HD12	12	0.22
(1,1160)	1:290:A:PRO:HB3	1:310:A:LEU:HD13	12	0.22
(1,1160)	1:290:A:PRO:HB3	1:310:A:LEU:HD21	12	0.22
(1,1160)	1:290:A:PRO:HB3	1:310:A:LEU:HD22	12	0.22
(1,1160)	1:290:A:PRO:HB3	1:310:A:LEU:HD23	12	0.22
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB2	3	0.22
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB3	3	0.22
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB2	3	0.22
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB3	3	0.22
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB2	3	0.22
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB3	3	0.22
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	8	0.22
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	8	0.22
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	8	0.22
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	8	0.22
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	8	0.22
(1,1116)	1:267:A:LEU:HD11	1:329:A:VAL:HG21	15	0.22
(1,1116)	1:267:A:LEU:HD11	1:329:A:VAL:HG22	15	0.22
(1,1116)	1:267:A:LEU:HD11	1:329:A:VAL:HG23	15	0.22
(1,1116)	1:267:A:LEU:HD12	1:329:A:VAL:HG21	15	0.22
(1,1116)	1:267:A:LEU:HD12	1:329:A:VAL:HG22	15	0.22
(1,1116)	1:267:A:LEU:HD12	1:329:A:VAL:HG23	15	0.22
(1,1116)	1:267:A:LEU:HD13	1:329:A:VAL:HG21	15	0.22
(1,1116)	1:267:A:LEU:HD13	1:329:A:VAL:HG22	15	0.22
(1,1116)	1:267:A:LEU:HD13	1:329:A:VAL:HG23	15	0.22
(1,1116)	1:267:A:LEU:HD21	1:329:A:VAL:HG21	15	0.22
(1,1116)	1:267:A:LEU:HD21	1:329:A:VAL:HG22	15	0.22
(1,1116)	1:267:A:LEU:HD21	1:329:A:VAL:HG23	15	0.22
(1,1116)	1:267:A:LEU:HD22	1:329:A:VAL:HG21	15	0.22
(1,1116)	1:267:A:LEU:HD22	1:329:A:VAL:HG22	15	0.22
(1,1116)	1:267:A:LEU:HD22	1:329:A:VAL:HG23	15	0.22
(1,1116)	1:267:A:LEU:HD23	1:329:A:VAL:HG21	15	0.22
(1,1116)	1:267:A:LEU:HD23	1:329:A:VAL:HG22	15	0.22
(1,1116)	1:267:A:LEU:HD23	1:329:A:VAL:HG23	15	0.22
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG21	13	0.22
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG22	13	0.22
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG23	13	0.22
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG21	13	0.22
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG22	13	0.22
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG23	13	0.22
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG21	13	0.22
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG22	13	0.22
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG23	13	0.22
(1,942)	1:251:A:ILE:HD11	1:327:A:GLY:HA3	6	0.22
(1,942)	1:251:A:ILE:HD12	1:327:A:GLY:HA3	6	0.22
(1,942)	1:251:A:ILE:HD13	1:327:A:GLY:HA3	6	0.22
(1,905)	1:247:A:PRO:HD2	1:322:A:ILE:HG12	3	0.22
(1,905)	1:247:A:PRO:HD3	1:322:A:ILE:HG12	3	0.22
(1,905)	1:247:A:PRO:HD2	1:322:A:ILE:HG12	11	0.22
(1,905)	1:247:A:PRO:HD3	1:322:A:ILE:HG12	11	0.22
(1,876)	1:315:A:ILE:HD11	1:328:A:GLN:HA	11	0.22
(1,876)	1:315:A:ILE:HD12	1:328:A:GLN:HA	11	0.22
(1,876)	1:315:A:ILE:HD13	1:328:A:GLN:HA	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	13	0.22
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	13	0.22
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	13	0.22
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	15	0.22
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	15	0.22
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	15	0.22
(1,863)	1:315:A:ILE:HG21	1:326:A:SER:HB2	19	0.22
(1,863)	1:315:A:ILE:HG22	1:326:A:SER:HB2	19	0.22
(1,863)	1:315:A:ILE:HG23	1:326:A:SER:HB2	19	0.22
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	20	0.22
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	20	0.22
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	20	0.22
(1,790)	1:284:A:THR:HG21	1:314:A:TYR:HD2	10	0.22
(1,790)	1:284:A:THR:HG22	1:314:A:TYR:HD2	10	0.22
(1,790)	1:284:A:THR:HG23	1:314:A:TYR:HD2	10	0.22
(1,757)	1:245:A:TYR:HD1	1:273:A:ALA:HA	14	0.22
(1,732)	1:267:A:LEU:HB2	1:302:A:PHE:HD1	17	0.22
(1,732)	1:267:A:LEU:HB3	1:302:A:PHE:HD1	17	0.22
(1,727)	1:266:A:LYS:HG3	1:267:A:LEU:H	2	0.22
(1,727)	1:266:A:LYS:HG3	1:267:A:LEU:H	8	0.22
(1,718)	1:266:A:LYS:HB2	1:301:A:PHE:HZ	8	0.22
(1,718)	1:266:A:LYS:HB3	1:301:A:PHE:HZ	8	0.22
(1,718)	1:266:A:LYS:HB2	1:301:A:PHE:HZ	20	0.22
(1,718)	1:266:A:LYS:HB3	1:301:A:PHE:HZ	20	0.22
(1,703)	1:265:A:VAL:HG21	1:306:A:ILE:HD11	4	0.22
(1,703)	1:265:A:VAL:HG21	1:306:A:ILE:HD12	4	0.22
(1,703)	1:265:A:VAL:HG21	1:306:A:ILE:HD13	4	0.22
(1,703)	1:265:A:VAL:HG22	1:306:A:ILE:HD11	4	0.22
(1,703)	1:265:A:VAL:HG22	1:306:A:ILE:HD12	4	0.22
(1,703)	1:265:A:VAL:HG22	1:306:A:ILE:HD13	4	0.22
(1,703)	1:265:A:VAL:HG23	1:306:A:ILE:HD11	4	0.22
(1,703)	1:265:A:VAL:HG23	1:306:A:ILE:HD12	4	0.22
(1,703)	1:265:A:VAL:HG23	1:306:A:ILE:HD13	4	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	6	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	6	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	6	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	9	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	9	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	9	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	12	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	12	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	12	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	16	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	16	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	16	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	18	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	18	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	18	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	19	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	19	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	19	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	20	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	20	0.22
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	20	0.22
(1,655)	1:301:A:PHE:HA	1:302:A:PHE:HE1	13	0.22
(1,645)	1:251:A:ILE:HD11	1:314:A:TYR:H	20	0.22
(1,645)	1:251:A:ILE:HD12	1:314:A:TYR:H	20	0.22
(1,645)	1:251:A:ILE:HD13	1:314:A:TYR:H	20	0.22
(1,641)	1:251:A:ILE:HD11	1:316:A:CYS:HA	20	0.22
(1,641)	1:251:A:ILE:HD12	1:316:A:CYS:HA	20	0.22
(1,641)	1:251:A:ILE:HD13	1:316:A:CYS:HA	20	0.22
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	7	0.22
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	7	0.22
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	7	0.22
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	7	0.22
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	7	0.22
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	7	0.22
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	7	0.22
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	7	0.22
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	7	0.22
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	8	0.22
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	8	0.22
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	8	0.22
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	8	0.22
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	8	0.22
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	8	0.22
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	8	0.22
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	8	0.22
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	8	0.22
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	13	0.22
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	13	0.22
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	13	0.22
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	13	0.22
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	13	0.22
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	13	0.22
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	13	0.22
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	13	0.22
(1,632)	1:251:A:ILE:HG21	1:328:A:GLN:HA	3	0.22
(1,632)	1:251:A:ILE:HG22	1:328:A:GLN:HA	3	0.22
(1,632)	1:251:A:ILE:HG23	1:328:A:GLN:HA	3	0.22
(1,612)	1:250:A:THR:HB	1:270:A:LYS:HB2	13	0.22
(1,513)	1:333:A:ILE:HB	1:334:A:THR:H	16	0.22
(1,495)	1:331:A:VAL:HB	1:332:A:ASN:H	19	0.22
(1,420)	1:318:A:ALA:HB1	1:320:A:ASN:H	3	0.22
(1,420)	1:318:A:ALA:HB2	1:320:A:ASN:H	3	0.22
(1,420)	1:318:A:ALA:HB3	1:320:A:ASN:H	3	0.22
(1,397)	1:318:A:ALA:H	1:326:A:SER:HB3	16	0.22
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	4	0.22
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	18	0.22
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	13	0.22
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	13	0.22
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	13	0.22
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	20	0.22
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	20	0.22
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	20	0.22
(1,290)	1:265:A:VAL:H	1:302:A:PHE:H	10	0.22
(1,157)	1:268:A:THR:H	1:269:A:CYS:HB2	9	0.22
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	14	0.22
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD11	3	0.22
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD12	3	0.22
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD13	3	0.22
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD11	9	0.22
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD12	9	0.22
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD13	9	0.22
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD11	16	0.22
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD12	16	0.22
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD13	16	0.22
(1,1208)	1:310:A:LEU:HD11	1:314:A:TYR:HE1	4	0.21
(1,1208)	1:310:A:LEU:HD12	1:314:A:TYR:HE1	4	0.21
(1,1208)	1:310:A:LEU:HD13	1:314:A:TYR:HE1	4	0.21
(1,1208)	1:310:A:LEU:HD21	1:314:A:TYR:HE1	4	0.21
(1,1208)	1:310:A:LEU:HD22	1:314:A:TYR:HE1	4	0.21
(1,1208)	1:310:A:LEU:HD23	1:314:A:TYR:HE1	4	0.21
(1,1208)	1:310:A:LEU:HD11	1:314:A:TYR:HE1	6	0.21
(1,1208)	1:310:A:LEU:HD12	1:314:A:TYR:HE1	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1208)	1:310:A:LEU:HD13	1:314:A:TYR:HE1	6	0.21
(1,1208)	1:310:A:LEU:HD21	1:314:A:TYR:HE1	6	0.21
(1,1208)	1:310:A:LEU:HD22	1:314:A:TYR:HE1	6	0.21
(1,1208)	1:310:A:LEU:HD23	1:314:A:TYR:HE1	6	0.21
(1,1208)	1:310:A:LEU:HD11	1:314:A:TYR:HE1	8	0.21
(1,1208)	1:310:A:LEU:HD12	1:314:A:TYR:HE1	8	0.21
(1,1208)	1:310:A:LEU:HD13	1:314:A:TYR:HE1	8	0.21
(1,1208)	1:310:A:LEU:HD21	1:314:A:TYR:HE1	8	0.21
(1,1208)	1:310:A:LEU:HD22	1:314:A:TYR:HE1	8	0.21
(1,1208)	1:310:A:LEU:HD23	1:314:A:TYR:HE1	8	0.21
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	17	0.21
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	17	0.21
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	17	0.21
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	17	0.21
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	17	0.21
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	17	0.21
(1,1173)	1:293:A:VAL:HG11	1:294:A:GLU:H	16	0.21
(1,1173)	1:293:A:VAL:HG12	1:294:A:GLU:H	16	0.21
(1,1173)	1:293:A:VAL:HG13	1:294:A:GLU:H	16	0.21
(1,1173)	1:293:A:VAL:HG21	1:294:A:GLU:H	16	0.21
(1,1173)	1:293:A:VAL:HG22	1:294:A:GLU:H	16	0.21
(1,1173)	1:293:A:VAL:HG23	1:294:A:GLU:H	16	0.21
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD11	17	0.21
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD12	17	0.21
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD13	17	0.21
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD21	17	0.21
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD22	17	0.21
(1,1149)	1:285:A:LEU:HA	1:285:A:LEU:HD23	17	0.21
(1,1130)	1:273:A:ALA:HB1	1:320:A:ASN:HB2	11	0.21
(1,1130)	1:273:A:ALA:HB1	1:320:A:ASN:HB3	11	0.21
(1,1130)	1:273:A:ALA:HB2	1:320:A:ASN:HB2	11	0.21
(1,1130)	1:273:A:ALA:HB2	1:320:A:ASN:HB3	11	0.21
(1,1130)	1:273:A:ALA:HB3	1:320:A:ASN:HB2	11	0.21
(1,1130)	1:273:A:ALA:HB3	1:320:A:ASN:HB3	11	0.21
(1,1112)	1:267:A:LEU:HD11	1:302:A:PHE:HZ	8	0.21
(1,1112)	1:267:A:LEU:HD12	1:302:A:PHE:HZ	8	0.21
(1,1112)	1:267:A:LEU:HD13	1:302:A:PHE:HZ	8	0.21
(1,1112)	1:267:A:LEU:HD21	1:302:A:PHE:HZ	8	0.21
(1,1112)	1:267:A:LEU:HD22	1:302:A:PHE:HZ	8	0.21
(1,1112)	1:267:A:LEU:HD23	1:302:A:PHE:HZ	8	0.21
(1,1004)	1:244:A:GLN:HG2	1:322:A:ILE:HG13	1	0.21
(1,1004)	1:244:A:GLN:HG3	1:322:A:ILE:HG13	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD11	19	0.21
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD12	19	0.21
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD13	19	0.21
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD11	19	0.21
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD12	19	0.21
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD13	19	0.21
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	11	0.21
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	11	0.21
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	11	0.21
(1,876)	1:315:A:ILE:HD11	1:328:A:GLN:HA	1	0.21
(1,876)	1:315:A:ILE:HD12	1:328:A:GLN:HA	1	0.21
(1,876)	1:315:A:ILE:HD13	1:328:A:GLN:HA	1	0.21
(1,876)	1:315:A:ILE:HD11	1:328:A:GLN:HA	7	0.21
(1,876)	1:315:A:ILE:HD12	1:328:A:GLN:HA	7	0.21
(1,876)	1:315:A:ILE:HD13	1:328:A:GLN:HA	7	0.21
(1,876)	1:315:A:ILE:HD11	1:328:A:GLN:HA	13	0.21
(1,876)	1:315:A:ILE:HD12	1:328:A:GLN:HA	13	0.21
(1,876)	1:315:A:ILE:HD13	1:328:A:GLN:HA	13	0.21
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	8	0.21
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	8	0.21
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	8	0.21
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	14	0.21
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	14	0.21
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	14	0.21
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	7	0.21
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	7	0.21
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	7	0.21
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	12	0.21
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	19	0.21
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	4	0.21
(1,831)	1:260:A:LEU:HA	1:306:A:ILE:HB	14	0.21
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	20	0.21
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB1	10	0.21
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB2	10	0.21
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB3	10	0.21
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB1	12	0.21
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB2	12	0.21
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB3	12	0.21
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD2	2	0.21
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD3	2	0.21
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD2	2	0.21
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD3	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD2	2	0.21
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD3	2	0.21
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD2	6	0.21
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD3	6	0.21
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD2	6	0.21
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD3	6	0.21
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD2	6	0.21
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD3	6	0.21
(1,732)	1:267:A:LEU:HB2	1:302:A:PHE:HD1	11	0.21
(1,732)	1:267:A:LEU:HB3	1:302:A:PHE:HD1	11	0.21
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	1	0.21
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	1	0.21
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	1	0.21
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	7	0.21
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	7	0.21
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	7	0.21
(1,655)	1:301:A:PHE:HA	1:302:A:PHE:HE1	9	0.21
(1,645)	1:251:A:ILE:HD11	1:314:A:TYR:H	16	0.21
(1,645)	1:251:A:ILE:HD12	1:314:A:TYR:H	16	0.21
(1,645)	1:251:A:ILE:HD13	1:314:A:TYR:H	16	0.21
(1,644)	1:251:A:ILE:HD11	1:328:A:GLN:HA	1	0.21
(1,644)	1:251:A:ILE:HD12	1:328:A:GLN:HA	1	0.21
(1,644)	1:251:A:ILE:HD13	1:328:A:GLN:HA	1	0.21
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	2	0.21
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	2	0.21
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	2	0.21
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	2	0.21
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	2	0.21
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	2	0.21
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	2	0.21
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	2	0.21
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	2	0.21
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	5	0.21
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	5	0.21
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	5	0.21
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	5	0.21
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	5	0.21
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	5	0.21
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	5	0.21
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	5	0.21
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	5	0.21
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	15	0.21
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	15	0.21
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	15	0.21
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	15	0.21
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	15	0.21
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	15	0.21
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	15	0.21
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	15	0.21
(1,632)	1:251:A:ILE:HG21	1:328:A:GLN:HA	9	0.21
(1,632)	1:251:A:ILE:HG22	1:328:A:GLN:HA	9	0.21
(1,632)	1:251:A:ILE:HG23	1:328:A:GLN:HA	9	0.21
(1,632)	1:251:A:ILE:HG21	1:328:A:GLN:HA	19	0.21
(1,632)	1:251:A:ILE:HG22	1:328:A:GLN:HA	19	0.21
(1,632)	1:251:A:ILE:HG23	1:328:A:GLN:HA	19	0.21
(1,614)	1:251:A:ILE:HA	1:268:A:THR:H	12	0.21
(1,612)	1:250:A:THR:HB	1:270:A:LYS:HB2	15	0.21
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB1	11	0.21
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB2	11	0.21
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB3	11	0.21
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB1	11	0.21
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB2	11	0.21
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB3	11	0.21
(1,560)	1:249:A:VAL:HG21	1:316:A:CYS:HB3	2	0.21
(1,560)	1:249:A:VAL:HG22	1:316:A:CYS:HB3	2	0.21
(1,560)	1:249:A:VAL:HG23	1:316:A:CYS:HB3	2	0.21
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	15	0.21
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	15	0.21
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	15	0.21
(1,477)	1:328:A:GLN:HB3	1:329:A:VAL:H	2	0.21
(1,441)	1:246:A:GLU:HB2	1:324:A:THR:H	15	0.21
(1,441)	1:246:A:GLU:HB3	1:324:A:THR:H	15	0.21
(1,290)	1:265:A:VAL:H	1:302:A:PHE:H	20	0.21
(1,123)	1:265:A:VAL:H	1:266:A:LYS:HG2	7	0.21
(1,65)	1:251:A:ILE:HG21	1:254:A:PHE:H	15	0.21
(1,65)	1:251:A:ILE:HG22	1:254:A:PHE:H	15	0.21
(1,65)	1:251:A:ILE:HG23	1:254:A:PHE:H	15	0.21
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD11	8	0.21
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD12	8	0.21
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD13	8	0.21
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	11	0.21
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	12	0.21
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:245:A:TYR:H	1:273:A:ALA:HA	3	0.21
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG21	18	0.2
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG22	18	0.2
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG23	18	0.2
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	18	0.2
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	18	0.2
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	18	0.2
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	20	0.2
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	20	0.2
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	20	0.2
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	20	0.2
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	20	0.2
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	20	0.2
(1,1173)	1:293:A:VAL:HG11	1:294:A:GLU:H	3	0.2
(1,1173)	1:293:A:VAL:HG12	1:294:A:GLU:H	3	0.2
(1,1173)	1:293:A:VAL:HG13	1:294:A:GLU:H	3	0.2
(1,1173)	1:293:A:VAL:HG21	1:294:A:GLU:H	3	0.2
(1,1173)	1:293:A:VAL:HG22	1:294:A:GLU:H	3	0.2
(1,1173)	1:293:A:VAL:HG23	1:294:A:GLU:H	3	0.2
(1,1155)	1:285:A:LEU:HD11	1:315:A:ILE:HD11	13	0.2
(1,1155)	1:285:A:LEU:HD11	1:315:A:ILE:HD12	13	0.2
(1,1155)	1:285:A:LEU:HD11	1:315:A:ILE:HD13	13	0.2
(1,1155)	1:285:A:LEU:HD12	1:315:A:ILE:HD11	13	0.2
(1,1155)	1:285:A:LEU:HD12	1:315:A:ILE:HD12	13	0.2
(1,1155)	1:285:A:LEU:HD12	1:315:A:ILE:HD13	13	0.2
(1,1155)	1:285:A:LEU:HD13	1:315:A:ILE:HD11	13	0.2
(1,1155)	1:285:A:LEU:HD13	1:315:A:ILE:HD12	13	0.2
(1,1155)	1:285:A:LEU:HD13	1:315:A:ILE:HD13	13	0.2
(1,1155)	1:285:A:LEU:HD21	1:315:A:ILE:HD11	13	0.2
(1,1155)	1:285:A:LEU:HD21	1:315:A:ILE:HD12	13	0.2
(1,1155)	1:285:A:LEU:HD21	1:315:A:ILE:HD13	13	0.2
(1,1155)	1:285:A:LEU:HD22	1:315:A:ILE:HD11	13	0.2
(1,1155)	1:285:A:LEU:HD22	1:315:A:ILE:HD12	13	0.2
(1,1155)	1:285:A:LEU:HD22	1:315:A:ILE:HD13	13	0.2
(1,1155)	1:285:A:LEU:HD23	1:315:A:ILE:HD11	13	0.2
(1,1155)	1:285:A:LEU:HD23	1:315:A:ILE:HD12	13	0.2
(1,1155)	1:285:A:LEU:HD23	1:315:A:ILE:HD13	13	0.2
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG21	2	0.2
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG22	2	0.2
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG23	2	0.2
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG21	2	0.2
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG22	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG23	2	0.2
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG21	8	0.2
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG22	8	0.2
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG23	8	0.2
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG21	8	0.2
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG22	8	0.2
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG23	8	0.2
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG21	10	0.2
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG22	10	0.2
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG23	10	0.2
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG21	10	0.2
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG22	10	0.2
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG23	10	0.2
(1,1076)	1:260:A:LEU:HD11	1:306:A:ILE:H	20	0.2
(1,1076)	1:260:A:LEU:HD12	1:306:A:ILE:H	20	0.2
(1,1076)	1:260:A:LEU:HD13	1:306:A:ILE:H	20	0.2
(1,1076)	1:260:A:LEU:HD21	1:306:A:ILE:H	20	0.2
(1,1076)	1:260:A:LEU:HD22	1:306:A:ILE:H	20	0.2
(1,1076)	1:260:A:LEU:HD23	1:306:A:ILE:H	20	0.2
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD11	4	0.2
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD12	4	0.2
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD13	4	0.2
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD21	4	0.2
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD22	4	0.2
(1,1055)	1:255:A:ASP:H	1:267:A:LEU:HD23	4	0.2
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG21	8	0.2
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG22	8	0.2
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG23	8	0.2
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG21	9	0.2
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG22	9	0.2
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG23	9	0.2
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG21	14	0.2
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG22	14	0.2
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG23	14	0.2
(1,942)	1:251:A:ILE:HD11	1:327:A:GLY:HA3	9	0.2
(1,942)	1:251:A:ILE:HD12	1:327:A:GLY:HA3	9	0.2
(1,942)	1:251:A:ILE:HD13	1:327:A:GLY:HA3	9	0.2
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	2	0.2
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	2	0.2
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	2	0.2
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	3	0.2
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	3	0.2
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	6	0.2
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	6	0.2
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	6	0.2
(1,871)	1:315:A:ILE:HD11	1:328:A:GLN:HB3	8	0.2
(1,871)	1:315:A:ILE:HD12	1:328:A:GLN:HB3	8	0.2
(1,871)	1:315:A:ILE:HD13	1:328:A:GLN:HB3	8	0.2
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	18	0.2
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	18	0.2
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	18	0.2
(1,853)	1:313:A:THR:HG21	1:328:A:GLN:HA	12	0.2
(1,853)	1:313:A:THR:HG22	1:328:A:GLN:HA	12	0.2
(1,853)	1:313:A:THR:HG23	1:328:A:GLN:HA	12	0.2
(1,827)	1:261:A:GLN:HA	1:305:A:PRO:HB2	6	0.2
(1,776)	1:273:A:ALA:HB1	1:277:A:ALA:HA	16	0.2
(1,776)	1:273:A:ALA:HB2	1:277:A:ALA:HA	16	0.2
(1,776)	1:273:A:ALA:HB3	1:277:A:ALA:HA	16	0.2
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD2	11	0.2
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD3	11	0.2
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD2	11	0.2
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD3	11	0.2
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD2	11	0.2
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD3	11	0.2
(1,746)	1:268:A:THR:HG21	1:270:A:LYS:HG2	17	0.2
(1,746)	1:268:A:THR:HG22	1:270:A:LYS:HG2	17	0.2
(1,746)	1:268:A:THR:HG23	1:270:A:LYS:HG2	17	0.2
(1,746)	1:268:A:THR:HG21	1:270:A:LYS:HG3	17	0.2
(1,746)	1:268:A:THR:HG22	1:270:A:LYS:HG3	17	0.2
(1,746)	1:268:A:THR:HG23	1:270:A:LYS:HG3	17	0.2
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	1	0.2
(1,683)	1:247:A:PRO:HB2	1:325:A:ARG:HB2	6	0.2
(1,683)	1:247:A:PRO:HB2	1:325:A:ARG:HB2	14	0.2
(1,682)	1:262:A:ARG:HA	1:262:A:ARG:HD2	9	0.2
(1,682)	1:262:A:ARG:HA	1:262:A:ARG:HD3	9	0.2
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	17	0.2
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	17	0.2
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	17	0.2
(1,645)	1:251:A:ILE:HD11	1:314:A:TYR:H	10	0.2
(1,645)	1:251:A:ILE:HD12	1:314:A:TYR:H	10	0.2
(1,645)	1:251:A:ILE:HD13	1:314:A:TYR:H	10	0.2
(1,639)	1:251:A:ILE:HD11	1:314:A:TYR:HB3	13	0.2
(1,639)	1:251:A:ILE:HD12	1:314:A:TYR:HB3	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:251:A:ILE:HD13	1:314:A:TYR:HB3	13	0.2
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	3	0.2
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	3	0.2
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	3	0.2
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	3	0.2
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	3	0.2
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	3	0.2
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	3	0.2
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	3	0.2
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	3	0.2
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	16	0.2
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	16	0.2
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	16	0.2
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	16	0.2
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	16	0.2
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	16	0.2
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	16	0.2
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	16	0.2
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	16	0.2
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	18	0.2
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	18	0.2
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	18	0.2
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	18	0.2
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	18	0.2
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	18	0.2
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	18	0.2
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	18	0.2
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	18	0.2
(1,630)	1:251:A:ILE:HG21	1:268:A:THR:HB	20	0.2
(1,630)	1:251:A:ILE:HG22	1:268:A:THR:HB	20	0.2
(1,630)	1:251:A:ILE:HG23	1:268:A:THR:HB	20	0.2
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	20	0.2
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	20	0.2
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	20	0.2
(1,627)	1:251:A:ILE:HG21	1:267:A:LEU:HG	13	0.2
(1,627)	1:251:A:ILE:HG22	1:267:A:LEU:HG	13	0.2
(1,627)	1:251:A:ILE:HG23	1:267:A:LEU:HG	13	0.2
(1,608)	1:250:A:THR:HA	1:251:A:ILE:HG13	19	0.2
(1,588)	1:247:A:PRO:HA	1:318:A:ALA:HB1	11	0.2
(1,588)	1:247:A:PRO:HA	1:318:A:ALA:HB2	11	0.2
(1,588)	1:247:A:PRO:HA	1:318:A:ALA:HB3	11	0.2
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB1	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB2	15	0.2
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB3	15	0.2
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB1	15	0.2
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB2	15	0.2
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB3	15	0.2
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB1	19	0.2
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB2	19	0.2
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB3	19	0.2
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB1	19	0.2
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB2	19	0.2
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB3	19	0.2
(1,555)	1:300:A:LEU:HB2	1:314:A:TYR:HB2	13	0.2
(1,555)	1:300:A:LEU:HB3	1:314:A:TYR:HB2	13	0.2
(1,542)	1:268:A:THR:HG21	1:269:A:CYS:HB2	9	0.2
(1,542)	1:268:A:THR:HG22	1:269:A:CYS:HB2	9	0.2
(1,542)	1:268:A:THR:HG23	1:269:A:CYS:HB2	9	0.2
(1,535)	1:249:A:VAL:HG11	1:316:A:CYS:HB3	7	0.2
(1,535)	1:249:A:VAL:HG12	1:316:A:CYS:HB3	7	0.2
(1,535)	1:249:A:VAL:HG13	1:316:A:CYS:HB3	7	0.2
(1,535)	1:249:A:VAL:HG11	1:316:A:CYS:HB3	12	0.2
(1,535)	1:249:A:VAL:HG12	1:316:A:CYS:HB3	12	0.2
(1,535)	1:249:A:VAL:HG13	1:316:A:CYS:HB3	12	0.2
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	7	0.2
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	16	0.2
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	16	0.2
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	16	0.2
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	19	0.2
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	19	0.2
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	19	0.2
(1,190)	1:245:A:TYR:H	1:274:A:ASN:H	11	0.2
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	18	0.2
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	12	0.2
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	12	0.2
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	12	0.2
(1,77)	1:258:A:TRP:H	1:333:A:ILE:HD11	9	0.2
(1,77)	1:258:A:TRP:H	1:333:A:ILE:HD12	9	0.2
(1,77)	1:258:A:TRP:H	1:333:A:ILE:HD13	9	0.2
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	17	0.2
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	2	0.2
(1,1245)	1:325:A:ARG:HD2	1:326:A:SER:H	12	0.19
(1,1245)	1:325:A:ARG:HD3	1:326:A:SER:H	12	0.19
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG21	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG22	12	0.19
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG23	12	0.19
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	12	0.19
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	12	0.19
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	12	0.19
(1,1192)	1:303:A:ARG:HG2	1:304:A:GLY:H	11	0.19
(1,1192)	1:303:A:ARG:HG3	1:304:A:GLY:H	11	0.19
(1,1175)	1:293:A:VAL:HG11	1:302:A:PHE:H	12	0.19
(1,1175)	1:293:A:VAL:HG12	1:302:A:PHE:H	12	0.19
(1,1175)	1:293:A:VAL:HG13	1:302:A:PHE:H	12	0.19
(1,1175)	1:293:A:VAL:HG21	1:302:A:PHE:H	12	0.19
(1,1175)	1:293:A:VAL:HG22	1:302:A:PHE:H	12	0.19
(1,1175)	1:293:A:VAL:HG23	1:302:A:PHE:H	12	0.19
(1,1155)	1:285:A:LEU:HD11	1:315:A:ILE:HD11	19	0.19
(1,1155)	1:285:A:LEU:HD11	1:315:A:ILE:HD12	19	0.19
(1,1155)	1:285:A:LEU:HD11	1:315:A:ILE:HD13	19	0.19
(1,1155)	1:285:A:LEU:HD12	1:315:A:ILE:HD11	19	0.19
(1,1155)	1:285:A:LEU:HD12	1:315:A:ILE:HD12	19	0.19
(1,1155)	1:285:A:LEU:HD12	1:315:A:ILE:HD13	19	0.19
(1,1155)	1:285:A:LEU:HD13	1:315:A:ILE:HD11	19	0.19
(1,1155)	1:285:A:LEU:HD13	1:315:A:ILE:HD12	19	0.19
(1,1155)	1:285:A:LEU:HD13	1:315:A:ILE:HD13	19	0.19
(1,1155)	1:285:A:LEU:HD21	1:315:A:ILE:HD11	19	0.19
(1,1155)	1:285:A:LEU:HD21	1:315:A:ILE:HD12	19	0.19
(1,1155)	1:285:A:LEU:HD21	1:315:A:ILE:HD13	19	0.19
(1,1155)	1:285:A:LEU:HD22	1:315:A:ILE:HD11	19	0.19
(1,1155)	1:285:A:LEU:HD22	1:315:A:ILE:HD12	19	0.19
(1,1155)	1:285:A:LEU:HD22	1:315:A:ILE:HD13	19	0.19
(1,1155)	1:285:A:LEU:HD23	1:315:A:ILE:HD11	19	0.19
(1,1155)	1:285:A:LEU:HD23	1:315:A:ILE:HD12	19	0.19
(1,1155)	1:285:A:LEU:HD23	1:315:A:ILE:HD13	19	0.19
(1,1154)	1:285:A:LEU:HD11	1:313:A:THR:HB	5	0.19
(1,1154)	1:285:A:LEU:HD12	1:313:A:THR:HB	5	0.19
(1,1154)	1:285:A:LEU:HD13	1:313:A:THR:HB	5	0.19
(1,1154)	1:285:A:LEU:HD21	1:313:A:THR:HB	5	0.19
(1,1154)	1:285:A:LEU:HD22	1:313:A:THR:HB	5	0.19
(1,1154)	1:285:A:LEU:HD23	1:313:A:THR:HB	5	0.19
(1,1154)	1:285:A:LEU:HD11	1:313:A:THR:HB	15	0.19
(1,1154)	1:285:A:LEU:HD12	1:313:A:THR:HB	15	0.19
(1,1154)	1:285:A:LEU:HD13	1:313:A:THR:HB	15	0.19
(1,1154)	1:285:A:LEU:HD21	1:313:A:THR:HB	15	0.19
(1,1154)	1:285:A:LEU:HD22	1:313:A:THR:HB	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1154)	1:285:A:LEU:HD23	1:313:A:THR:HB	15	0.19
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB1	19	0.19
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB2	19	0.19
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB3	19	0.19
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB1	19	0.19
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB2	19	0.19
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB3	19	0.19
(1,1124)	1:270:A:LYS:HB3	1:270:A:LYS:HD2	2	0.19
(1,1124)	1:270:A:LYS:HB3	1:270:A:LYS:HD3	2	0.19
(1,1080)	1:260:A:LEU:HD11	1:308:A:TYR:HA	19	0.19
(1,1080)	1:260:A:LEU:HD12	1:308:A:TYR:HA	19	0.19
(1,1080)	1:260:A:LEU:HD13	1:308:A:TYR:HA	19	0.19
(1,1080)	1:260:A:LEU:HD21	1:308:A:TYR:HA	19	0.19
(1,1080)	1:260:A:LEU:HD22	1:308:A:TYR:HA	19	0.19
(1,1080)	1:260:A:LEU:HD23	1:308:A:TYR:HA	19	0.19
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	4	0.19
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	4	0.19
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	4	0.19
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	5	0.19
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	5	0.19
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	5	0.19
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	9	0.19
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	9	0.19
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	9	0.19
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	20	0.19
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	20	0.19
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	20	0.19
(1,853)	1:313:A:THR:HG21	1:328:A:GLN:HA	9	0.19
(1,853)	1:313:A:THR:HG22	1:328:A:GLN:HA	9	0.19
(1,853)	1:313:A:THR:HG23	1:328:A:GLN:HA	9	0.19
(1,853)	1:313:A:THR:HG21	1:328:A:GLN:HA	17	0.19
(1,853)	1:313:A:THR:HG22	1:328:A:GLN:HA	17	0.19
(1,853)	1:313:A:THR:HG23	1:328:A:GLN:HA	17	0.19
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD11	16	0.19
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD12	16	0.19
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD13	16	0.19
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD11	16	0.19
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD12	16	0.19
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD13	16	0.19
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD11	16	0.19
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD12	16	0.19
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD13	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	1	0.19
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	4	0.19
(1,802)	1:290:A:PRO:HA	1:291:A:LYS:HB2	14	0.19
(1,802)	1:290:A:PRO:HA	1:291:A:LYS:HB3	14	0.19
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB1	8	0.19
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB2	8	0.19
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB3	8	0.19
(1,732)	1:267:A:LEU:HB2	1:302:A:PHE:HD1	7	0.19
(1,732)	1:267:A:LEU:HB3	1:302:A:PHE:HD1	7	0.19
(1,732)	1:267:A:LEU:HB2	1:302:A:PHE:HD1	12	0.19
(1,732)	1:267:A:LEU:HB3	1:302:A:PHE:HD1	12	0.19
(1,727)	1:266:A:LYS:HG3	1:267:A:LEU:H	4	0.19
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG11	6	0.19
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG12	6	0.19
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG13	6	0.19
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	18	0.19
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	4	0.19
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	4	0.19
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	4	0.19
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	5	0.19
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	5	0.19
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	5	0.19
(1,655)	1:301:A:PHE:HA	1:302:A:PHE:HE1	8	0.19
(1,644)	1:251:A:ILE:HD11	1:328:A:GLN:HA	7	0.19
(1,644)	1:251:A:ILE:HD12	1:328:A:GLN:HA	7	0.19
(1,644)	1:251:A:ILE:HD13	1:328:A:GLN:HA	7	0.19
(1,644)	1:251:A:ILE:HD11	1:328:A:GLN:HA	16	0.19
(1,644)	1:251:A:ILE:HD12	1:328:A:GLN:HA	16	0.19
(1,644)	1:251:A:ILE:HD13	1:328:A:GLN:HA	16	0.19
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD11	4	0.19
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD12	4	0.19
(1,635)	1:250:A:THR:HG21	1:251:A:ILE:HD13	4	0.19
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD11	4	0.19
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD12	4	0.19
(1,635)	1:250:A:THR:HG22	1:251:A:ILE:HD13	4	0.19
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD11	4	0.19
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD12	4	0.19
(1,635)	1:250:A:THR:HG23	1:251:A:ILE:HD13	4	0.19
(1,630)	1:251:A:ILE:HG21	1:268:A:THR:HB	12	0.19
(1,630)	1:251:A:ILE:HG22	1:268:A:THR:HB	12	0.19
(1,630)	1:251:A:ILE:HG23	1:268:A:THR:HB	12	0.19
(1,627)	1:251:A:ILE:HG21	1:267:A:LEU:HG	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,627)	1:251:A:ILE:HG22	1:267:A:LEU:HG	14	0.19
(1,627)	1:251:A:ILE:HG23	1:267:A:LEU:HG	14	0.19
(1,627)	1:251:A:ILE:HG21	1:267:A:LEU:HG	18	0.19
(1,627)	1:251:A:ILE:HG22	1:267:A:LEU:HG	18	0.19
(1,627)	1:251:A:ILE:HG23	1:267:A:LEU:HG	18	0.19
(1,608)	1:250:A:THR:HA	1:251:A:ILE:HG13	15	0.19
(1,575)	1:243:A:VAL:HG11	1:244:A:GLN:HG3	14	0.19
(1,575)	1:243:A:VAL:HG12	1:244:A:GLN:HG3	14	0.19
(1,575)	1:243:A:VAL:HG13	1:244:A:GLN:HG3	14	0.19
(1,575)	1:243:A:VAL:HG21	1:244:A:GLN:HG3	14	0.19
(1,575)	1:243:A:VAL:HG22	1:244:A:GLN:HG3	14	0.19
(1,575)	1:243:A:VAL:HG23	1:244:A:GLN:HG3	14	0.19
(1,541)	1:251:A:ILE:HG21	1:269:A:CYS:HB2	16	0.19
(1,541)	1:251:A:ILE:HG22	1:269:A:CYS:HB2	16	0.19
(1,541)	1:251:A:ILE:HG23	1:269:A:CYS:HB2	16	0.19
(1,535)	1:249:A:VAL:HG11	1:316:A:CYS:HB3	17	0.19
(1,535)	1:249:A:VAL:HG12	1:316:A:CYS:HB3	17	0.19
(1,535)	1:249:A:VAL:HG13	1:316:A:CYS:HB3	17	0.19
(1,532)	1:266:A:LYS:H	1:301:A:PHE:HA	20	0.19
(1,480)	1:313:A:THR:HG21	1:329:A:VAL:H	16	0.19
(1,480)	1:313:A:THR:HG22	1:329:A:VAL:H	16	0.19
(1,480)	1:313:A:THR:HG23	1:329:A:VAL:H	16	0.19
(1,480)	1:313:A:THR:HG21	1:329:A:VAL:H	17	0.19
(1,480)	1:313:A:THR:HG22	1:329:A:VAL:H	17	0.19
(1,480)	1:313:A:THR:HG23	1:329:A:VAL:H	17	0.19
(1,462)	1:316:A:CYS:HB3	1:327:A:GLY:H	6	0.19
(1,420)	1:318:A:ALA:HB1	1:320:A:ASN:H	5	0.19
(1,420)	1:318:A:ALA:HB2	1:320:A:ASN:H	5	0.19
(1,420)	1:318:A:ALA:HB3	1:320:A:ASN:H	5	0.19
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	16	0.19
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	14	0.19
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	19	0.19
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD11	17	0.19
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD12	17	0.19
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD13	17	0.19
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	9	0.19
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG11	12	0.18
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG12	12	0.18
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG13	12	0.18
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG21	12	0.18
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG22	12	0.18
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG23	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD11	10	0.18
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD12	10	0.18
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD13	10	0.18
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD11	10	0.18
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD12	10	0.18
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD13	10	0.18
(1,1208)	1:310:A:LEU:HD11	1:314:A:TYR:HE1	12	0.18
(1,1208)	1:310:A:LEU:HD12	1:314:A:TYR:HE1	12	0.18
(1,1208)	1:310:A:LEU:HD13	1:314:A:TYR:HE1	12	0.18
(1,1208)	1:310:A:LEU:HD21	1:314:A:TYR:HE1	12	0.18
(1,1208)	1:310:A:LEU:HD22	1:314:A:TYR:HE1	12	0.18
(1,1208)	1:310:A:LEU:HD23	1:314:A:TYR:HE1	12	0.18
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG21	15	0.18
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG22	15	0.18
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG23	15	0.18
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	15	0.18
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	15	0.18
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	15	0.18
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	2	0.18
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	2	0.18
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	2	0.18
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	2	0.18
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	2	0.18
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	2	0.18
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	18	0.18
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	18	0.18
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	18	0.18
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	18	0.18
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	18	0.18
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	18	0.18
(1,1192)	1:303:A:ARG:HG2	1:304:A:GLY:H	9	0.18
(1,1192)	1:303:A:ARG:HG3	1:304:A:GLY:H	9	0.18
(1,1173)	1:293:A:VAL:HG11	1:294:A:GLU:H	7	0.18
(1,1173)	1:293:A:VAL:HG12	1:294:A:GLU:H	7	0.18
(1,1173)	1:293:A:VAL:HG13	1:294:A:GLU:H	7	0.18
(1,1173)	1:293:A:VAL:HG21	1:294:A:GLU:H	7	0.18
(1,1173)	1:293:A:VAL:HG22	1:294:A:GLU:H	7	0.18
(1,1173)	1:293:A:VAL:HG23	1:294:A:GLU:H	7	0.18
(1,1154)	1:285:A:LEU:HD11	1:313:A:THR:HB	12	0.18
(1,1154)	1:285:A:LEU:HD12	1:313:A:THR:HB	12	0.18
(1,1154)	1:285:A:LEU:HD13	1:313:A:THR:HB	12	0.18
(1,1154)	1:285:A:LEU:HD21	1:313:A:THR:HB	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1154)	1:285:A:LEU:HD22	1:313:A:THR:HB	12	0.18
(1,1154)	1:285:A:LEU:HD23	1:313:A:THR:HB	12	0.18
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB2	20	0.18
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB3	20	0.18
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB2	20	0.18
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB3	20	0.18
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB2	20	0.18
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB3	20	0.18
(1,1131)	1:276:A:PRO:HD2	1:277:A:ALA:H	11	0.18
(1,1131)	1:276:A:PRO:HD3	1:277:A:ALA:H	11	0.18
(1,1130)	1:273:A:ALA:HB1	1:320:A:ASN:HB2	4	0.18
(1,1130)	1:273:A:ALA:HB1	1:320:A:ASN:HB3	4	0.18
(1,1130)	1:273:A:ALA:HB2	1:320:A:ASN:HB2	4	0.18
(1,1130)	1:273:A:ALA:HB2	1:320:A:ASN:HB3	4	0.18
(1,1130)	1:273:A:ALA:HB3	1:320:A:ASN:HB2	4	0.18
(1,1130)	1:273:A:ALA:HB3	1:320:A:ASN:HB3	4	0.18
(1,1112)	1:267:A:LEU:HD11	1:302:A:PHE:HZ	2	0.18
(1,1112)	1:267:A:LEU:HD12	1:302:A:PHE:HZ	2	0.18
(1,1112)	1:267:A:LEU:HD13	1:302:A:PHE:HZ	2	0.18
(1,1112)	1:267:A:LEU:HD21	1:302:A:PHE:HZ	2	0.18
(1,1112)	1:267:A:LEU:HD22	1:302:A:PHE:HZ	2	0.18
(1,1112)	1:267:A:LEU:HD23	1:302:A:PHE:HZ	2	0.18
(1,1100)	1:266:A:LYS:HE2	1:267:A:LEU:H	3	0.18
(1,1100)	1:266:A:LYS:HE3	1:267:A:LEU:H	3	0.18
(1,1047)	1:252:A:GLU:H	1:270:A:LYS:HD2	2	0.18
(1,1047)	1:252:A:GLU:H	1:270:A:LYS:HD3	2	0.18
(1,1010)	1:246:A:GLU:HB2	1:325:A:ARG:HD2	1	0.18
(1,1010)	1:246:A:GLU:HB2	1:325:A:ARG:HD3	1	0.18
(1,1010)	1:246:A:GLU:HB3	1:325:A:ARG:HD2	1	0.18
(1,1010)	1:246:A:GLU:HB3	1:325:A:ARG:HD3	1	0.18
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD11	15	0.18
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD12	15	0.18
(1,988)	1:244:A:GLN:HG2	1:322:A:ILE:HD13	15	0.18
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG21	20	0.18
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG22	20	0.18
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG23	20	0.18
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG21	11	0.18
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG22	11	0.18
(1,966)	1:259:A:TYR:HB3	1:333:A:ILE:HG23	11	0.18
(1,900)	1:244:A:GLN:HB3	1:322:A:ILE:HA	17	0.18
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	10	0.18
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	10	0.18
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	1	0.18
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	1	0.18
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	1	0.18
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	12	0.18
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	12	0.18
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	12	0.18
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	16	0.18
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	16	0.18
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	16	0.18
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	18	0.18
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	18	0.18
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	18	0.18
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	19	0.18
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	19	0.18
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	19	0.18
(1,853)	1:313:A:THR:HG21	1:328:A:GLN:HA	11	0.18
(1,853)	1:313:A:THR:HG22	1:328:A:GLN:HA	11	0.18
(1,853)	1:313:A:THR:HG23	1:328:A:GLN:HA	11	0.18
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	3	0.18
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	7	0.18
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	8	0.18
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB1	1	0.18
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB2	1	0.18
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB3	1	0.18
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB1	5	0.18
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB2	5	0.18
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB3	5	0.18
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB1	14	0.18
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB2	14	0.18
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB3	14	0.18
(1,765)	1:245:A:TYR:HD1	1:273:A:ALA:HB1	11	0.18
(1,765)	1:245:A:TYR:HD1	1:273:A:ALA:HB2	11	0.18
(1,765)	1:245:A:TYR:HD1	1:273:A:ALA:HB3	11	0.18
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD2	4	0.18
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD3	4	0.18
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD2	4	0.18
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD3	4	0.18
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD2	4	0.18
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD3	4	0.18
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD2	7	0.18
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD3	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD2	7	0.18
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD3	7	0.18
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD2	7	0.18
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD3	7	0.18
(1,731)	1:267:A:LEU:HB2	1:314:A:TYR:HE2	11	0.18
(1,731)	1:267:A:LEU:HB3	1:314:A:TYR:HE2	11	0.18
(1,703)	1:265:A:VAL:HG21	1:306:A:ILE:HD11	20	0.18
(1,703)	1:265:A:VAL:HG21	1:306:A:ILE:HD12	20	0.18
(1,703)	1:265:A:VAL:HG21	1:306:A:ILE:HD13	20	0.18
(1,703)	1:265:A:VAL:HG22	1:306:A:ILE:HD11	20	0.18
(1,703)	1:265:A:VAL:HG22	1:306:A:ILE:HD12	20	0.18
(1,703)	1:265:A:VAL:HG22	1:306:A:ILE:HD13	20	0.18
(1,703)	1:265:A:VAL:HG23	1:306:A:ILE:HD11	20	0.18
(1,703)	1:265:A:VAL:HG23	1:306:A:ILE:HD12	20	0.18
(1,703)	1:265:A:VAL:HG23	1:306:A:ILE:HD13	20	0.18
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	10	0.18
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	10	0.18
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	10	0.18
(1,644)	1:251:A:ILE:HD11	1:328:A:GLN:HA	9	0.18
(1,644)	1:251:A:ILE:HD12	1:328:A:GLN:HA	9	0.18
(1,644)	1:251:A:ILE:HD13	1:328:A:GLN:HA	9	0.18
(1,633)	1:251:A:ILE:HG21	1:268:A:THR:H	12	0.18
(1,633)	1:251:A:ILE:HG22	1:268:A:THR:H	12	0.18
(1,633)	1:251:A:ILE:HG23	1:268:A:THR:H	12	0.18
(1,627)	1:251:A:ILE:HG21	1:267:A:LEU:HG	17	0.18
(1,627)	1:251:A:ILE:HG22	1:267:A:LEU:HG	17	0.18
(1,627)	1:251:A:ILE:HG23	1:267:A:LEU:HG	17	0.18
(1,612)	1:250:A:THR:HB	1:270:A:LYS:HB2	19	0.18
(1,608)	1:250:A:THR:HA	1:251:A:ILE:HG13	13	0.18
(1,608)	1:250:A:THR:HA	1:251:A:ILE:HG13	14	0.18
(1,565)	1:243:A:VAL:HA	1:243:A:VAL:HB	7	0.18
(1,565)	1:243:A:VAL:HA	1:243:A:VAL:HB	11	0.18
(1,546)	1:267:A:LEU:HB2	1:300:A:LEU:HA	16	0.18
(1,546)	1:267:A:LEU:HB3	1:300:A:LEU:HA	16	0.18
(1,532)	1:266:A:LYS:H	1:301:A:PHE:HA	19	0.18
(1,511)	1:259:A:TYR:HB3	1:334:A:THR:H	3	0.18
(1,495)	1:331:A:VAL:HB	1:332:A:ASN:H	17	0.18
(1,482)	1:251:A:ILE:HD11	1:329:A:VAL:H	16	0.18
(1,482)	1:251:A:ILE:HD12	1:329:A:VAL:H	16	0.18
(1,482)	1:251:A:ILE:HD13	1:329:A:VAL:H	16	0.18
(1,420)	1:318:A:ALA:HB1	1:320:A:ASN:H	2	0.18
(1,420)	1:318:A:ALA:HB2	1:320:A:ASN:H	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,420)	1:318:A:ALA:HB3	1:320:A:ASN:H	2	0.18
(1,420)	1:318:A:ALA:HB1	1:320:A:ASN:H	15	0.18
(1,420)	1:318:A:ALA:HB2	1:320:A:ASN:H	15	0.18
(1,420)	1:318:A:ALA:HB3	1:320:A:ASN:H	15	0.18
(1,397)	1:318:A:ALA:H	1:326:A:SER:HB3	4	0.18
(1,397)	1:318:A:ALA:H	1:326:A:SER:HB3	9	0.18
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	9	0.18
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	14	0.18
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	20	0.18
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	12	0.18
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	12	0.18
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	12	0.18
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	18	0.18
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	18	0.18
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	18	0.18
(1,275)	1:267:A:LEU:HB2	1:300:A:LEU:H	10	0.18
(1,275)	1:267:A:LEU:HB3	1:300:A:LEU:H	10	0.18
(1,270)	1:296:A:GLN:HG2	1:299:A:THR:H	11	0.18
(1,270)	1:296:A:GLN:HG3	1:299:A:THR:H	11	0.18
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG2	1	0.18
(1,204)	1:279:A:GLU:H	1:279:A:GLU:HG3	1	0.18
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	8	0.18
(1,101)	1:261:A:GLN:H	1:305:A:PRO:HB2	4	0.18
(1,101)	1:261:A:GLN:H	1:305:A:PRO:HB2	5	0.18
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	2	0.18
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	5	0.18
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	18	0.18
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	19	0.18
(1,65)	1:251:A:ILE:HG21	1:254:A:PHE:H	20	0.18
(1,65)	1:251:A:ILE:HG22	1:254:A:PHE:H	20	0.18
(1,65)	1:251:A:ILE:HG23	1:254:A:PHE:H	20	0.18
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD11	6	0.18
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD12	6	0.18
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD13	6	0.18
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD11	18	0.18
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD12	18	0.18
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD13	18	0.18
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD11	19	0.18
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD12	19	0.18
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD13	19	0.18
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	20	0.18
(1,13)	1:244:A:GLN:H	1:244:A:GLN:HB2	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1250)	1:330:A:GLU:HB2	1:331:A:VAL:H	12	0.17
(1,1250)	1:330:A:GLU:HB3	1:331:A:VAL:H	12	0.17
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD11	2	0.17
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD12	2	0.17
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD13	2	0.17
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD11	2	0.17
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD12	2	0.17
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD13	2	0.17
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG2	9	0.17
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG3	9	0.17
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG2	9	0.17
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG3	9	0.17
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG2	9	0.17
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG3	9	0.17
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	3	0.17
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	3	0.17
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	3	0.17
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	3	0.17
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	3	0.17
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	3	0.17
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	11	0.17
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	11	0.17
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	11	0.17
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	11	0.17
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	11	0.17
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	11	0.17
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB2	12	0.17
(1,1198)	1:306:A:ILE:HG21	1:310:A:LEU:HB3	12	0.17
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB2	12	0.17
(1,1198)	1:306:A:ILE:HG22	1:310:A:LEU:HB3	12	0.17
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB2	12	0.17
(1,1198)	1:306:A:ILE:HG23	1:310:A:LEU:HB3	12	0.17
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	15	0.17
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	15	0.17
(1,1142)	1:280:A:TYR:H	1:281:A:HIS:HB2	12	0.17
(1,1142)	1:280:A:TYR:H	1:281:A:HIS:HB3	12	0.17
(1,1122)	1:270:A:LYS:HB2	1:270:A:LYS:HD2	17	0.17
(1,1122)	1:270:A:LYS:HB2	1:270:A:LYS:HD3	17	0.17
(1,1109)	1:267:A:LEU:HD11	1:268:A:THR:H	12	0.17
(1,1109)	1:267:A:LEU:HD12	1:268:A:THR:H	12	0.17
(1,1109)	1:267:A:LEU:HD13	1:268:A:THR:H	12	0.17
(1,1109)	1:267:A:LEU:HD21	1:268:A:THR:H	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1109)	1:267:A:LEU:HD22	1:268:A:THR:H	12	0.17
(1,1109)	1:267:A:LEU:HD23	1:268:A:THR:H	12	0.17
(1,1015)	1:246:A:GLU:HG2	1:325:A:ARG:HG2	8	0.17
(1,1015)	1:246:A:GLU:HG3	1:325:A:ARG:HG2	8	0.17
(1,1015)	1:246:A:GLU:HG2	1:325:A:ARG:HG2	19	0.17
(1,1015)	1:246:A:GLU:HG3	1:325:A:ARG:HG2	19	0.17
(1,999)	1:243:A:VAL:HG11	1:245:A:TYR:HB2	9	0.17
(1,999)	1:243:A:VAL:HG11	1:245:A:TYR:HB3	9	0.17
(1,999)	1:243:A:VAL:HG12	1:245:A:TYR:HB2	9	0.17
(1,999)	1:243:A:VAL:HG12	1:245:A:TYR:HB3	9	0.17
(1,999)	1:243:A:VAL:HG13	1:245:A:TYR:HB2	9	0.17
(1,999)	1:243:A:VAL:HG13	1:245:A:TYR:HB3	9	0.17
(1,999)	1:243:A:VAL:HG21	1:245:A:TYR:HB2	9	0.17
(1,999)	1:243:A:VAL:HG21	1:245:A:TYR:HB3	9	0.17
(1,999)	1:243:A:VAL:HG22	1:245:A:TYR:HB2	9	0.17
(1,999)	1:243:A:VAL:HG22	1:245:A:TYR:HB3	9	0.17
(1,999)	1:243:A:VAL:HG23	1:245:A:TYR:HB2	9	0.17
(1,999)	1:243:A:VAL:HG23	1:245:A:TYR:HB3	9	0.17
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG21	2	0.17
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG22	2	0.17
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG23	2	0.17
(1,967)	1:308:A:TYR:HB2	1:333:A:ILE:HG21	12	0.17
(1,967)	1:308:A:TYR:HB2	1:333:A:ILE:HG22	12	0.17
(1,967)	1:308:A:TYR:HB2	1:333:A:ILE:HG23	12	0.17
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD11	11	0.17
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD12	11	0.17
(1,912)	1:244:A:GLN:HB3	1:322:A:ILE:HD13	11	0.17
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD11	11	0.17
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD12	11	0.17
(1,912)	1:244:A:GLN:HB2	1:322:A:ILE:HD13	11	0.17
(1,853)	1:313:A:THR:HG21	1:328:A:GLN:HA	4	0.17
(1,853)	1:313:A:THR:HG22	1:328:A:GLN:HA	4	0.17
(1,853)	1:313:A:THR:HG23	1:328:A:GLN:HA	4	0.17
(1,853)	1:313:A:THR:HG21	1:328:A:GLN:HA	8	0.17
(1,853)	1:313:A:THR:HG22	1:328:A:GLN:HA	8	0.17
(1,853)	1:313:A:THR:HG23	1:328:A:GLN:HA	8	0.17
(1,853)	1:313:A:THR:HG21	1:328:A:GLN:HA	14	0.17
(1,853)	1:313:A:THR:HG22	1:328:A:GLN:HA	14	0.17
(1,853)	1:313:A:THR:HG23	1:328:A:GLN:HA	14	0.17
(1,853)	1:313:A:THR:HG21	1:328:A:GLN:HA	15	0.17
(1,853)	1:313:A:THR:HG22	1:328:A:GLN:HA	15	0.17
(1,853)	1:313:A:THR:HG23	1:328:A:GLN:HA	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD11	3	0.17
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD12	3	0.17
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD13	3	0.17
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD11	3	0.17
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD12	3	0.17
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD13	3	0.17
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD11	3	0.17
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD12	3	0.17
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD13	3	0.17
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD11	15	0.17
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD12	15	0.17
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD13	15	0.17
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD11	15	0.17
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD12	15	0.17
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD13	15	0.17
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD11	15	0.17
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD12	15	0.17
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD13	15	0.17
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	6	0.17
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	16	0.17
(1,787)	1:283:A:THR:HA	1:284:A:THR:HG21	7	0.17
(1,787)	1:283:A:THR:HA	1:284:A:THR:HG22	7	0.17
(1,787)	1:283:A:THR:HA	1:284:A:THR:HG23	7	0.17
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB1	3	0.17
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB2	3	0.17
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB3	3	0.17
(1,770)	1:274:A:ASN:HB2	1:322:A:ILE:HG13	3	0.17
(1,770)	1:274:A:ASN:HB3	1:322:A:ILE:HG13	3	0.17
(1,757)	1:245:A:TYR:HD1	1:273:A:ALA:HA	10	0.17
(1,732)	1:267:A:LEU:HB2	1:302:A:PHE:HD1	2	0.17
(1,732)	1:267:A:LEU:HB3	1:302:A:PHE:HD1	2	0.17
(1,727)	1:266:A:LYS:HG3	1:267:A:LEU:H	18	0.17
(1,717)	1:266:A:LYS:HB3	1:302:A:PHE:HE1	4	0.17
(1,717)	1:266:A:LYS:HB2	1:302:A:PHE:HE1	4	0.17
(1,695)	1:265:A:VAL:HB	1:302:A:PHE:HB3	13	0.17
(1,645)	1:251:A:ILE:HD11	1:314:A:TYR:H	3	0.17
(1,645)	1:251:A:ILE:HD12	1:314:A:TYR:H	3	0.17
(1,645)	1:251:A:ILE:HD13	1:314:A:TYR:H	3	0.17
(1,639)	1:251:A:ILE:HD11	1:314:A:TYR:HB3	16	0.17
(1,639)	1:251:A:ILE:HD12	1:314:A:TYR:HB3	16	0.17
(1,639)	1:251:A:ILE:HD13	1:314:A:TYR:HB3	16	0.17
(1,630)	1:251:A:ILE:HG21	1:268:A:THR:HB	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,630)	1:251:A:ILE:HG22	1:268:A:THR:HB	17	0.17
(1,630)	1:251:A:ILE:HG23	1:268:A:THR:HB	17	0.17
(1,613)	1:250:A:THR:HG21	1:252:A:GLU:HG2	5	0.17
(1,613)	1:250:A:THR:HG21	1:252:A:GLU:HG3	5	0.17
(1,613)	1:250:A:THR:HG22	1:252:A:GLU:HG2	5	0.17
(1,613)	1:250:A:THR:HG22	1:252:A:GLU:HG3	5	0.17
(1,613)	1:250:A:THR:HG23	1:252:A:GLU:HG2	5	0.17
(1,613)	1:250:A:THR:HG23	1:252:A:GLU:HG3	5	0.17
(1,608)	1:250:A:THR:HA	1:251:A:ILE:HG13	10	0.17
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB1	13	0.17
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB2	13	0.17
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB3	13	0.17
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB1	13	0.17
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB2	13	0.17
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB3	13	0.17
(1,565)	1:243:A:VAL:HA	1:243:A:VAL:HB	8	0.17
(1,565)	1:243:A:VAL:HA	1:243:A:VAL:HB	12	0.17
(1,565)	1:243:A:VAL:HA	1:243:A:VAL:HB	16	0.17
(1,513)	1:333:A:ILE:HB	1:334:A:THR:H	13	0.17
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	2	0.17
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	6	0.17
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	16	0.17
(1,289)	1:294:A:GLU:H	1:302:A:PHE:H	16	0.17
(1,96)	1:260:A:LEU:H	1:333:A:ILE:HG21	20	0.17
(1,96)	1:260:A:LEU:H	1:333:A:ILE:HG22	20	0.17
(1,96)	1:260:A:LEU:H	1:333:A:ILE:HG23	20	0.17
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD11	2	0.17
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD12	2	0.17
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD13	2	0.17
(1,21)	1:244:A:GLN:HB3	1:245:A:TYR:H	16	0.17
(1,15)	1:251:A:ILE:HD11	1:316:A:CYS:H	19	0.17
(1,15)	1:251:A:ILE:HD12	1:316:A:CYS:H	19	0.17
(1,15)	1:251:A:ILE:HD13	1:316:A:CYS:H	19	0.17
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD11	7	0.16
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD12	7	0.16
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD13	7	0.16
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD11	7	0.16
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD12	7	0.16
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD13	7	0.16
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG2	5	0.16
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG3	5	0.16
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG2	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG3	5	0.16
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG2	5	0.16
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG3	5	0.16
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG21	6	0.16
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG22	6	0.16
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG23	6	0.16
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	6	0.16
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	6	0.16
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	6	0.16
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG21	17	0.16
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG22	17	0.16
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG23	17	0.16
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	17	0.16
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	17	0.16
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	17	0.16
(1,1173)	1:293:A:VAL:HG11	1:294:A:GLU:H	18	0.16
(1,1173)	1:293:A:VAL:HG12	1:294:A:GLU:H	18	0.16
(1,1173)	1:293:A:VAL:HG13	1:294:A:GLU:H	18	0.16
(1,1173)	1:293:A:VAL:HG21	1:294:A:GLU:H	18	0.16
(1,1173)	1:293:A:VAL:HG22	1:294:A:GLU:H	18	0.16
(1,1173)	1:293:A:VAL:HG23	1:294:A:GLU:H	18	0.16
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB1	1	0.16
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB2	1	0.16
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB3	1	0.16
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB1	1	0.16
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB2	1	0.16
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB3	1	0.16
(1,1109)	1:267:A:LEU:HD11	1:268:A:THR:H	3	0.16
(1,1109)	1:267:A:LEU:HD12	1:268:A:THR:H	3	0.16
(1,1109)	1:267:A:LEU:HD13	1:268:A:THR:H	3	0.16
(1,1109)	1:267:A:LEU:HD21	1:268:A:THR:H	3	0.16
(1,1109)	1:267:A:LEU:HD22	1:268:A:THR:H	3	0.16
(1,1109)	1:267:A:LEU:HD23	1:268:A:THR:H	3	0.16
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG21	15	0.16
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG22	15	0.16
(1,1073)	1:260:A:LEU:HB2	1:333:A:ILE:HG23	15	0.16
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG21	15	0.16
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG22	15	0.16
(1,1073)	1:260:A:LEU:HB3	1:333:A:ILE:HG23	15	0.16
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG11	9	0.16
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG12	9	0.16
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG13	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG21	9	0.16
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG22	9	0.16
(1,1054)	1:254:A:PHE:HB2	1:331:A:VAL:HG23	9	0.16
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG11	9	0.16
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG12	9	0.16
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG13	9	0.16
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG21	9	0.16
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG22	9	0.16
(1,1054)	1:254:A:PHE:HB3	1:331:A:VAL:HG23	9	0.16
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD11	3	0.16
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD12	3	0.16
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD13	3	0.16
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD21	3	0.16
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD22	3	0.16
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD23	3	0.16
(1,1003)	1:244:A:GLN:HG2	1:274:A:ASN:HB3	11	0.16
(1,1003)	1:244:A:GLN:HG3	1:274:A:ASN:HB3	11	0.16
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG21	3	0.16
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG22	3	0.16
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG23	3	0.16
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG21	11	0.16
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG22	11	0.16
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG23	11	0.16
(1,937)	1:316:A:CYS:H	1:326:A:SER:HB3	15	0.16
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG21	14	0.16
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG22	14	0.16
(1,908)	1:244:A:GLN:HB3	1:322:A:ILE:HG23	14	0.16
(1,870)	1:285:A:LEU:HB2	1:315:A:ILE:HD11	6	0.16
(1,870)	1:285:A:LEU:HB2	1:315:A:ILE:HD12	6	0.16
(1,870)	1:285:A:LEU:HB2	1:315:A:ILE:HD13	6	0.16
(1,870)	1:285:A:LEU:HB3	1:315:A:ILE:HD11	6	0.16
(1,870)	1:285:A:LEU:HB3	1:315:A:ILE:HD12	6	0.16
(1,870)	1:285:A:LEU:HB3	1:315:A:ILE:HD13	6	0.16
(1,870)	1:285:A:LEU:HB2	1:315:A:ILE:HD11	9	0.16
(1,870)	1:285:A:LEU:HB2	1:315:A:ILE:HD12	9	0.16
(1,870)	1:285:A:LEU:HB2	1:315:A:ILE:HD13	9	0.16
(1,870)	1:285:A:LEU:HB3	1:315:A:ILE:HD11	9	0.16
(1,870)	1:285:A:LEU:HB3	1:315:A:ILE:HD12	9	0.16
(1,870)	1:285:A:LEU:HB3	1:315:A:ILE:HD13	9	0.16
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD11	4	0.16
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD12	4	0.16
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD13	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD11	4	0.16
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD12	4	0.16
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD13	4	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD11	4	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD12	4	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD13	4	0.16
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD11	5	0.16
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD12	5	0.16
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD13	5	0.16
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD11	5	0.16
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD12	5	0.16
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD13	5	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD11	5	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD12	5	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD13	5	0.16
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD11	6	0.16
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD12	6	0.16
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD13	6	0.16
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD11	6	0.16
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD12	6	0.16
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD13	6	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD11	6	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD12	6	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD13	6	0.16
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD11	9	0.16
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD12	9	0.16
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD13	9	0.16
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD11	9	0.16
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD12	9	0.16
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD13	9	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD11	9	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD12	9	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD13	9	0.16
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD11	13	0.16
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD12	13	0.16
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD13	13	0.16
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD11	13	0.16
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD12	13	0.16
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD13	13	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD11	13	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD12	13	0.16
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD13	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:285:A:LEU:HB2	1:313:A:THR:HG21	12	0.16
(1,849)	1:285:A:LEU:HB2	1:313:A:THR:HG22	12	0.16
(1,849)	1:285:A:LEU:HB2	1:313:A:THR:HG23	12	0.16
(1,849)	1:285:A:LEU:HB3	1:313:A:THR:HG21	12	0.16
(1,849)	1:285:A:LEU:HB3	1:313:A:THR:HG22	12	0.16
(1,849)	1:285:A:LEU:HB3	1:313:A:THR:HG23	12	0.16
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	17	0.16
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	18	0.16
(1,839)	1:302:A:PHE:HE1	1:306:A:ILE:HD11	15	0.16
(1,839)	1:302:A:PHE:HE1	1:306:A:ILE:HD12	15	0.16
(1,839)	1:302:A:PHE:HE1	1:306:A:ILE:HD13	15	0.16
(1,820)	1:300:A:LEU:HG	1:314:A:TYR:HE2	11	0.16
(1,816)	1:299:A:THR:HG21	1:301:A:PHE:HZ	9	0.16
(1,816)	1:299:A:THR:HG22	1:301:A:PHE:HZ	9	0.16
(1,816)	1:299:A:THR:HG23	1:301:A:PHE:HZ	9	0.16
(1,810)	1:296:A:GLN:HG2	1:299:A:THR:HB	1	0.16
(1,810)	1:296:A:GLN:HG3	1:299:A:THR:HB	1	0.16
(1,787)	1:283:A:THR:HA	1:284:A:THR:HG21	15	0.16
(1,787)	1:283:A:THR:HA	1:284:A:THR:HG22	15	0.16
(1,787)	1:283:A:THR:HA	1:284:A:THR:HG23	15	0.16
(1,778)	1:277:A:ALA:HB1	1:320:A:ASN:HA	14	0.16
(1,778)	1:277:A:ALA:HB2	1:320:A:ASN:HA	14	0.16
(1,778)	1:277:A:ALA:HB3	1:320:A:ASN:HA	14	0.16
(1,778)	1:277:A:ALA:HB1	1:320:A:ASN:HA	17	0.16
(1,778)	1:277:A:ALA:HB2	1:320:A:ASN:HA	17	0.16
(1,778)	1:277:A:ALA:HB3	1:320:A:ASN:HA	17	0.16
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB1	18	0.16
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB2	18	0.16
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB3	18	0.16
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD2	15	0.16
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD3	15	0.16
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD2	15	0.16
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD3	15	0.16
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD2	15	0.16
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD3	15	0.16
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD2	20	0.16
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD3	20	0.16
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD2	20	0.16
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD3	20	0.16
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD2	20	0.16
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD3	20	0.16
(1,732)	1:267:A:LEU:HB2	1:302:A:PHE:HD1	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,732)	1:267:A:LEU:HB3	1:302:A:PHE:HD1	5	0.16
(1,732)	1:267:A:LEU:HB2	1:302:A:PHE:HD1	18	0.16
(1,732)	1:267:A:LEU:HB3	1:302:A:PHE:HD1	18	0.16
(1,727)	1:266:A:LYS:HG3	1:267:A:LEU:H	20	0.16
(1,726)	1:266:A:LYS:HG3	1:301:A:PHE:HD1	6	0.16
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG21	15	0.16
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG22	15	0.16
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG23	15	0.16
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG21	15	0.16
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG22	15	0.16
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG23	15	0.16
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG21	18	0.16
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG22	18	0.16
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG23	18	0.16
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG21	18	0.16
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG22	18	0.16
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG23	18	0.16
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	13	0.16
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	13	0.16
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	13	0.16
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG11	13	0.16
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG12	13	0.16
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG13	13	0.16
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	16	0.16
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	16	0.16
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	16	0.16
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	4	0.16
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	4	0.16
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	4	0.16
(1,627)	1:251:A:ILE:HG21	1:267:A:LEU:HG	4	0.16
(1,627)	1:251:A:ILE:HG22	1:267:A:LEU:HG	4	0.16
(1,627)	1:251:A:ILE:HG23	1:267:A:LEU:HG	4	0.16
(1,627)	1:251:A:ILE:HG21	1:267:A:LEU:HG	20	0.16
(1,627)	1:251:A:ILE:HG22	1:267:A:LEU:HG	20	0.16
(1,627)	1:251:A:ILE:HG23	1:267:A:LEU:HG	20	0.16
(1,613)	1:250:A:THR:HG21	1:252:A:GLU:HG2	3	0.16
(1,613)	1:250:A:THR:HG21	1:252:A:GLU:HG3	3	0.16
(1,613)	1:250:A:THR:HG22	1:252:A:GLU:HG2	3	0.16
(1,613)	1:250:A:THR:HG22	1:252:A:GLU:HG3	3	0.16
(1,613)	1:250:A:THR:HG23	1:252:A:GLU:HG2	3	0.16
(1,613)	1:250:A:THR:HG23	1:252:A:GLU:HG3	3	0.16
(1,613)	1:250:A:THR:HG21	1:252:A:GLU:HG2	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,613)	1:250:A:THR:HG21	1:252:A:GLU:HG3	8	0.16
(1,613)	1:250:A:THR:HG22	1:252:A:GLU:HG2	8	0.16
(1,613)	1:250:A:THR:HG22	1:252:A:GLU:HG3	8	0.16
(1,613)	1:250:A:THR:HG23	1:252:A:GLU:HG2	8	0.16
(1,613)	1:250:A:THR:HG23	1:252:A:GLU:HG3	8	0.16
(1,612)	1:250:A:THR:HB	1:270:A:LYS:HB2	2	0.16
(1,612)	1:250:A:THR:HB	1:270:A:LYS:HB2	3	0.16
(1,612)	1:250:A:THR:HB	1:270:A:LYS:HB2	11	0.16
(1,612)	1:250:A:THR:HB	1:270:A:LYS:HB2	18	0.16
(1,608)	1:250:A:THR:HA	1:251:A:ILE:HG13	2	0.16
(1,608)	1:250:A:THR:HA	1:251:A:ILE:HG13	6	0.16
(1,608)	1:250:A:THR:HA	1:251:A:ILE:HG13	9	0.16
(1,565)	1:243:A:VAL:HA	1:243:A:VAL:HB	13	0.16
(1,565)	1:243:A:VAL:HA	1:243:A:VAL:HB	19	0.16
(1,546)	1:267:A:LEU:HB2	1:300:A:LEU:HA	4	0.16
(1,546)	1:267:A:LEU:HB3	1:300:A:LEU:HA	4	0.16
(1,544)	1:258:A:TRP:HA	1:259:A:TYR:HD1	13	0.16
(1,437)	1:246:A:GLU:HB2	1:323:A:GLY:H	16	0.16
(1,437)	1:246:A:GLU:HB3	1:323:A:GLY:H	16	0.16
(1,397)	1:318:A:ALA:H	1:326:A:SER:HB3	8	0.16
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	5	0.16
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	13	0.16
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	7	0.16
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	7	0.16
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	7	0.16
(1,301)	1:299:A:THR:HG21	1:302:A:PHE:H	7	0.16
(1,301)	1:299:A:THR:HG22	1:302:A:PHE:H	7	0.16
(1,301)	1:299:A:THR:HG23	1:302:A:PHE:H	7	0.16
(1,295)	1:302:A:PHE:H	1:303:A:ARG:HA	19	0.16
(1,285)	1:295:A:ALA:HB1	1:301:A:PHE:H	11	0.16
(1,285)	1:295:A:ALA:HB2	1:301:A:PHE:H	11	0.16
(1,285)	1:295:A:ALA:HB3	1:301:A:PHE:H	11	0.16
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	7	0.16
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	13	0.16
(1,136)	1:264:A:ASP:HB2	1:266:A:LYS:H	7	0.16
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG21	11	0.16
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG22	11	0.16
(1,85)	1:259:A:TYR:H	1:333:A:ILE:HG23	11	0.16
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	3	0.16
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	9	0.16
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	15	0.16
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD11	7	0.16
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD12	7	0.16
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD13	7	0.16
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD11	13	0.16
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD12	13	0.16
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD13	13	0.16
(1,9)	1:316:A:CYS:H	1:326:A:SER:HB2	20	0.16
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG2	10	0.15
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG3	10	0.15
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG2	10	0.15
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG3	10	0.15
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG2	10	0.15
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG3	10	0.15
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG21	4	0.15
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG22	4	0.15
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG23	4	0.15
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	4	0.15
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	4	0.15
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	4	0.15
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG21	14	0.15
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG22	14	0.15
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG23	14	0.15
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	14	0.15
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	14	0.15
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	14	0.15
(1,1192)	1:303:A:ARG:HG2	1:304:A:GLY:H	17	0.15
(1,1192)	1:303:A:ARG:HG3	1:304:A:GLY:H	17	0.15
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB1	3	0.15
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB2	3	0.15
(1,1143)	1:280:A:TYR:HB2	1:318:A:ALA:HB3	3	0.15
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB1	3	0.15
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB2	3	0.15
(1,1143)	1:280:A:TYR:HB3	1:318:A:ALA:HB3	3	0.15
(1,1142)	1:280:A:TYR:H	1:281:A:HIS:HB2	1	0.15
(1,1142)	1:280:A:TYR:H	1:281:A:HIS:HB3	1	0.15
(1,1142)	1:280:A:TYR:H	1:281:A:HIS:HB2	2	0.15
(1,1142)	1:280:A:TYR:H	1:281:A:HIS:HB3	2	0.15
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB2	5	0.15
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB3	5	0.15
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB2	5	0.15
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB3	5	0.15
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB2	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB3	5	0.15
(1,1089)	1:261:A:GLN:HB3	1:305:A:PRO:HG2	2	0.15
(1,1089)	1:261:A:GLN:HB3	1:305:A:PRO:HG3	2	0.15
(1,1081)	1:260:A:LEU:HD11	1:308:A:TYR:HB2	2	0.15
(1,1081)	1:260:A:LEU:HD11	1:308:A:TYR:HB3	2	0.15
(1,1081)	1:260:A:LEU:HD12	1:308:A:TYR:HB2	2	0.15
(1,1081)	1:260:A:LEU:HD12	1:308:A:TYR:HB3	2	0.15
(1,1081)	1:260:A:LEU:HD13	1:308:A:TYR:HB2	2	0.15
(1,1081)	1:260:A:LEU:HD13	1:308:A:TYR:HB3	2	0.15
(1,1081)	1:260:A:LEU:HD21	1:308:A:TYR:HB2	2	0.15
(1,1081)	1:260:A:LEU:HD21	1:308:A:TYR:HB3	2	0.15
(1,1081)	1:260:A:LEU:HD22	1:308:A:TYR:HB2	2	0.15
(1,1081)	1:260:A:LEU:HD22	1:308:A:TYR:HB3	2	0.15
(1,1081)	1:260:A:LEU:HD23	1:308:A:TYR:HB2	2	0.15
(1,1081)	1:260:A:LEU:HD23	1:308:A:TYR:HB3	2	0.15
(1,1081)	1:260:A:LEU:HD11	1:308:A:TYR:HB2	12	0.15
(1,1081)	1:260:A:LEU:HD11	1:308:A:TYR:HB3	12	0.15
(1,1081)	1:260:A:LEU:HD12	1:308:A:TYR:HB2	12	0.15
(1,1081)	1:260:A:LEU:HD12	1:308:A:TYR:HB3	12	0.15
(1,1081)	1:260:A:LEU:HD13	1:308:A:TYR:HB2	12	0.15
(1,1081)	1:260:A:LEU:HD13	1:308:A:TYR:HB3	12	0.15
(1,1081)	1:260:A:LEU:HD21	1:308:A:TYR:HB2	12	0.15
(1,1081)	1:260:A:LEU:HD21	1:308:A:TYR:HB3	12	0.15
(1,1081)	1:260:A:LEU:HD22	1:308:A:TYR:HB2	12	0.15
(1,1081)	1:260:A:LEU:HD22	1:308:A:TYR:HB3	12	0.15
(1,1081)	1:260:A:LEU:HD23	1:308:A:TYR:HB2	12	0.15
(1,1081)	1:260:A:LEU:HD23	1:308:A:TYR:HB3	12	0.15
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG21	18	0.15
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG22	18	0.15
(1,986)	1:308:A:TYR:HA	1:333:A:ILE:HG23	18	0.15
(1,953)	1:251:A:ILE:HB	1:329:A:VAL:HB	3	0.15
(1,953)	1:251:A:ILE:HB	1:329:A:VAL:HB	16	0.15
(1,905)	1:247:A:PRO:HD2	1:322:A:ILE:HG12	9	0.15
(1,905)	1:247:A:PRO:HD3	1:322:A:ILE:HG12	9	0.15
(1,905)	1:247:A:PRO:HD2	1:322:A:ILE:HG12	18	0.15
(1,905)	1:247:A:PRO:HD3	1:322:A:ILE:HG12	18	0.15
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	3	0.15
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	3	0.15
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	3	0.15
(1,876)	1:315:A:ILE:HD11	1:328:A:GLN:HA	16	0.15
(1,876)	1:315:A:ILE:HD12	1:328:A:GLN:HA	16	0.15
(1,876)	1:315:A:ILE:HD13	1:328:A:GLN:HA	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	7	0.15
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	7	0.15
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	7	0.15
(1,853)	1:313:A:THR:HG21	1:328:A:GLN:HA	3	0.15
(1,853)	1:313:A:THR:HG22	1:328:A:GLN:HA	3	0.15
(1,853)	1:313:A:THR:HG23	1:328:A:GLN:HA	3	0.15
(1,853)	1:313:A:THR:HG21	1:328:A:GLN:HA	18	0.15
(1,853)	1:313:A:THR:HG22	1:328:A:GLN:HA	18	0.15
(1,853)	1:313:A:THR:HG23	1:328:A:GLN:HA	18	0.15
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD11	8	0.15
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD12	8	0.15
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD13	8	0.15
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD11	8	0.15
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD12	8	0.15
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD13	8	0.15
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD11	8	0.15
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD12	8	0.15
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD13	8	0.15
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD11	11	0.15
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD12	11	0.15
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD13	11	0.15
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD11	11	0.15
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD12	11	0.15
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD13	11	0.15
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD11	11	0.15
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD12	11	0.15
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD13	11	0.15
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD11	17	0.15
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD12	17	0.15
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD13	17	0.15
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD11	17	0.15
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD12	17	0.15
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD13	17	0.15
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD11	17	0.15
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD12	17	0.15
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD13	17	0.15
(1,828)	1:263:A:THR:HG21	1:305:A:PRO:HB3	13	0.15
(1,828)	1:263:A:THR:HG22	1:305:A:PRO:HB3	13	0.15
(1,828)	1:263:A:THR:HG23	1:305:A:PRO:HB3	13	0.15
(1,810)	1:296:A:GLN:HG2	1:299:A:THR:HB	10	0.15
(1,810)	1:296:A:GLN:HG3	1:299:A:THR:HB	10	0.15
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB1	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB2	7	0.15
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB3	7	0.15
(1,731)	1:267:A:LEU:HB2	1:314:A:TYR:HE2	12	0.15
(1,731)	1:267:A:LEU:HB3	1:314:A:TYR:HE2	12	0.15
(1,703)	1:265:A:VAL:HG21	1:306:A:ILE:HD11	2	0.15
(1,703)	1:265:A:VAL:HG21	1:306:A:ILE:HD12	2	0.15
(1,703)	1:265:A:VAL:HG21	1:306:A:ILE:HD13	2	0.15
(1,703)	1:265:A:VAL:HG22	1:306:A:ILE:HD11	2	0.15
(1,703)	1:265:A:VAL:HG22	1:306:A:ILE:HD12	2	0.15
(1,703)	1:265:A:VAL:HG22	1:306:A:ILE:HD13	2	0.15
(1,703)	1:265:A:VAL:HG23	1:306:A:ILE:HD11	2	0.15
(1,703)	1:265:A:VAL:HG23	1:306:A:ILE:HD12	2	0.15
(1,703)	1:265:A:VAL:HG23	1:306:A:ILE:HD13	2	0.15
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	13	0.15
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	13	0.15
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	13	0.15
(1,641)	1:251:A:ILE:HD11	1:316:A:CYS:HA	3	0.15
(1,641)	1:251:A:ILE:HD12	1:316:A:CYS:HA	3	0.15
(1,641)	1:251:A:ILE:HD13	1:316:A:CYS:HA	3	0.15
(1,641)	1:251:A:ILE:HD11	1:316:A:CYS:HA	14	0.15
(1,641)	1:251:A:ILE:HD12	1:316:A:CYS:HA	14	0.15
(1,641)	1:251:A:ILE:HD13	1:316:A:CYS:HA	14	0.15
(1,613)	1:250:A:THR:HG21	1:252:A:GLU:HG2	18	0.15
(1,613)	1:250:A:THR:HG21	1:252:A:GLU:HG3	18	0.15
(1,613)	1:250:A:THR:HG22	1:252:A:GLU:HG2	18	0.15
(1,613)	1:250:A:THR:HG22	1:252:A:GLU:HG3	18	0.15
(1,613)	1:250:A:THR:HG23	1:252:A:GLU:HG2	18	0.15
(1,613)	1:250:A:THR:HG23	1:252:A:GLU:HG3	18	0.15
(1,612)	1:250:A:THR:HB	1:270:A:LYS:HB2	6	0.15
(1,608)	1:250:A:THR:HA	1:251:A:ILE:HG13	17	0.15
(1,566)	1:243:A:VAL:HA	1:244:A:GLN:HG2	15	0.15
(1,565)	1:243:A:VAL:HA	1:243:A:VAL:HB	1	0.15
(1,541)	1:251:A:ILE:HG21	1:269:A:CYS:HB2	2	0.15
(1,541)	1:251:A:ILE:HG22	1:269:A:CYS:HB2	2	0.15
(1,541)	1:251:A:ILE:HG23	1:269:A:CYS:HB2	2	0.15
(1,532)	1:266:A:LYS:H	1:301:A:PHE:HA	14	0.15
(1,480)	1:313:A:THR:HG21	1:329:A:VAL:H	19	0.15
(1,480)	1:313:A:THR:HG22	1:329:A:VAL:H	19	0.15
(1,480)	1:313:A:THR:HG23	1:329:A:VAL:H	19	0.15
(1,382)	1:315:A:ILE:H	1:328:A:GLN:HB3	10	0.15
(1,290)	1:265:A:VAL:H	1:302:A:PHE:H	3	0.15
(1,285)	1:295:A:ALA:HB1	1:301:A:PHE:H	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,285)	1:295:A:ALA:HB2	1:301:A:PHE:H	15	0.15
(1,285)	1:295:A:ALA:HB3	1:301:A:PHE:H	15	0.15
(1,261)	1:294:A:GLU:H	1:303:A:ARG:HB2	3	0.15
(1,261)	1:294:A:GLU:H	1:303:A:ARG:HB3	3	0.15
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	5	0.15
(1,101)	1:261:A:GLN:H	1:305:A:PRO:HB2	7	0.15
(1,70)	1:257:A:ASN:H	1:258:A:TRP:HA	6	0.15
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	10	0.15
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	11	0.15
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	12	0.15
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD11	5	0.15
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD12	5	0.15
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD13	5	0.15
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	10	0.15
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	15	0.15
(1,18)	1:245:A:TYR:H	1:273:A:ALA:HA	11	0.15
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG11	18	0.14
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG12	18	0.14
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG13	18	0.14
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG21	18	0.14
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG22	18	0.14
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG23	18	0.14
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD11	16	0.14
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD12	16	0.14
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD13	16	0.14
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD11	16	0.14
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD12	16	0.14
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD13	16	0.14
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG21	3	0.14
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG22	3	0.14
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG23	3	0.14
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	3	0.14
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	3	0.14
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	3	0.14
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG21	8	0.14
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG22	8	0.14
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG23	8	0.14
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	8	0.14
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	8	0.14
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	8	0.14
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG21	11	0.14
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG22	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1204)	1:308:A:TYR:HB2	1:333:A:ILE:HG23	11	0.14
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	11	0.14
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	11	0.14
(1,1204)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	11	0.14
(1,1121)	1:270:A:LYS:HA	1:270:A:LYS:HE2	15	0.14
(1,1121)	1:270:A:LYS:HA	1:270:A:LYS:HE3	15	0.14
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	15	0.14
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	15	0.14
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	15	0.14
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	15	0.14
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	15	0.14
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	15	0.14
(1,1109)	1:267:A:LEU:HD11	1:268:A:THR:H	1	0.14
(1,1109)	1:267:A:LEU:HD12	1:268:A:THR:H	1	0.14
(1,1109)	1:267:A:LEU:HD13	1:268:A:THR:H	1	0.14
(1,1109)	1:267:A:LEU:HD21	1:268:A:THR:H	1	0.14
(1,1109)	1:267:A:LEU:HD22	1:268:A:THR:H	1	0.14
(1,1109)	1:267:A:LEU:HD23	1:268:A:THR:H	1	0.14
(1,1022)	1:248:A:GLU:HG2	1:249:A:VAL:H	10	0.14
(1,1022)	1:248:A:GLU:HG3	1:249:A:VAL:H	10	0.14
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG21	5	0.14
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG22	5	0.14
(1,969)	1:308:A:TYR:HE1	1:333:A:ILE:HG23	5	0.14
(1,876)	1:315:A:ILE:HD11	1:328:A:GLN:HA	19	0.14
(1,876)	1:315:A:ILE:HD12	1:328:A:GLN:HA	19	0.14
(1,876)	1:315:A:ILE:HD13	1:328:A:GLN:HA	19	0.14
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	17	0.14
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	17	0.14
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	17	0.14
(1,870)	1:285:A:LEU:HB2	1:315:A:ILE:HD11	12	0.14
(1,870)	1:285:A:LEU:HB2	1:315:A:ILE:HD12	12	0.14
(1,870)	1:285:A:LEU:HB2	1:315:A:ILE:HD13	12	0.14
(1,870)	1:285:A:LEU:HB3	1:315:A:ILE:HD11	12	0.14
(1,870)	1:285:A:LEU:HB3	1:315:A:ILE:HD12	12	0.14
(1,870)	1:285:A:LEU:HB3	1:315:A:ILE:HD13	12	0.14
(1,853)	1:313:A:THR:HG21	1:328:A:GLN:HA	13	0.14
(1,853)	1:313:A:THR:HG22	1:328:A:GLN:HA	13	0.14
(1,853)	1:313:A:THR:HG23	1:328:A:GLN:HA	13	0.14
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD11	7	0.14
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD12	7	0.14
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD13	7	0.14
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD11	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD12	7	0.14
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD13	7	0.14
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD11	7	0.14
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD12	7	0.14
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD13	7	0.14
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD11	12	0.14
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD12	12	0.14
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD13	12	0.14
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD11	12	0.14
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD12	12	0.14
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD13	12	0.14
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD11	12	0.14
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD12	12	0.14
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD13	12	0.14
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD11	14	0.14
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD12	14	0.14
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD13	14	0.14
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD11	14	0.14
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD12	14	0.14
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD13	14	0.14
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD11	14	0.14
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD12	14	0.14
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD13	14	0.14
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD11	20	0.14
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD12	20	0.14
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD13	20	0.14
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD11	20	0.14
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD12	20	0.14
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD13	20	0.14
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD11	20	0.14
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD12	20	0.14
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD13	20	0.14
(1,828)	1:263:A:THR:HG21	1:305:A:PRO:HB3	8	0.14
(1,828)	1:263:A:THR:HG22	1:305:A:PRO:HB3	8	0.14
(1,828)	1:263:A:THR:HG23	1:305:A:PRO:HB3	8	0.14
(1,776)	1:273:A:ALA:HB1	1:277:A:ALA:HA	2	0.14
(1,776)	1:273:A:ALA:HB2	1:277:A:ALA:HA	2	0.14
(1,776)	1:273:A:ALA:HB3	1:277:A:ALA:HA	2	0.14
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB1	6	0.14
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB2	6	0.14
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB3	6	0.14
(1,765)	1:245:A:TYR:HD1	1:273:A:ALA:HB1	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,765)	1:245:A:TYR:HD1	1:273:A:ALA:HB2	5	0.14
(1,765)	1:245:A:TYR:HD1	1:273:A:ALA:HB3	5	0.14
(1,690)	1:263:A:THR:HB	1:264:A:ASP:HB2	6	0.14
(1,683)	1:247:A:PRO:HB2	1:325:A:ARG:HB2	10	0.14
(1,655)	1:301:A:PHE:HA	1:302:A:PHE:HE1	16	0.14
(1,646)	1:259:A:TYR:HB3	1:259:A:TYR:HE1	3	0.14
(1,646)	1:259:A:TYR:HB3	1:259:A:TYR:HE1	4	0.14
(1,646)	1:259:A:TYR:HB3	1:259:A:TYR:HE1	7	0.14
(1,646)	1:259:A:TYR:HB3	1:259:A:TYR:HE1	8	0.14
(1,646)	1:259:A:TYR:HB3	1:259:A:TYR:HE1	14	0.14
(1,630)	1:251:A:ILE:HG21	1:268:A:THR:HB	9	0.14
(1,630)	1:251:A:ILE:HG22	1:268:A:THR:HB	9	0.14
(1,630)	1:251:A:ILE:HG23	1:268:A:THR:HB	9	0.14
(1,627)	1:251:A:ILE:HG21	1:267:A:LEU:HG	10	0.14
(1,627)	1:251:A:ILE:HG22	1:267:A:LEU:HG	10	0.14
(1,627)	1:251:A:ILE:HG23	1:267:A:LEU:HG	10	0.14
(1,613)	1:250:A:THR:HG21	1:252:A:GLU:HG2	17	0.14
(1,613)	1:250:A:THR:HG21	1:252:A:GLU:HG3	17	0.14
(1,613)	1:250:A:THR:HG22	1:252:A:GLU:HG2	17	0.14
(1,613)	1:250:A:THR:HG22	1:252:A:GLU:HG3	17	0.14
(1,613)	1:250:A:THR:HG23	1:252:A:GLU:HG2	17	0.14
(1,613)	1:250:A:THR:HG23	1:252:A:GLU:HG3	17	0.14
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB1	14	0.14
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB2	14	0.14
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB3	14	0.14
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB1	14	0.14
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB2	14	0.14
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB3	14	0.14
(1,565)	1:243:A:VAL:HA	1:243:A:VAL:HB	3	0.14
(1,565)	1:243:A:VAL:HA	1:243:A:VAL:HB	6	0.14
(1,542)	1:268:A:THR:HG21	1:269:A:CYS:HB2	3	0.14
(1,542)	1:268:A:THR:HG22	1:269:A:CYS:HB2	3	0.14
(1,542)	1:268:A:THR:HG23	1:269:A:CYS:HB2	3	0.14
(1,539)	1:267:A:LEU:HB2	1:269:A:CYS:HB2	13	0.14
(1,539)	1:267:A:LEU:HB3	1:269:A:CYS:HB2	13	0.14
(1,480)	1:313:A:THR:HG21	1:329:A:VAL:H	4	0.14
(1,480)	1:313:A:THR:HG22	1:329:A:VAL:H	4	0.14
(1,480)	1:313:A:THR:HG23	1:329:A:VAL:H	4	0.14
(1,420)	1:318:A:ALA:HB1	1:320:A:ASN:H	10	0.14
(1,420)	1:318:A:ALA:HB2	1:320:A:ASN:H	10	0.14
(1,420)	1:318:A:ALA:HB3	1:320:A:ASN:H	10	0.14
(1,370)	1:314:A:TYR:H	1:328:A:GLN:HB3	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	19	0.14
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	10	0.14
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	10	0.14
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	10	0.14
(1,284)	1:294:A:GLU:HG3	1:301:A:PHE:H	12	0.14
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	6	0.14
(1,158)	1:252:A:GLU:HG2	1:268:A:THR:H	4	0.14
(1,158)	1:252:A:GLU:HG3	1:268:A:THR:H	4	0.14
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG21	17	0.14
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG22	17	0.14
(1,151)	1:267:A:LEU:H	1:299:A:THR:HG23	17	0.14
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD11	12	0.14
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD12	12	0.14
(1,55)	1:251:A:ILE:H	1:251:A:ILE:HD13	12	0.14
(1,20)	1:245:A:TYR:H	1:274:A:ASN:HB3	11	0.14
(1,20)	1:245:A:TYR:H	1:274:A:ASN:HB2	11	0.14
(1,1250)	1:330:A:GLU:HB2	1:331:A:VAL:H	11	0.13
(1,1250)	1:330:A:GLU:HB3	1:331:A:VAL:H	11	0.13
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD11	8	0.13
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD12	8	0.13
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD13	8	0.13
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD11	8	0.13
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD12	8	0.13
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD13	8	0.13
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG2	18	0.13
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG3	18	0.13
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG2	18	0.13
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG3	18	0.13
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG2	18	0.13
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG3	18	0.13
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	11	0.13
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	11	0.13
(1,1122)	1:270:A:LYS:HB2	1:270:A:LYS:HD2	7	0.13
(1,1122)	1:270:A:LYS:HB2	1:270:A:LYS:HD3	7	0.13
(1,1119)	1:270:A:LYS:H	1:270:A:LYS:HD2	15	0.13
(1,1119)	1:270:A:LYS:H	1:270:A:LYS:HD3	15	0.13
(1,1081)	1:260:A:LEU:HD11	1:308:A:TYR:HB2	18	0.13
(1,1081)	1:260:A:LEU:HD11	1:308:A:TYR:HB3	18	0.13
(1,1081)	1:260:A:LEU:HD12	1:308:A:TYR:HB2	18	0.13
(1,1081)	1:260:A:LEU:HD12	1:308:A:TYR:HB3	18	0.13
(1,1081)	1:260:A:LEU:HD13	1:308:A:TYR:HB2	18	0.13
(1,1081)	1:260:A:LEU:HD13	1:308:A:TYR:HB3	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1081)	1:260:A:LEU:HD21	1:308:A:TYR:HB2	18	0.13
(1,1081)	1:260:A:LEU:HD21	1:308:A:TYR:HB3	18	0.13
(1,1081)	1:260:A:LEU:HD22	1:308:A:TYR:HB2	18	0.13
(1,1081)	1:260:A:LEU:HD22	1:308:A:TYR:HB3	18	0.13
(1,1081)	1:260:A:LEU:HD23	1:308:A:TYR:HB2	18	0.13
(1,1081)	1:260:A:LEU:HD23	1:308:A:TYR:HB3	18	0.13
(1,1076)	1:260:A:LEU:HD11	1:306:A:ILE:H	17	0.13
(1,1076)	1:260:A:LEU:HD12	1:306:A:ILE:H	17	0.13
(1,1076)	1:260:A:LEU:HD13	1:306:A:ILE:H	17	0.13
(1,1076)	1:260:A:LEU:HD21	1:306:A:ILE:H	17	0.13
(1,1076)	1:260:A:LEU:HD22	1:306:A:ILE:H	17	0.13
(1,1076)	1:260:A:LEU:HD23	1:306:A:ILE:H	17	0.13
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD11	8	0.13
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD12	8	0.13
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD13	8	0.13
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD21	8	0.13
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD22	8	0.13
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD23	8	0.13
(1,1019)	1:248:A:GLU:H	1:272:A:ASP:HB2	2	0.13
(1,1019)	1:248:A:GLU:H	1:272:A:ASP:HB3	2	0.13
(1,905)	1:247:A:PRO:HD2	1:322:A:ILE:HG12	13	0.13
(1,905)	1:247:A:PRO:HD3	1:322:A:ILE:HG12	13	0.13
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD11	20	0.13
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD12	20	0.13
(1,877)	1:313:A:THR:H	1:315:A:ILE:HD13	20	0.13
(1,876)	1:315:A:ILE:HD11	1:328:A:GLN:HA	3	0.13
(1,876)	1:315:A:ILE:HD12	1:328:A:GLN:HA	3	0.13
(1,876)	1:315:A:ILE:HD13	1:328:A:GLN:HA	3	0.13
(1,876)	1:315:A:ILE:HD11	1:328:A:GLN:HA	18	0.13
(1,876)	1:315:A:ILE:HD12	1:328:A:GLN:HA	18	0.13
(1,876)	1:315:A:ILE:HD13	1:328:A:GLN:HA	18	0.13
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD11	10	0.13
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD12	10	0.13
(1,874)	1:284:A:THR:HB	1:315:A:ILE:HD13	10	0.13
(1,865)	1:285:A:LEU:HA	1:315:A:ILE:HG21	6	0.13
(1,865)	1:285:A:LEU:HA	1:315:A:ILE:HG22	6	0.13
(1,865)	1:285:A:LEU:HA	1:315:A:ILE:HG23	6	0.13
(1,853)	1:313:A:THR:HG21	1:328:A:GLN:HA	1	0.13
(1,853)	1:313:A:THR:HG22	1:328:A:GLN:HA	1	0.13
(1,853)	1:313:A:THR:HG23	1:328:A:GLN:HA	1	0.13
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD11	2	0.13
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD12	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:313:A:THR:HG21	1:315:A:ILE:HD13	2	0.13
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD11	2	0.13
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD12	2	0.13
(1,850)	1:313:A:THR:HG22	1:315:A:ILE:HD13	2	0.13
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD11	2	0.13
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD12	2	0.13
(1,850)	1:313:A:THR:HG23	1:315:A:ILE:HD13	2	0.13
(1,849)	1:285:A:LEU:HB2	1:313:A:THR:HG21	5	0.13
(1,849)	1:285:A:LEU:HB2	1:313:A:THR:HG22	5	0.13
(1,849)	1:285:A:LEU:HB2	1:313:A:THR:HG23	5	0.13
(1,849)	1:285:A:LEU:HB3	1:313:A:THR:HG21	5	0.13
(1,849)	1:285:A:LEU:HB3	1:313:A:THR:HG22	5	0.13
(1,849)	1:285:A:LEU:HB3	1:313:A:THR:HG23	5	0.13
(1,849)	1:285:A:LEU:HB2	1:313:A:THR:HG21	11	0.13
(1,849)	1:285:A:LEU:HB2	1:313:A:THR:HG22	11	0.13
(1,849)	1:285:A:LEU:HB2	1:313:A:THR:HG23	11	0.13
(1,849)	1:285:A:LEU:HB3	1:313:A:THR:HG21	11	0.13
(1,849)	1:285:A:LEU:HB3	1:313:A:THR:HG22	11	0.13
(1,849)	1:285:A:LEU:HB3	1:313:A:THR:HG23	11	0.13
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	14	0.13
(1,828)	1:263:A:THR:HG21	1:305:A:PRO:HB3	3	0.13
(1,828)	1:263:A:THR:HG22	1:305:A:PRO:HB3	3	0.13
(1,828)	1:263:A:THR:HG23	1:305:A:PRO:HB3	3	0.13
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	16	0.13
(1,805)	1:290:A:PRO:HD3	1:314:A:TYR:HE1	3	0.13
(1,805)	1:290:A:PRO:HD2	1:314:A:TYR:HE1	3	0.13
(1,790)	1:284:A:THR:HG21	1:314:A:TYR:HD2	17	0.13
(1,790)	1:284:A:THR:HG22	1:314:A:TYR:HD2	17	0.13
(1,790)	1:284:A:THR:HG23	1:314:A:TYR:HD2	17	0.13
(1,768)	1:244:A:GLN:HB2	1:274:A:ASN:HB3	14	0.13
(1,732)	1:267:A:LEU:HB2	1:302:A:PHE:HD1	1	0.13
(1,732)	1:267:A:LEU:HB3	1:302:A:PHE:HD1	1	0.13
(1,726)	1:266:A:LYS:HG3	1:301:A:PHE:HD1	5	0.13
(1,726)	1:266:A:LYS:HG3	1:301:A:PHE:HD1	17	0.13
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG21	8	0.13
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG22	8	0.13
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG23	8	0.13
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG21	8	0.13
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG22	8	0.13
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG23	8	0.13
(1,718)	1:266:A:LYS:HB2	1:301:A:PHE:HZ	14	0.13
(1,718)	1:266:A:LYS:HB3	1:301:A:PHE:HZ	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,682)	1:262:A:ARG:HA	1:262:A:ARG:HD2	1	0.13
(1,682)	1:262:A:ARG:HA	1:262:A:ARG:HD3	1	0.13
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG21	2	0.13
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG22	2	0.13
(1,650)	1:308:A:TYR:HB3	1:333:A:ILE:HG23	2	0.13
(1,646)	1:259:A:TYR:HB3	1:259:A:TYR:HE1	1	0.13
(1,645)	1:251:A:ILE:HD11	1:314:A:TYR:H	4	0.13
(1,645)	1:251:A:ILE:HD12	1:314:A:TYR:H	4	0.13
(1,645)	1:251:A:ILE:HD13	1:314:A:TYR:H	4	0.13
(1,641)	1:251:A:ILE:HD11	1:316:A:CYS:HA	5	0.13
(1,641)	1:251:A:ILE:HD12	1:316:A:CYS:HA	5	0.13
(1,641)	1:251:A:ILE:HD13	1:316:A:CYS:HA	5	0.13
(1,637)	1:251:A:ILE:HD11	1:329:A:VAL:HB	19	0.13
(1,637)	1:251:A:ILE:HD12	1:329:A:VAL:HB	19	0.13
(1,637)	1:251:A:ILE:HD13	1:329:A:VAL:HB	19	0.13
(1,627)	1:251:A:ILE:HG21	1:267:A:LEU:HG	12	0.13
(1,627)	1:251:A:ILE:HG22	1:267:A:LEU:HG	12	0.13
(1,627)	1:251:A:ILE:HG23	1:267:A:LEU:HG	12	0.13
(1,612)	1:250:A:THR:HB	1:270:A:LYS:HB2	9	0.13
(1,599)	1:247:A:PRO:HD2	1:277:A:ALA:HB1	15	0.13
(1,599)	1:247:A:PRO:HD2	1:277:A:ALA:HB2	15	0.13
(1,599)	1:247:A:PRO:HD2	1:277:A:ALA:HB3	15	0.13
(1,599)	1:247:A:PRO:HD3	1:277:A:ALA:HB1	15	0.13
(1,599)	1:247:A:PRO:HD3	1:277:A:ALA:HB2	15	0.13
(1,599)	1:247:A:PRO:HD3	1:277:A:ALA:HB3	15	0.13
(1,594)	1:246:A:GLU:HA	1:247:A:PRO:HB2	12	0.13
(1,573)	1:244:A:GLN:HA	1:245:A:TYR:HD1	9	0.13
(1,565)	1:243:A:VAL:HA	1:243:A:VAL:HB	5	0.13
(1,565)	1:243:A:VAL:HA	1:243:A:VAL:HB	14	0.13
(1,555)	1:300:A:LEU:HB2	1:314:A:TYR:HB2	6	0.13
(1,555)	1:300:A:LEU:HB3	1:314:A:TYR:HB2	6	0.13
(1,546)	1:267:A:LEU:HB2	1:300:A:LEU:HA	13	0.13
(1,546)	1:267:A:LEU:HB3	1:300:A:LEU:HA	13	0.13
(1,541)	1:251:A:ILE:HG21	1:269:A:CYS:HB2	20	0.13
(1,541)	1:251:A:ILE:HG22	1:269:A:CYS:HB2	20	0.13
(1,541)	1:251:A:ILE:HG23	1:269:A:CYS:HB2	20	0.13
(1,532)	1:266:A:LYS:H	1:301:A:PHE:HA	10	0.13
(1,528)	1:324:A:THR:H	1:325:A:ARG:HG2	19	0.13
(1,420)	1:318:A:ALA:HB1	1:320:A:ASN:H	7	0.13
(1,420)	1:318:A:ALA:HB2	1:320:A:ASN:H	7	0.13
(1,420)	1:318:A:ALA:HB3	1:320:A:ASN:H	7	0.13
(1,403)	1:281:A:HIS:H	1:319:A:THR:H	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,334)	1:307:A:THR:H	1:307:A:THR:HB	8	0.13
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	1	0.13
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	1	0.13
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	1	0.13
(1,290)	1:265:A:VAL:H	1:302:A:PHE:H	9	0.13
(1,285)	1:295:A:ALA:HB1	1:301:A:PHE:H	12	0.13
(1,285)	1:295:A:ALA:HB2	1:301:A:PHE:H	12	0.13
(1,285)	1:295:A:ALA:HB3	1:301:A:PHE:H	12	0.13
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	11	0.13
(1,136)	1:264:A:ASP:HB2	1:266:A:LYS:H	3	0.13
(1,123)	1:265:A:VAL:H	1:266:A:LYS:HG2	14	0.13
(1,123)	1:265:A:VAL:H	1:266:A:LYS:HG2	15	0.13
(1,115)	1:263:A:THR:HG21	1:264:A:ASP:H	20	0.13
(1,115)	1:263:A:THR:HG22	1:264:A:ASP:H	20	0.13
(1,115)	1:263:A:THR:HG23	1:264:A:ASP:H	20	0.13
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD11	2	0.13
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD12	2	0.13
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD13	2	0.13
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	5	0.13
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	6	0.13
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	14	0.13
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG11	5	0.12
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG12	5	0.12
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG13	5	0.12
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG21	5	0.12
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG22	5	0.12
(1,1249)	1:330:A:GLU:H	1:331:A:VAL:HG23	5	0.12
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD11	18	0.12
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD12	18	0.12
(1,1242)	1:321:A:PRO:HB2	1:322:A:ILE:HD13	18	0.12
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD11	18	0.12
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD12	18	0.12
(1,1242)	1:321:A:PRO:HB3	1:322:A:ILE:HD13	18	0.12
(1,1195)	1:306:A:ILE:H	1:306:A:ILE:HG12	8	0.12
(1,1195)	1:306:A:ILE:H	1:306:A:ILE:HG13	8	0.12
(1,1175)	1:293:A:VAL:HG11	1:302:A:PHE:H	14	0.12
(1,1175)	1:293:A:VAL:HG12	1:302:A:PHE:H	14	0.12
(1,1175)	1:293:A:VAL:HG13	1:302:A:PHE:H	14	0.12
(1,1175)	1:293:A:VAL:HG21	1:302:A:PHE:H	14	0.12
(1,1175)	1:293:A:VAL:HG22	1:302:A:PHE:H	14	0.12
(1,1175)	1:293:A:VAL:HG23	1:302:A:PHE:H	14	0.12
(1,1173)	1:293:A:VAL:HG11	1:294:A:GLU:H	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1173)	1:293:A:VAL:HG12	1:294:A:GLU:H	20	0.12
(1,1173)	1:293:A:VAL:HG13	1:294:A:GLU:H	20	0.12
(1,1173)	1:293:A:VAL:HG21	1:294:A:GLU:H	20	0.12
(1,1173)	1:293:A:VAL:HG22	1:294:A:GLU:H	20	0.12
(1,1173)	1:293:A:VAL:HG23	1:294:A:GLU:H	20	0.12
(1,1168)	1:291:A:LYS:HA	1:291:A:LYS:HG2	14	0.12
(1,1168)	1:291:A:LYS:HA	1:291:A:LYS:HG3	14	0.12
(1,1146)	1:281:A:HIS:HB2	1:317:A:GLU:HB3	4	0.12
(1,1146)	1:281:A:HIS:HB3	1:317:A:GLU:HB3	4	0.12
(1,1144)	1:280:A:TYR:HB2	1:319:A:THR:H	10	0.12
(1,1144)	1:280:A:TYR:HB3	1:319:A:THR:H	10	0.12
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB2	19	0.12
(1,1134)	1:277:A:ALA:HB1	1:320:A:ASN:HB3	19	0.12
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB2	19	0.12
(1,1134)	1:277:A:ALA:HB2	1:320:A:ASN:HB3	19	0.12
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB2	19	0.12
(1,1134)	1:277:A:ALA:HB3	1:320:A:ASN:HB3	19	0.12
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG2	20	0.12
(1,1118)	1:268:A:THR:HG21	1:270:A:LYS:HG3	20	0.12
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG2	20	0.12
(1,1118)	1:268:A:THR:HG22	1:270:A:LYS:HG3	20	0.12
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG2	20	0.12
(1,1118)	1:268:A:THR:HG23	1:270:A:LYS:HG3	20	0.12
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD11	19	0.12
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD12	19	0.12
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD13	19	0.12
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD21	19	0.12
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD22	19	0.12
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD23	19	0.12
(1,1003)	1:244:A:GLN:HG2	1:274:A:ASN:HB3	2	0.12
(1,1003)	1:244:A:GLN:HG3	1:274:A:ASN:HB3	2	0.12
(1,1001)	1:243:A:VAL:HG11	1:245:A:TYR:HE1	5	0.12
(1,1001)	1:243:A:VAL:HG12	1:245:A:TYR:HE1	5	0.12
(1,1001)	1:243:A:VAL:HG13	1:245:A:TYR:HE1	5	0.12
(1,1001)	1:243:A:VAL:HG21	1:245:A:TYR:HE1	5	0.12
(1,1001)	1:243:A:VAL:HG22	1:245:A:TYR:HE1	5	0.12
(1,1001)	1:243:A:VAL:HG23	1:245:A:TYR:HE1	5	0.12
(1,997)	1:243:A:VAL:HG11	1:244:A:GLN:HA	15	0.12
(1,997)	1:243:A:VAL:HG12	1:244:A:GLN:HA	15	0.12
(1,997)	1:243:A:VAL:HG13	1:244:A:GLN:HA	15	0.12
(1,997)	1:243:A:VAL:HG21	1:244:A:GLN:HA	15	0.12
(1,997)	1:243:A:VAL:HG22	1:244:A:GLN:HA	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,997)	1:243:A:VAL:HG23	1:244:A:GLN:HA	15	0.12
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD11	14	0.12
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD12	14	0.12
(1,979)	1:308:A:TYR:HD1	1:333:A:ILE:HD13	14	0.12
(1,905)	1:247:A:PRO:HD2	1:322:A:ILE:HG12	7	0.12
(1,905)	1:247:A:PRO:HD3	1:322:A:ILE:HG12	7	0.12
(1,870)	1:285:A:LEU:HB2	1:315:A:ILE:HD11	20	0.12
(1,870)	1:285:A:LEU:HB2	1:315:A:ILE:HD12	20	0.12
(1,870)	1:285:A:LEU:HB2	1:315:A:ILE:HD13	20	0.12
(1,870)	1:285:A:LEU:HB3	1:315:A:ILE:HD11	20	0.12
(1,870)	1:285:A:LEU:HB3	1:315:A:ILE:HD12	20	0.12
(1,870)	1:285:A:LEU:HB3	1:315:A:ILE:HD13	20	0.12
(1,853)	1:313:A:THR:HG21	1:328:A:GLN:HA	6	0.12
(1,853)	1:313:A:THR:HG22	1:328:A:GLN:HA	6	0.12
(1,853)	1:313:A:THR:HG23	1:328:A:GLN:HA	6	0.12
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	9	0.12
(1,839)	1:302:A:PHE:HE1	1:306:A:ILE:HD11	2	0.12
(1,839)	1:302:A:PHE:HE1	1:306:A:ILE:HD12	2	0.12
(1,839)	1:302:A:PHE:HE1	1:306:A:ILE:HD13	2	0.12
(1,828)	1:263:A:THR:HG21	1:305:A:PRO:HB3	11	0.12
(1,828)	1:263:A:THR:HG22	1:305:A:PRO:HB3	11	0.12
(1,828)	1:263:A:THR:HG23	1:305:A:PRO:HB3	11	0.12
(1,828)	1:263:A:THR:HG21	1:305:A:PRO:HB3	17	0.12
(1,828)	1:263:A:THR:HG22	1:305:A:PRO:HB3	17	0.12
(1,828)	1:263:A:THR:HG23	1:305:A:PRO:HB3	17	0.12
(1,827)	1:261:A:GLN:HA	1:305:A:PRO:HB2	3	0.12
(1,819)	1:300:A:LEU:HG	1:314:A:TYR:HB3	14	0.12
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB1	13	0.12
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB2	13	0.12
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB3	13	0.12
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB1	1	0.12
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB2	1	0.12
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB3	1	0.12
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB1	5	0.12
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB2	5	0.12
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB3	5	0.12
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB1	9	0.12
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB2	9	0.12
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB3	9	0.12
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD2	10	0.12
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD3	10	0.12
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD2	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD3	10	0.12
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD2	10	0.12
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD3	10	0.12
(1,732)	1:267:A:LEU:HB2	1:302:A:PHE:HD1	4	0.12
(1,732)	1:267:A:LEU:HB3	1:302:A:PHE:HD1	4	0.12
(1,731)	1:267:A:LEU:HB2	1:314:A:TYR:HE2	6	0.12
(1,731)	1:267:A:LEU:HB3	1:314:A:TYR:HE2	6	0.12
(1,727)	1:266:A:LYS:HG3	1:267:A:LEU:H	12	0.12
(1,727)	1:266:A:LYS:HG3	1:267:A:LEU:H	16	0.12
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG21	1	0.12
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG22	1	0.12
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG23	1	0.12
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG21	1	0.12
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG22	1	0.12
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG23	1	0.12
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG21	20	0.12
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG22	20	0.12
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG23	20	0.12
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG21	20	0.12
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG22	20	0.12
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG23	20	0.12
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG21	5	0.12
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG22	5	0.12
(1,714)	1:266:A:LYS:HB2	1:299:A:THR:HG23	5	0.12
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG11	10	0.12
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG12	10	0.12
(1,699)	1:259:A:TYR:HB3	1:265:A:VAL:HG13	10	0.12
(1,683)	1:247:A:PRO:HB2	1:325:A:ARG:HB2	15	0.12
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG21	2	0.12
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG22	2	0.12
(1,676)	1:262:A:ARG:HA	1:263:A:THR:HG23	2	0.12
(1,646)	1:259:A:TYR:HB3	1:259:A:TYR:HE1	10	0.12
(1,646)	1:259:A:TYR:HB3	1:259:A:TYR:HE1	12	0.12
(1,646)	1:259:A:TYR:HB3	1:259:A:TYR:HE1	15	0.12
(1,630)	1:251:A:ILE:HG21	1:268:A:THR:HB	3	0.12
(1,630)	1:251:A:ILE:HG22	1:268:A:THR:HB	3	0.12
(1,630)	1:251:A:ILE:HG23	1:268:A:THR:HB	3	0.12
(1,630)	1:251:A:ILE:HG21	1:268:A:THR:HB	4	0.12
(1,630)	1:251:A:ILE:HG22	1:268:A:THR:HB	4	0.12
(1,630)	1:251:A:ILE:HG23	1:268:A:THR:HB	4	0.12
(1,627)	1:251:A:ILE:HG21	1:267:A:LEU:HG	3	0.12
(1,627)	1:251:A:ILE:HG22	1:267:A:LEU:HG	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,627)	1:251:A:ILE:HG23	1:267:A:LEU:HG	3	0.12
(1,627)	1:251:A:ILE:HG21	1:267:A:LEU:HG	7	0.12
(1,627)	1:251:A:ILE:HG22	1:267:A:LEU:HG	7	0.12
(1,627)	1:251:A:ILE:HG23	1:267:A:LEU:HG	7	0.12
(1,609)	1:250:A:THR:HB	1:270:A:LYS:HA	6	0.12
(1,609)	1:250:A:THR:HB	1:270:A:LYS:HA	20	0.12
(1,608)	1:250:A:THR:HA	1:251:A:ILE:HG13	5	0.12
(1,594)	1:246:A:GLU:HA	1:247:A:PRO:HB2	1	0.12
(1,594)	1:246:A:GLU:HA	1:247:A:PRO:HB2	8	0.12
(1,594)	1:246:A:GLU:HA	1:247:A:PRO:HB2	9	0.12
(1,594)	1:246:A:GLU:HA	1:247:A:PRO:HB2	11	0.12
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB1	16	0.12
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB2	16	0.12
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB3	16	0.12
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB1	16	0.12
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB2	16	0.12
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB3	16	0.12
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB1	20	0.12
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB2	20	0.12
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB3	20	0.12
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB1	20	0.12
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB2	20	0.12
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB3	20	0.12
(1,565)	1:243:A:VAL:HA	1:243:A:VAL:HB	9	0.12
(1,565)	1:243:A:VAL:HA	1:243:A:VAL:HB	20	0.12
(1,546)	1:267:A:LEU:HB2	1:300:A:LEU:HA	8	0.12
(1,546)	1:267:A:LEU:HB3	1:300:A:LEU:HA	8	0.12
(1,539)	1:267:A:LEU:HB2	1:269:A:CYS:HB2	3	0.12
(1,539)	1:267:A:LEU:HB3	1:269:A:CYS:HB2	3	0.12
(1,513)	1:333:A:ILE:HB	1:334:A:THR:H	10	0.12
(1,403)	1:281:A:HIS:H	1:319:A:THR:H	18	0.12
(1,397)	1:318:A:ALA:H	1:326:A:SER:HB3	13	0.12
(1,259)	1:294:A:GLU:H	1:294:A:GLU:HG3	8	0.12
(1,259)	1:294:A:GLU:H	1:294:A:GLU:HG2	8	0.12
(1,259)	1:294:A:GLU:H	1:294:A:GLU:HG3	15	0.12
(1,259)	1:294:A:GLU:H	1:294:A:GLU:HG2	15	0.12
(1,242)	1:286:A:ASN:HA	1:288:A:SER:H	9	0.12
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	16	0.12
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	17	0.12
(1,157)	1:268:A:THR:H	1:269:A:CYS:HB2	13	0.12
(1,136)	1:264:A:ASP:HB2	1:266:A:LYS:H	1	0.12
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG21	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG22	5	0.12
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG23	5	0.12
(1,15)	1:251:A:ILE:HD11	1:316:A:CYS:H	3	0.12
(1,15)	1:251:A:ILE:HD12	1:316:A:CYS:H	3	0.12
(1,15)	1:251:A:ILE:HD13	1:316:A:CYS:H	3	0.12
(1,1250)	1:330:A:GLU:HB2	1:331:A:VAL:H	10	0.11
(1,1250)	1:330:A:GLU:HB3	1:331:A:VAL:H	10	0.11
(1,1243)	1:325:A:ARG:H	1:325:A:ARG:HD2	6	0.11
(1,1243)	1:325:A:ARG:H	1:325:A:ARG:HD3	6	0.11
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG2	12	0.11
(1,1226)	1:315:A:ILE:HG21	1:328:A:GLN:HG3	12	0.11
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG2	12	0.11
(1,1226)	1:315:A:ILE:HG22	1:328:A:GLN:HG3	12	0.11
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG2	12	0.11
(1,1226)	1:315:A:ILE:HG23	1:328:A:GLN:HG3	12	0.11
(1,1208)	1:310:A:LEU:HD11	1:314:A:TYR:HE1	16	0.11
(1,1208)	1:310:A:LEU:HD12	1:314:A:TYR:HE1	16	0.11
(1,1208)	1:310:A:LEU:HD13	1:314:A:TYR:HE1	16	0.11
(1,1208)	1:310:A:LEU:HD21	1:314:A:TYR:HE1	16	0.11
(1,1208)	1:310:A:LEU:HD22	1:314:A:TYR:HE1	16	0.11
(1,1208)	1:310:A:LEU:HD23	1:314:A:TYR:HE1	16	0.11
(1,1195)	1:306:A:ILE:H	1:306:A:ILE:HG12	10	0.11
(1,1195)	1:306:A:ILE:H	1:306:A:ILE:HG13	10	0.11
(1,1195)	1:306:A:ILE:H	1:306:A:ILE:HG12	14	0.11
(1,1195)	1:306:A:ILE:H	1:306:A:ILE:HG13	14	0.11
(1,1195)	1:306:A:ILE:H	1:306:A:ILE:HG12	19	0.11
(1,1195)	1:306:A:ILE:H	1:306:A:ILE:HG13	19	0.11
(1,1195)	1:306:A:ILE:H	1:306:A:ILE:HG12	20	0.11
(1,1195)	1:306:A:ILE:H	1:306:A:ILE:HG13	20	0.11
(1,1192)	1:303:A:ARG:HG2	1:304:A:GLY:H	7	0.11
(1,1192)	1:303:A:ARG:HG3	1:304:A:GLY:H	7	0.11
(1,1173)	1:293:A:VAL:HG11	1:294:A:GLU:H	4	0.11
(1,1173)	1:293:A:VAL:HG12	1:294:A:GLU:H	4	0.11
(1,1173)	1:293:A:VAL:HG13	1:294:A:GLU:H	4	0.11
(1,1173)	1:293:A:VAL:HG21	1:294:A:GLU:H	4	0.11
(1,1173)	1:293:A:VAL:HG22	1:294:A:GLU:H	4	0.11
(1,1173)	1:293:A:VAL:HG23	1:294:A:GLU:H	4	0.11
(1,1146)	1:281:A:HIS:HB2	1:317:A:GLU:HB3	12	0.11
(1,1146)	1:281:A:HIS:HB3	1:317:A:GLU:HB3	12	0.11
(1,1133)	1:277:A:ALA:HA	1:320:A:ASN:HB2	10	0.11
(1,1133)	1:277:A:ALA:HA	1:320:A:ASN:HB3	10	0.11
(1,1133)	1:277:A:ALA:HA	1:320:A:ASN:HB2	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1133)	1:277:A:ALA:HA	1:320:A:ASN:HB3	14	0.11
(1,1119)	1:270:A:LYS:H	1:270:A:LYS:HD2	16	0.11
(1,1119)	1:270:A:LYS:H	1:270:A:LYS:HD3	16	0.11
(1,1109)	1:267:A:LEU:HD11	1:268:A:THR:H	13	0.11
(1,1109)	1:267:A:LEU:HD12	1:268:A:THR:H	13	0.11
(1,1109)	1:267:A:LEU:HD13	1:268:A:THR:H	13	0.11
(1,1109)	1:267:A:LEU:HD21	1:268:A:THR:H	13	0.11
(1,1109)	1:267:A:LEU:HD22	1:268:A:THR:H	13	0.11
(1,1109)	1:267:A:LEU:HD23	1:268:A:THR:H	13	0.11
(1,1104)	1:266:A:LYS:HE2	1:301:A:PHE:HE1	4	0.11
(1,1104)	1:266:A:LYS:HE3	1:301:A:PHE:HE1	4	0.11
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG21	14	0.11
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG22	14	0.11
(1,1101)	1:266:A:LYS:HE2	1:299:A:THR:HG23	14	0.11
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG21	14	0.11
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG22	14	0.11
(1,1101)	1:266:A:LYS:HE3	1:299:A:THR:HG23	14	0.11
(1,1095)	1:262:A:ARG:HG2	1:264:A:ASP:HB3	7	0.11
(1,1095)	1:262:A:ARG:HG3	1:264:A:ASP:HB3	7	0.11
(1,1082)	1:260:A:LEU:HD11	1:308:A:TYR:HD1	9	0.11
(1,1082)	1:260:A:LEU:HD12	1:308:A:TYR:HD1	9	0.11
(1,1082)	1:260:A:LEU:HD13	1:308:A:TYR:HD1	9	0.11
(1,1082)	1:260:A:LEU:HD21	1:308:A:TYR:HD1	9	0.11
(1,1082)	1:260:A:LEU:HD22	1:308:A:TYR:HD1	9	0.11
(1,1082)	1:260:A:LEU:HD23	1:308:A:TYR:HD1	9	0.11
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD11	18	0.11
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD12	18	0.11
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD13	18	0.11
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD21	18	0.11
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD22	18	0.11
(1,1046)	1:252:A:GLU:H	1:267:A:LEU:HD23	18	0.11
(1,993)	1:243:A:VAL:H	1:244:A:GLN:HG2	18	0.11
(1,993)	1:243:A:VAL:H	1:244:A:GLN:HG3	18	0.11
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG21	17	0.11
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG22	17	0.11
(1,971)	1:308:A:TYR:HD1	1:333:A:ILE:HG23	17	0.11
(1,871)	1:315:A:ILE:HD11	1:328:A:GLN:HB3	7	0.11
(1,871)	1:315:A:ILE:HD12	1:328:A:GLN:HB3	7	0.11
(1,871)	1:315:A:ILE:HD13	1:328:A:GLN:HB3	7	0.11
(1,871)	1:315:A:ILE:HD11	1:328:A:GLN:HB3	14	0.11
(1,871)	1:315:A:ILE:HD12	1:328:A:GLN:HB3	14	0.11
(1,871)	1:315:A:ILE:HD13	1:328:A:GLN:HB3	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,854)	1:313:A:THR:HG21	1:314:A:TYR:HB2	10	0.11
(1,854)	1:313:A:THR:HG22	1:314:A:TYR:HB2	10	0.11
(1,854)	1:313:A:THR:HG23	1:314:A:TYR:HB2	10	0.11
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	5	0.11
(1,841)	1:306:A:ILE:H	1:307:A:THR:HA	17	0.11
(1,839)	1:302:A:PHE:HE1	1:306:A:ILE:HD11	4	0.11
(1,839)	1:302:A:PHE:HE1	1:306:A:ILE:HD12	4	0.11
(1,839)	1:302:A:PHE:HE1	1:306:A:ILE:HD13	4	0.11
(1,828)	1:263:A:THR:HG21	1:305:A:PRO:HB3	4	0.11
(1,828)	1:263:A:THR:HG22	1:305:A:PRO:HB3	4	0.11
(1,828)	1:263:A:THR:HG23	1:305:A:PRO:HB3	4	0.11
(1,828)	1:263:A:THR:HG21	1:305:A:PRO:HB3	19	0.11
(1,828)	1:263:A:THR:HG22	1:305:A:PRO:HB3	19	0.11
(1,828)	1:263:A:THR:HG23	1:305:A:PRO:HB3	19	0.11
(1,827)	1:261:A:GLN:HA	1:305:A:PRO:HB2	12	0.11
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB1	16	0.11
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB2	16	0.11
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB3	16	0.11
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB1	18	0.11
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB2	18	0.11
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB3	18	0.11
(1,770)	1:274:A:ASN:HB2	1:322:A:ILE:HG13	7	0.11
(1,770)	1:274:A:ASN:HB3	1:322:A:ILE:HG13	7	0.11
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB1	11	0.11
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB2	11	0.11
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB3	11	0.11
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB1	20	0.11
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB2	20	0.11
(1,766)	1:272:A:ASP:H	1:273:A:ALA:HB3	20	0.11
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD2	17	0.11
(1,763)	1:273:A:ALA:HB1	1:321:A:PRO:HD3	17	0.11
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD2	17	0.11
(1,763)	1:273:A:ALA:HB2	1:321:A:PRO:HD3	17	0.11
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD2	17	0.11
(1,763)	1:273:A:ALA:HB3	1:321:A:PRO:HD3	17	0.11
(1,718)	1:266:A:LYS:HB2	1:301:A:PHE:HZ	4	0.11
(1,718)	1:266:A:LYS:HB3	1:301:A:PHE:HZ	4	0.11
(1,682)	1:262:A:ARG:HA	1:262:A:ARG:HD2	6	0.11
(1,682)	1:262:A:ARG:HA	1:262:A:ARG:HD3	6	0.11
(1,655)	1:301:A:PHE:HA	1:302:A:PHE:HE1	18	0.11
(1,645)	1:251:A:ILE:HD11	1:314:A:TYR:H	7	0.11
(1,645)	1:251:A:ILE:HD12	1:314:A:TYR:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,645)	1:251:A:ILE:HD13	1:314:A:TYR:H	7	0.11
(1,613)	1:250:A:THR:HG21	1:252:A:GLU:HG2	1	0.11
(1,613)	1:250:A:THR:HG21	1:252:A:GLU:HG3	1	0.11
(1,613)	1:250:A:THR:HG22	1:252:A:GLU:HG2	1	0.11
(1,613)	1:250:A:THR:HG22	1:252:A:GLU:HG3	1	0.11
(1,613)	1:250:A:THR:HG23	1:252:A:GLU:HG2	1	0.11
(1,613)	1:250:A:THR:HG23	1:252:A:GLU:HG3	1	0.11
(1,612)	1:250:A:THR:HB	1:270:A:LYS:HB2	4	0.11
(1,612)	1:250:A:THR:HB	1:270:A:LYS:HB2	8	0.11
(1,608)	1:250:A:THR:HA	1:251:A:ILE:HG13	4	0.11
(1,608)	1:250:A:THR:HA	1:251:A:ILE:HG13	7	0.11
(1,594)	1:246:A:GLU:HA	1:247:A:PRO:HB2	2	0.11
(1,594)	1:246:A:GLU:HA	1:247:A:PRO:HB2	4	0.11
(1,594)	1:246:A:GLU:HA	1:247:A:PRO:HB2	10	0.11
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB1	4	0.11
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB2	4	0.11
(1,582)	1:246:A:GLU:HB2	1:273:A:ALA:HB3	4	0.11
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB1	4	0.11
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB2	4	0.11
(1,582)	1:246:A:GLU:HB3	1:273:A:ALA:HB3	4	0.11
(1,565)	1:243:A:VAL:HA	1:243:A:VAL:HB	4	0.11
(1,555)	1:300:A:LEU:HB2	1:314:A:TYR:HB2	10	0.11
(1,555)	1:300:A:LEU:HB3	1:314:A:TYR:HB2	10	0.11
(1,551)	1:268:A:THR:HA	1:300:A:LEU:HA	12	0.11
(1,546)	1:267:A:LEU:HB2	1:300:A:LEU:HA	7	0.11
(1,546)	1:267:A:LEU:HB3	1:300:A:LEU:HA	7	0.11
(1,542)	1:268:A:THR:HG21	1:269:A:CYS:HB2	13	0.11
(1,542)	1:268:A:THR:HG22	1:269:A:CYS:HB2	13	0.11
(1,542)	1:268:A:THR:HG23	1:269:A:CYS:HB2	13	0.11
(1,530)	1:269:A:CYS:H	1:299:A:THR:H	11	0.11
(1,447)	1:325:A:ARG:H	1:325:A:ARG:HG2	13	0.11
(1,441)	1:246:A:GLU:HB2	1:324:A:THR:H	7	0.11
(1,441)	1:246:A:GLU:HB3	1:324:A:THR:H	7	0.11
(1,437)	1:246:A:GLU:HB2	1:323:A:GLY:H	14	0.11
(1,437)	1:246:A:GLU:HB3	1:323:A:GLY:H	14	0.11
(1,405)	1:280:A:TYR:HA	1:319:A:THR:H	16	0.11
(1,403)	1:281:A:HIS:H	1:319:A:THR:H	2	0.11
(1,403)	1:281:A:HIS:H	1:319:A:THR:H	4	0.11
(1,402)	1:319:A:THR:H	1:320:A:ASN:H	8	0.11
(1,343)	1:310:A:LEU:H	1:310:A:LEU:HB3	14	0.11
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD11	17	0.11
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD12	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:306:A:ILE:H	1:306:A:ILE:HD13	17	0.11
(1,301)	1:299:A:THR:HG21	1:302:A:PHE:H	1	0.11
(1,301)	1:299:A:THR:HG22	1:302:A:PHE:H	1	0.11
(1,301)	1:299:A:THR:HG23	1:302:A:PHE:H	1	0.11
(1,301)	1:299:A:THR:HG21	1:302:A:PHE:H	3	0.11
(1,301)	1:299:A:THR:HG22	1:302:A:PHE:H	3	0.11
(1,301)	1:299:A:THR:HG23	1:302:A:PHE:H	3	0.11
(1,270)	1:296:A:GLN:HG2	1:299:A:THR:H	13	0.11
(1,270)	1:296:A:GLN:HG3	1:299:A:THR:H	13	0.11
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	2	0.11
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	9	0.11
(1,157)	1:268:A:THR:H	1:269:A:CYS:HB2	1	0.11
(1,123)	1:265:A:VAL:H	1:266:A:LYS:HG2	19	0.11
(1,115)	1:263:A:THR:HG21	1:264:A:ASP:H	3	0.11
(1,115)	1:263:A:THR:HG22	1:264:A:ASP:H	3	0.11
(1,115)	1:263:A:THR:HG23	1:264:A:ASP:H	3	0.11
(1,115)	1:263:A:THR:HG21	1:264:A:ASP:H	8	0.11
(1,115)	1:263:A:THR:HG22	1:264:A:ASP:H	8	0.11
(1,115)	1:263:A:THR:HG23	1:264:A:ASP:H	8	0.11
(1,115)	1:263:A:THR:HG21	1:264:A:ASP:H	16	0.11
(1,115)	1:263:A:THR:HG22	1:264:A:ASP:H	16	0.11
(1,115)	1:263:A:THR:HG23	1:264:A:ASP:H	16	0.11
(1,101)	1:261:A:GLN:H	1:305:A:PRO:HB2	1	0.11
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD11	5	0.11
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD12	5	0.11
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD13	5	0.11
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD11	13	0.11
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD12	13	0.11
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD13	13	0.11
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD11	16	0.11
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD12	16	0.11
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD13	16	0.11
(1,77)	1:258:A:TRP:H	1:333:A:ILE:HD11	20	0.11
(1,77)	1:258:A:TRP:H	1:333:A:ILE:HD12	20	0.11
(1,77)	1:258:A:TRP:H	1:333:A:ILE:HD13	20	0.11
(1,72)	1:258:A:TRP:H	1:334:A:THR:H	10	0.11
(1,69)	1:257:A:ASN:H	1:258:A:TRP:H	16	0.11
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	3	0.11
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	4	0.11
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	18	0.11
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG21	8	0.11
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG22	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG23	8	0.11
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG21	15	0.11
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG22	15	0.11
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG23	15	0.11
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG21	18	0.11
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG22	18	0.11
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG23	18	0.11
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG21	20	0.11
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG22	20	0.11
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG23	20	0.11
(1,32)	1:248:A:GLU:H	1:271:A:ALA:HA	11	0.11
(1,1195)	1:306:A:ILE:H	1:306:A:ILE:HG12	6	0.1
(1,1195)	1:306:A:ILE:H	1:306:A:ILE:HG13	6	0.1
(1,1133)	1:277:A:ALA:HA	1:320:A:ASN:HB2	17	0.1
(1,1133)	1:277:A:ALA:HA	1:320:A:ASN:HB3	17	0.1
(1,1119)	1:270:A:LYS:H	1:270:A:LYS:HD2	14	0.1
(1,1119)	1:270:A:LYS:H	1:270:A:LYS:HD3	14	0.1
(1,1031)	1:249:A:VAL:HG11	1:325:A:ARG:H	12	0.1
(1,1031)	1:249:A:VAL:HG12	1:325:A:ARG:H	12	0.1
(1,1031)	1:249:A:VAL:HG13	1:325:A:ARG:H	12	0.1
(1,1031)	1:249:A:VAL:HG21	1:325:A:ARG:H	12	0.1
(1,1031)	1:249:A:VAL:HG22	1:325:A:ARG:H	12	0.1
(1,1031)	1:249:A:VAL:HG23	1:325:A:ARG:H	12	0.1
(1,997)	1:243:A:VAL:HG11	1:244:A:GLN:HA	5	0.1
(1,997)	1:243:A:VAL:HG12	1:244:A:GLN:HA	5	0.1
(1,997)	1:243:A:VAL:HG13	1:244:A:GLN:HA	5	0.1
(1,997)	1:243:A:VAL:HG21	1:244:A:GLN:HA	5	0.1
(1,997)	1:243:A:VAL:HG22	1:244:A:GLN:HA	5	0.1
(1,997)	1:243:A:VAL:HG23	1:244:A:GLN:HA	5	0.1
(1,900)	1:244:A:GLN:HB3	1:322:A:ILE:HA	6	0.1
(1,876)	1:315:A:ILE:HD11	1:328:A:GLN:HA	15	0.1
(1,876)	1:315:A:ILE:HD12	1:328:A:GLN:HA	15	0.1
(1,876)	1:315:A:ILE:HD13	1:328:A:GLN:HA	15	0.1
(1,865)	1:285:A:LEU:HA	1:315:A:ILE:HG21	20	0.1
(1,865)	1:285:A:LEU:HA	1:315:A:ILE:HG22	20	0.1
(1,865)	1:285:A:LEU:HA	1:315:A:ILE:HG23	20	0.1
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	11	0.1
(1,843)	1:310:A:LEU:H	1:311:A:ALA:HA	15	0.1
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB1	2	0.1
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB2	2	0.1
(1,775)	1:276:A:PRO:HA	1:277:A:ALA:HB3	2	0.1
(1,770)	1:274:A:ASN:HB2	1:322:A:ILE:HG13	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,770)	1:274:A:ASN:HB3	1:322:A:ILE:HG13	20	0.1
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG21	6	0.1
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG22	6	0.1
(1,725)	1:266:A:LYS:HG2	1:299:A:THR:HG23	6	0.1
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG21	6	0.1
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG22	6	0.1
(1,725)	1:266:A:LYS:HG3	1:299:A:THR:HG23	6	0.1
(1,682)	1:262:A:ARG:HA	1:262:A:ARG:HD2	15	0.1
(1,682)	1:262:A:ARG:HA	1:262:A:ARG:HD3	15	0.1
(1,655)	1:301:A:PHE:HA	1:302:A:PHE:HE1	7	0.1
(1,655)	1:301:A:PHE:HA	1:302:A:PHE:HE1	15	0.1
(1,639)	1:251:A:ILE:HD11	1:314:A:TYR:HB3	11	0.1
(1,639)	1:251:A:ILE:HD12	1:314:A:TYR:HB3	11	0.1
(1,639)	1:251:A:ILE:HD13	1:314:A:TYR:HB3	11	0.1
(1,632)	1:251:A:ILE:HG21	1:328:A:GLN:HA	16	0.1
(1,632)	1:251:A:ILE:HG22	1:328:A:GLN:HA	16	0.1
(1,632)	1:251:A:ILE:HG23	1:328:A:GLN:HA	16	0.1
(1,630)	1:251:A:ILE:HG21	1:268:A:THR:HB	13	0.1
(1,630)	1:251:A:ILE:HG22	1:268:A:THR:HB	13	0.1
(1,630)	1:251:A:ILE:HG23	1:268:A:THR:HB	13	0.1
(1,629)	1:251:A:ILE:HG21	1:314:A:TYR:HB3	6	0.1
(1,629)	1:251:A:ILE:HG22	1:314:A:TYR:HB3	6	0.1
(1,629)	1:251:A:ILE:HG23	1:314:A:TYR:HB3	6	0.1
(1,609)	1:250:A:THR:HB	1:270:A:LYS:HA	9	0.1
(1,609)	1:250:A:THR:HB	1:270:A:LYS:HA	10	0.1
(1,594)	1:246:A:GLU:HA	1:247:A:PRO:HB2	3	0.1
(1,594)	1:246:A:GLU:HA	1:247:A:PRO:HB2	20	0.1
(1,546)	1:267:A:LEU:HB2	1:300:A:LEU:HA	1	0.1
(1,546)	1:267:A:LEU:HB3	1:300:A:LEU:HA	1	0.1
(1,546)	1:267:A:LEU:HB2	1:300:A:LEU:HA	12	0.1
(1,546)	1:267:A:LEU:HB3	1:300:A:LEU:HA	12	0.1
(1,539)	1:267:A:LEU:HB2	1:269:A:CYS:HB2	9	0.1
(1,539)	1:267:A:LEU:HB3	1:269:A:CYS:HB2	9	0.1
(1,535)	1:249:A:VAL:HG11	1:316:A:CYS:HB3	1	0.1
(1,535)	1:249:A:VAL:HG12	1:316:A:CYS:HB3	1	0.1
(1,535)	1:249:A:VAL:HG13	1:316:A:CYS:HB3	1	0.1
(1,437)	1:246:A:GLU:HB2	1:323:A:GLY:H	7	0.1
(1,437)	1:246:A:GLU:HB3	1:323:A:GLY:H	7	0.1
(1,382)	1:315:A:ILE:H	1:328:A:GLN:HB3	1	0.1
(1,354)	1:311:A:ALA:H	1:333:A:ILE:HG21	14	0.1
(1,354)	1:311:A:ALA:H	1:333:A:ILE:HG22	14	0.1
(1,354)	1:311:A:ALA:H	1:333:A:ILE:HG23	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:302:A:PHE:H	1:303:A:ARG:HA	3	0.1
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	15	0.1
(1,160)	1:267:A:LEU:HG	1:268:A:THR:H	20	0.1
(1,115)	1:263:A:THR:HG21	1:264:A:ASP:H	13	0.1
(1,115)	1:263:A:THR:HG22	1:264:A:ASP:H	13	0.1
(1,115)	1:263:A:THR:HG23	1:264:A:ASP:H	13	0.1
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD11	9	0.1
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD12	9	0.1
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD13	9	0.1
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD11	14	0.1
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD12	14	0.1
(1,84)	1:259:A:TYR:H	1:333:A:ILE:HD13	14	0.1
(1,54)	1:251:A:ILE:H	1:251:A:ILE:HG13	7	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG21	1	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG22	1	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG23	1	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG21	2	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG22	2	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG23	2	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG21	10	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG22	10	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG23	10	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG21	11	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG22	11	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG23	11	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG21	12	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG22	12	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG23	12	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG21	17	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG22	17	0.1
(1,53)	1:251:A:ILE:H	1:251:A:ILE:HG23	17	0.1
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	3	0.1
(1,45)	1:250:A:THR:H	1:316:A:CYS:HB3	13	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found