



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 03:33 PM EST

PDB ID : 2LF8  
BMRB ID : 17742  
Title : Intramolecular regulation of the ETS Domain within ETV6 sequence R335 to R458  
Authors : Coyne III, H.; Green, S.M.; Graves, B.J.; McIntosh, L.P.  
Deposited on : 2011-06-28

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.40

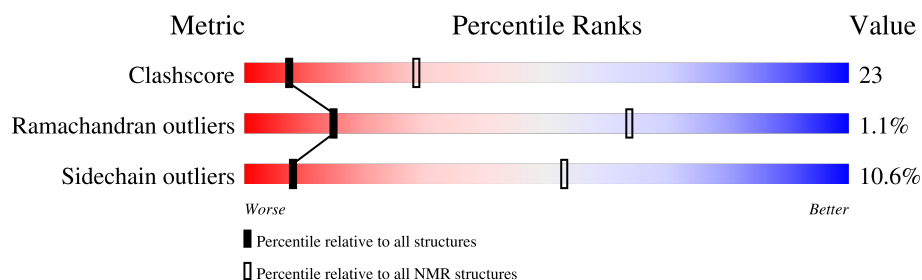
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 89%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain
1	A	128	<div> <div>42%</div> <div>34%</div> <div>•</div> <div>22%</div> </div>

## 2 Ensemble composition and analysis

This entry contains 19 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:336-A:382, A:386-A:438 (100)	0.38	3

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

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

The models can be grouped into 3 clusters and 3 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2173 atoms, of which 1076 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription factor ETV6.

Mol	Chain	Residues	Atoms						Trace
1	A	128	Total	C	H	N	O	S	0
			2173	693	1076	200	199	5	

There are 4 discrepancies between the modelled and reference sequences:

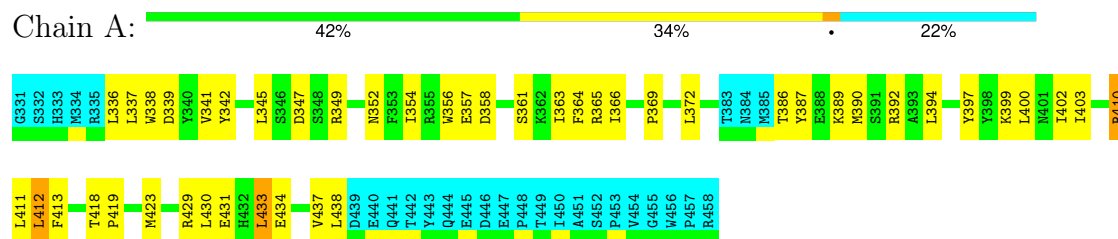
Chain	Residue	Modelled	Actual	Comment	Reference
A	331	GLY	-	expression tag	UNP P97360
A	332	SER	-	expression tag	UNP P97360
A	333	HIS	-	expression tag	UNP P97360
A	334	MET	-	expression tag	UNP P97360

## 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: Transcription factor ETV6

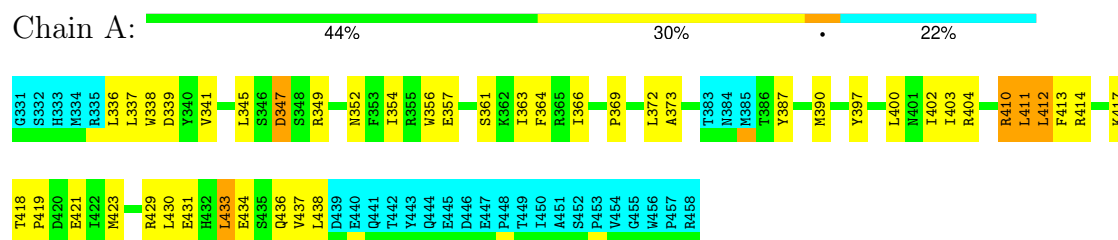


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

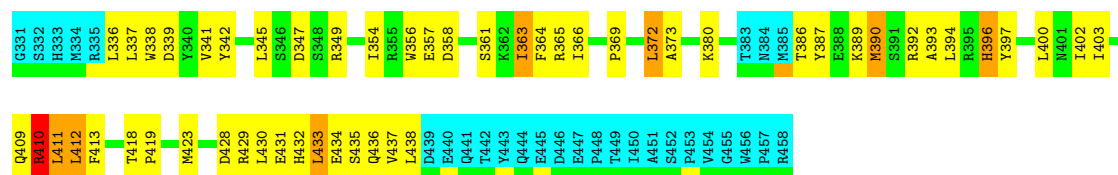
- Molecule 1: Transcription factor ETV6



#### 4.2.2 Score per residue for model 2

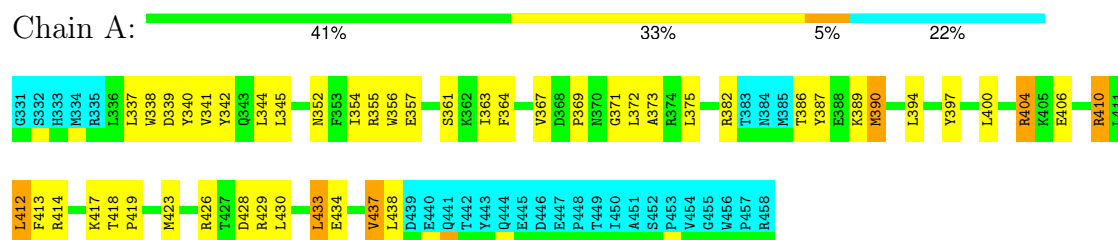
- Molecule 1: Transcription factor ETV6





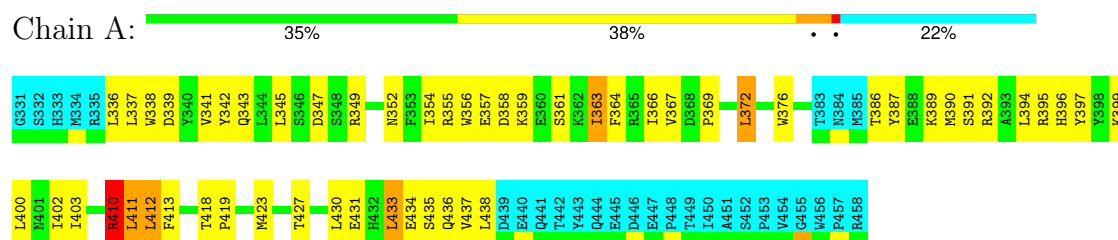
#### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Transcription factor ETV6



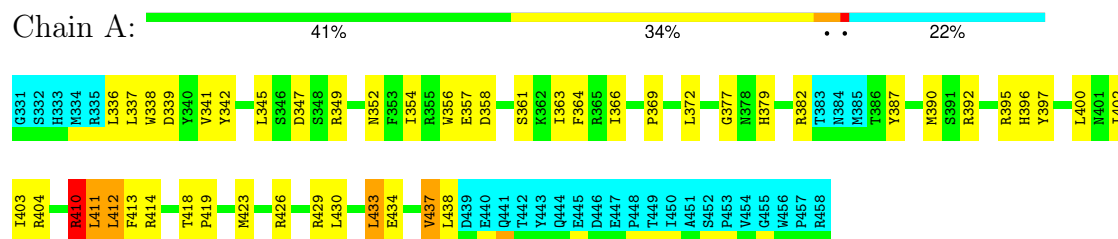
#### 4.2.4 Score per residue for model 4

- Molecule 1: Transcription factor ETV6



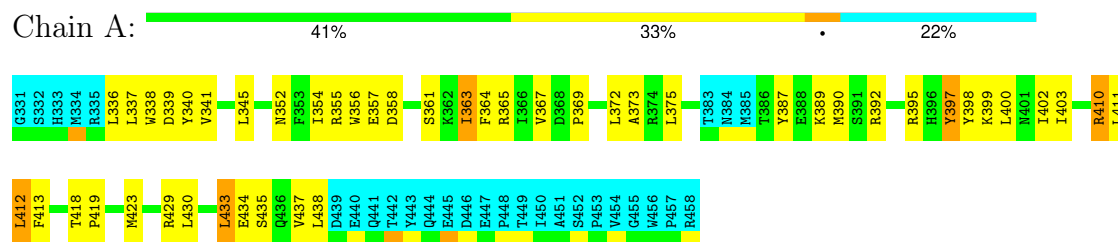
#### 4.2.5 Score per residue for model 5

- Molecule 1: Transcription factor ETV6



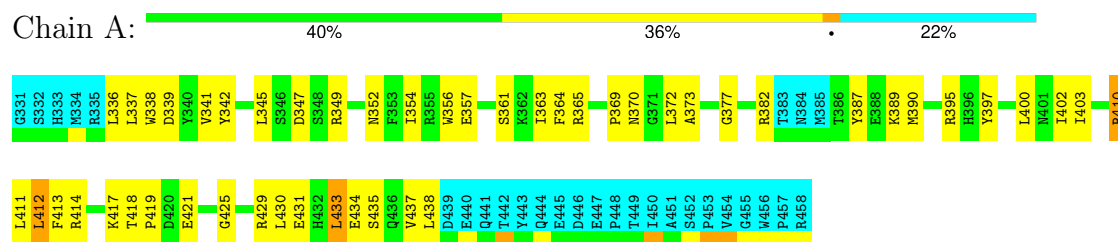
#### 4.2.6 Score per residue for model 6

- Molecule 1: Transcription factor ETV6



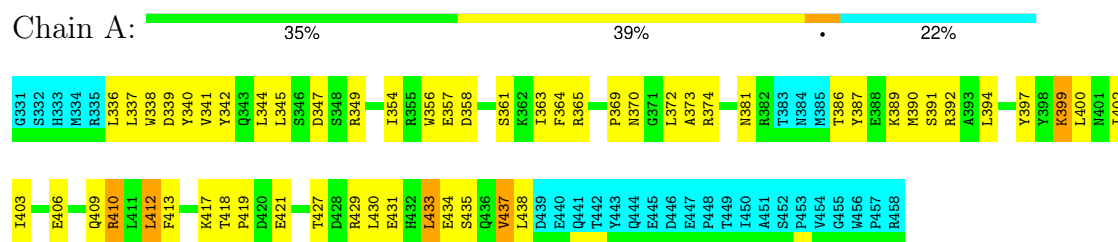
#### 4.2.7 Score per residue for model 7

- Molecule 1: Transcription factor ETV6



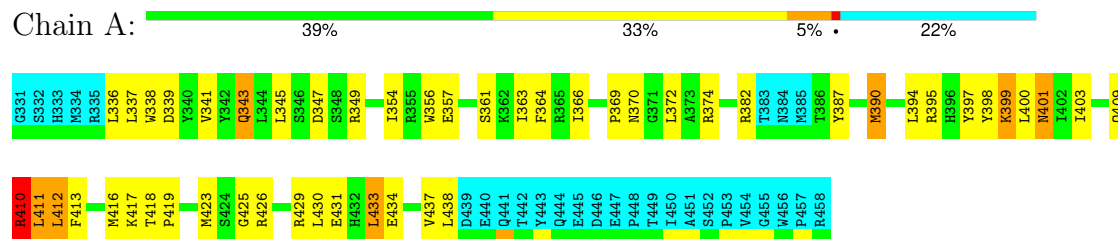
#### 4.2.8 Score per residue for model 8

- Molecule 1: Transcription factor ETV6



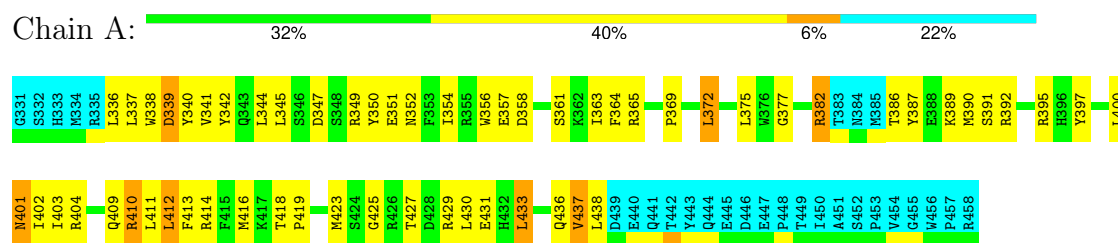
#### 4.2.9 Score per residue for model 9

- Molecule 1: Transcription factor ETV6



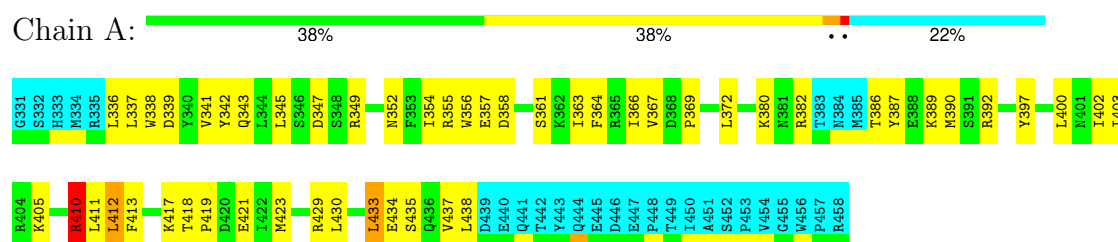
### 4.2.10 Score per residue for model 10

- Molecule 1: Transcription factor ETV6



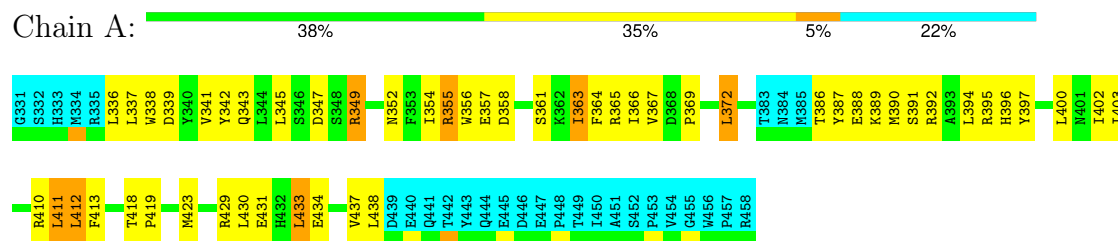
### 4.2.11 Score per residue for model 11

- Molecule 1: Transcription factor ETV6



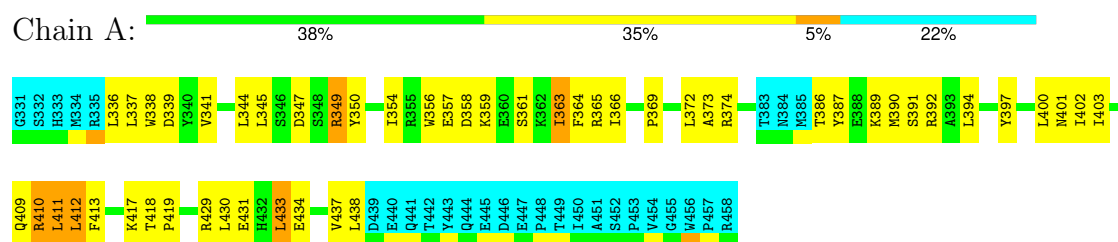
### 4.2.12 Score per residue for model 12

- Molecule 1: Transcription factor ETV6



### 4.2.13 Score per residue for model 13

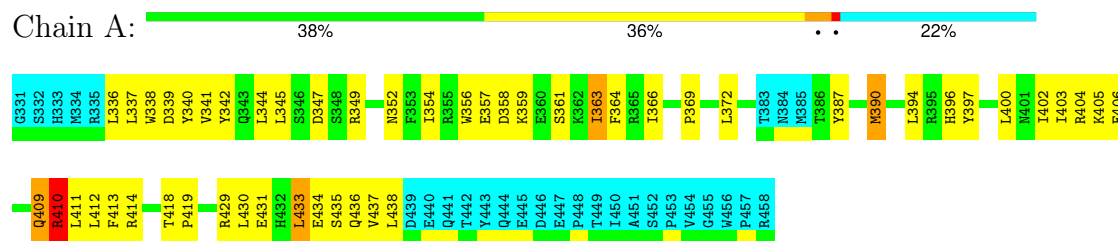
- Molecule 1: Transcription factor ETV6





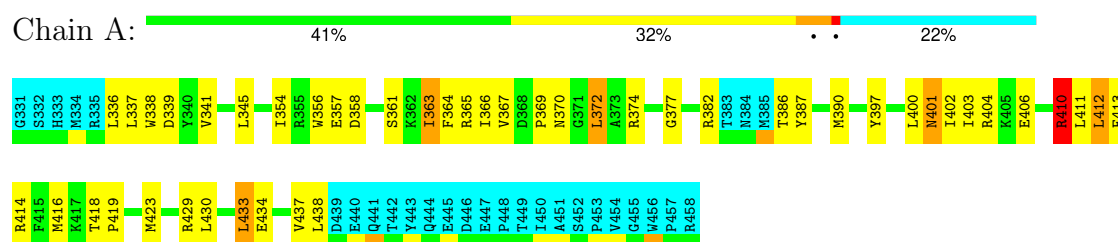
### 4.2.14 Score per residue for model 14

- Molecule 1: Transcription factor ETV6



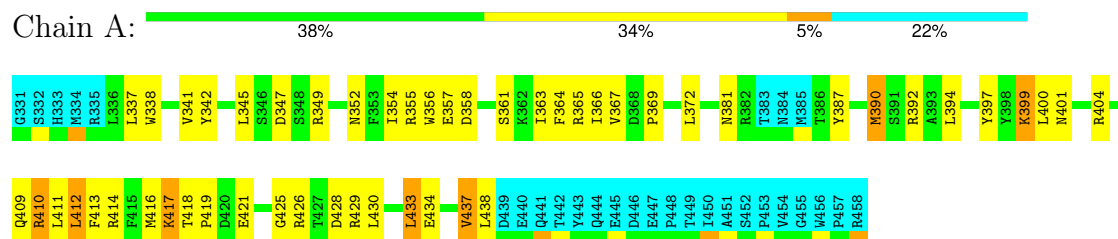
### 4.2.15 Score per residue for model 15

- Molecule 1: Transcription factor ETV6



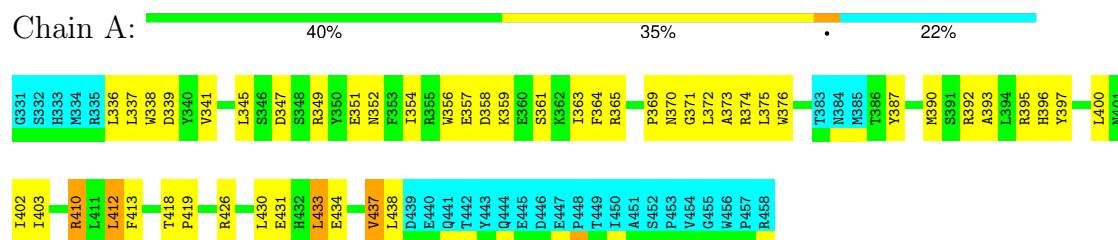
### 4.2.16 Score per residue for model 16

- Molecule 1: Transcription factor ETV6



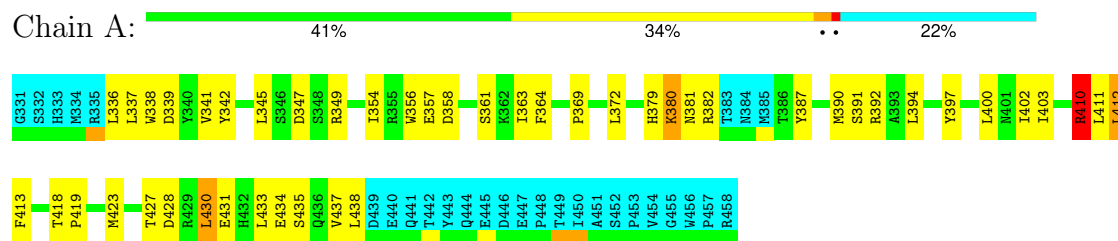
### 4.2.17 Score per residue for model 17

- Molecule 1: Transcription factor ETV6



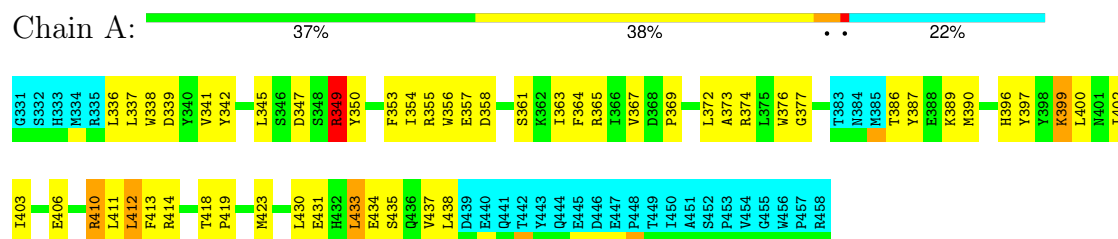
### 4.2.18 Score per residue for model 18

- Molecule 1: Transcription factor ETV6



### 4.2.19 Score per residue for model 19

- Molecule 1: Transcription factor ETV6



## 5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 19 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

Software name	Classification	Version
ARIA	structure solution	2.3
TALOS+	geometry optimization	
ARIA	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	1630
Number of shifts mapped to atoms	1630
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	349	ARG	Sidechain	1

### 6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	871	872	871	40±6
All	All	16549	16568	16549	759

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 23.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:347:ASP:HB3	1:A:349:ARG:CD	0.83	2.04	13	2
1:A:358:ASP:HB2	1:A:363:ILE:HB	0.80	1.53	17	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:349:ARG:NE	1:A:350:TYR:H	0.78	1.76	13	2
1:A:434:GLU:O	1:A:438:LEU:HG	0.75	1.81	2	18
1:A:400:LEU:HD11	1:A:430:LEU:HD21	0.75	1.58	2	18
1:A:349:ARG:HD2	1:A:350:TYR:CD2	0.74	2.17	19	1
1:A:397:TYR:HA	1:A:400:LEU:HD12	0.73	1.59	2	15
1:A:386:THR:H	1:A:389:LYS:HD2	0.71	1.44	3	6
1:A:410:ARG:HD3	1:A:411:LEU:H	0.70	1.45	14	4
1:A:386:THR:HB	1:A:389:LYS:HD2	0.70	1.64	11	2
1:A:349:ARG:NH1	1:A:350:TYR:HD2	0.69	1.85	13	2
1:A:349:ARG:HE	1:A:349:ARG:N	0.69	1.85	19	2
1:A:382:ARG:C	1:A:382:ARG:HD2	0.69	2.08	10	1
1:A:418:THR:HB	1:A:419:PRO:HD2	0.68	1.65	14	19
1:A:382:ARG:HD3	1:A:438:LEU:HD22	0.68	1.65	15	1
1:A:392:ARG:HB3	1:A:437:VAL:HG23	0.68	1.66	16	3
1:A:347:ASP:OD1	1:A:349:ARG:HG3	0.66	1.90	11	12
1:A:356:TRP:CE2	1:A:359:LYS:HD3	0.66	2.25	17	1
1:A:379:HIS:HB3	1:A:380:LYS:HD2	0.65	1.68	18	1
1:A:397:TYR:HD2	1:A:403:ILE:HD12	0.64	1.53	11	9
1:A:361:SER:HB3	1:A:363:ILE:HD13	0.64	1.70	18	13
1:A:349:ARG:CZ	1:A:350:TYR:HD2	0.64	2.06	13	2
1:A:361:SER:CB	1:A:363:ILE:HD13	0.63	2.23	7	17
1:A:337:LEU:O	1:A:341:VAL:HG12	0.63	1.94	4	18
1:A:369:PRO:HB3	1:A:387:TYR:CD2	0.62	2.29	18	19
1:A:392:ARG:HB3	1:A:437:VAL:CG2	0.62	2.25	18	1
1:A:392:ARG:HB2	1:A:437:VAL:HG23	0.62	1.70	8	6
1:A:370:ASN:O	1:A:374:ARG:HG2	0.62	1.94	15	4
1:A:355:ARG:HD2	1:A:367:VAL:CG2	0.61	2.25	12	1
1:A:410:ARG:CD	1:A:411:LEU:H	0.61	2.08	5	3
1:A:338:TRP:CZ3	1:A:339:ASP:HB3	0.61	2.30	9	4
1:A:376:TRP:CZ3	1:A:438:LEU:HD21	0.61	2.30	19	1
1:A:336:LEU:HD21	1:A:431:GLU:HG2	0.61	1.70	9	11
1:A:337:LEU:HB3	1:A:397:TYR:OH	0.61	1.96	9	19
1:A:433:LEU:HD13	1:A:434:GLU:N	0.61	2.10	17	1
1:A:400:LEU:CD1	1:A:430:LEU:HD21	0.60	2.25	5	16
1:A:347:ASP:HB3	1:A:349:ARG:HD3	0.60	1.71	19	2
1:A:349:ARG:HD2	1:A:350:TYR:CE2	0.60	2.32	19	1
1:A:406:GLU:HB2	1:A:409:GLN:HG3	0.59	1.72	8	1
1:A:354:ILE:HD11	1:A:364:PHE:CD2	0.59	2.31	1	19
1:A:343:GLN:HA	1:A:343:GLN:HE21	0.59	1.56	9	1
1:A:355:ARG:HD2	1:A:367:VAL:HG21	0.59	1.72	12	1
1:A:364:PHE:CE1	1:A:413:PHE:HB2	0.59	2.33	11	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:390:MET:HE2	1:A:394:LEU:HD11	0.59	1.72	14	5
1:A:433:LEU:HD22	1:A:433:LEU:O	0.59	1.97	17	1
1:A:357:GLU:HG3	1:A:412:LEU:HD21	0.58	1.73	15	17
1:A:391:SER:HA	1:A:394:LEU:HD12	0.58	1.75	8	4
1:A:393:ALA:HA	1:A:396:HIS:NE2	0.58	2.14	2	2
1:A:392:ARG:CB	1:A:437:VAL:HG23	0.58	2.29	8	5
1:A:427:THR:O	1:A:431:GLU:HG3	0.58	1.99	8	2
1:A:342:TYR:HA	1:A:345:LEU:HD12	0.58	1.76	14	11
1:A:339:ASP:O	1:A:343:GLN:HG2	0.57	1.98	11	2
1:A:347:ASP:HB3	1:A:349:ARG:HG3	0.57	1.74	17	1
1:A:410:ARG:HD2	1:A:411:LEU:H	0.57	1.59	15	1
1:A:417:LYS:HB2	1:A:421:GLU:HB2	0.57	1.77	1	5
1:A:426:ARG:HG3	1:A:426:ARG:O	0.57	1.99	5	1
1:A:429:ARG:O	1:A:433:LEU:HB2	0.57	1.99	5	15
1:A:377:GLY:HA3	1:A:382:ARG:NE	0.57	2.13	10	1
1:A:402:ILE:HG22	1:A:403:ILE:HG13	0.56	1.76	12	16
1:A:349:ARG:CZ	1:A:350:TYR:CD2	0.55	2.90	13	2
1:A:345:LEU:HB3	1:A:356:TRP:NE1	0.55	2.17	13	19
1:A:419:PRO:O	1:A:423:MET:HG3	0.55	2.02	3	12
1:A:386:THR:N	1:A:389:LYS:HD2	0.54	2.17	12	2
1:A:347:ASP:HB2	1:A:349:ARG:NH1	0.54	2.16	19	2
1:A:336:LEU:HD12	1:A:338:TRP:CZ2	0.54	2.38	15	16
1:A:357:GLU:HG3	1:A:412:LEU:HD11	0.54	1.78	5	4
1:A:434:GLU:HA	1:A:437:VAL:CG1	0.54	2.33	9	5
1:A:399:LYS:N	1:A:399:LYS:HD2	0.54	2.18	4	5
1:A:338:TRP:HA	1:A:341:VAL:CG1	0.53	2.33	9	13
1:A:358:ASP:HB3	1:A:361:SER:OG	0.53	2.02	15	4
1:A:396:HIS:O	1:A:400:LEU:HG	0.53	2.02	12	6
1:A:404:ARG:HG3	1:A:414:ARG:HB3	0.53	1.79	3	2
1:A:347:ASP:HB3	1:A:349:ARG:HD2	0.53	1.77	13	1
1:A:373:ALA:HB2	1:A:387:TYR:HA	0.52	1.80	13	9
1:A:391:SER:O	1:A:395:ARG:HG2	0.52	2.03	10	3
1:A:434:GLU:HA	1:A:437:VAL:HG12	0.52	1.80	18	3
1:A:433:LEU:O	1:A:437:VAL:HG12	0.52	2.04	16	16
1:A:336:LEU:HD13	1:A:430:LEU:CB	0.52	2.34	18	1
1:A:401:ASN:O	1:A:416:MET:HB2	0.52	2.05	9	4
1:A:338:TRP:CZ3	1:A:339:ASP:HB2	0.51	2.41	19	10
1:A:350:TYR:HB3	1:A:353:PHE:HB2	0.51	1.81	19	1
1:A:347:ASP:OD1	1:A:349:ARG:HD2	0.51	2.05	12	1
1:A:349:ARG:CD	1:A:350:TYR:CD2	0.51	2.93	19	1
1:A:365:ARG:HD2	1:A:367:VAL:HG22	0.51	1.82	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:417:LYS:HB2	1:A:421:GLU:CB	0.51	2.36	16	2
1:A:349:ARG:HG2	1:A:350:TYR:CD2	0.51	2.41	13	1
1:A:338:TRP:CZ3	1:A:419:PRO:HA	0.50	2.41	14	5
1:A:349:ARG:NE	1:A:349:ARG:N	0.50	2.60	13	2
1:A:365:ARG:HB2	1:A:412:LEU:HD22	0.50	1.82	16	7
1:A:354:ILE:HD11	1:A:364:PHE:CE2	0.50	2.42	1	12
1:A:410:ARG:HG2	1:A:411:LEU:H	0.49	1.67	9	1
1:A:357:GLU:HB2	1:A:363:ILE:HG22	0.49	1.83	5	4
1:A:363:ILE:HD11	1:A:414:ARG:CZ	0.49	2.38	14	4
1:A:392:ARG:HB2	1:A:437:VAL:CG2	0.49	2.37	6	7
1:A:356:TRP:CD1	1:A:359:LYS:HE2	0.49	2.42	14	1
1:A:347:ASP:HB3	1:A:349:ARG:NE	0.48	2.23	19	1
1:A:397:TYR:N	1:A:397:TYR:CD1	0.48	2.81	6	12
1:A:358:ASP:HB3	1:A:361:SER:HB2	0.48	1.85	17	1
1:A:340:TYR:O	1:A:344:LEU:HG	0.48	2.08	10	4
1:A:336:LEU:HD12	1:A:338:TRP:CE2	0.48	2.43	18	1
1:A:404:ARG:HG2	1:A:414:ARG:HB3	0.48	1.85	1	1
1:A:377:GLY:CA	1:A:382:ARG:HB2	0.47	2.39	15	2
1:A:338:TRP:O	1:A:342:TYR:HB2	0.47	2.10	19	3
1:A:365:ARG:HD3	1:A:410:ARG:NH2	0.47	2.24	2	1
1:A:355:ARG:HG2	1:A:367:VAL:CG2	0.47	2.40	19	6
1:A:366:ILE:HD12	1:A:413:PHE:CE2	0.47	2.45	9	10
1:A:377:GLY:HA2	1:A:382:ARG:HB2	0.47	1.87	7	2
1:A:410:ARG:N	1:A:410:ARG:HD3	0.47	2.25	9	1
1:A:405:LYS:HG2	1:A:413:PHE:CE1	0.47	2.44	11	2
1:A:344:LEU:HA	1:A:349:ARG:HH12	0.46	1.69	13	1
1:A:349:ARG:CD	1:A:349:ARG:N	0.46	2.78	13	1
1:A:426:ARG:O	1:A:430:LEU:HG	0.46	2.10	17	1
1:A:377:GLY:CA	1:A:382:ARG:HG3	0.46	2.40	10	1
1:A:388:GLU:O	1:A:392:ARG:HG2	0.46	2.11	12	1
1:A:392:ARG:HA	1:A:395:ARG:HG2	0.46	1.87	17	1
1:A:377:GLY:HA3	1:A:382:ARG:CZ	0.46	2.41	10	1
1:A:380:LYS:HZ1	1:A:434:GLU:HB3	0.45	1.70	2	1
1:A:338:TRP:HA	1:A:341:VAL:HG12	0.45	1.88	9	2
1:A:414:ARG:HD2	1:A:416:MET:SD	0.45	2.52	16	1
1:A:349:ARG:NH1	1:A:350:TYR:CD2	0.45	2.76	13	2
1:A:382:ARG:NH1	1:A:438:LEU:HB3	0.45	2.26	9	1
1:A:410:ARG:NE	1:A:411:LEU:H	0.44	2.10	1	1
1:A:386:THR:CB	1:A:389:LYS:HZ3	0.44	2.25	13	1
1:A:433:LEU:HD22	1:A:433:LEU:C	0.44	2.33	17	1
1:A:387:TYR:CE1	1:A:391:SER:HB3	0.44	2.47	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:338:TRP:CE3	1:A:339:ASP:N	0.44	2.85	7	11
1:A:418:THR:HB	1:A:419:PRO:CD	0.44	2.41	5	4
1:A:396:HIS:ND1	1:A:430:LEU:HD22	0.44	2.27	17	1
1:A:349:ARG:NE	1:A:350:TYR:N	0.44	2.57	13	1
1:A:365:ARG:HB2	1:A:412:LEU:CD2	0.44	2.43	16	2
1:A:400:LEU:HD11	1:A:430:LEU:CD2	0.44	2.38	17	1
1:A:403:ILE:HA	1:A:414:ARG:O	0.44	2.12	10	3
1:A:338:TRP:CZ3	1:A:419:PRO:HG3	0.44	2.48	16	1
1:A:433:LEU:O	1:A:433:LEU:HD13	0.43	2.13	16	7
1:A:359:LYS:O	1:A:359:LYS:HD2	0.43	2.13	17	1
1:A:371:GLY:O	1:A:375:LEU:HG	0.43	2.13	3	2
1:A:356:TRP:CD1	1:A:359:LYS:HD2	0.43	2.48	4	1
1:A:410:ARG:HG2	1:A:410:ARG:HH11	0.43	1.74	11	1
1:A:354:ILE:HB	1:A:372:LEU:CD2	0.43	2.44	2	5
1:A:354:ILE:HG13	1:A:365:ARG:O	0.43	2.14	2	3
1:A:400:LEU:HD13	1:A:430:LEU:HD21	0.43	1.89	18	1
1:A:357:GLU:HG2	1:A:412:LEU:HD21	0.43	1.90	4	1
1:A:406:GLU:HB3	1:A:409:GLN:NE2	0.43	2.29	14	1
1:A:358:ASP:HB3	1:A:363:ILE:HB	0.43	1.91	4	1
1:A:356:TRP:CE3	1:A:359:LYS:HA	0.43	2.49	13	1
1:A:404:ARG:CG	1:A:414:ARG:HB3	0.42	2.44	3	1
1:A:382:ARG:NH1	1:A:438:LEU:HA	0.42	2.29	15	1
1:A:380:LYS:O	1:A:382:ARG:HG2	0.42	2.14	11	1
1:A:433:LEU:HD13	1:A:433:LEU:C	0.42	2.35	17	1
1:A:400:LEU:HD22	1:A:426:ARG:HB3	0.42	1.90	9	2
1:A:366:ILE:HD13	1:A:387:TYR:HE2	0.42	1.74	13	1
1:A:376:TRP:CH2	1:A:438:LEU:HD21	0.42	2.49	4	1
1:A:402:ILE:HG12	1:A:417:LYS:HE2	0.42	1.92	7	2
1:A:386:THR:O	1:A:389:LYS:HB2	0.42	2.15	3	1
1:A:338:TRP:HD1	1:A:397:TYR:CE2	0.42	2.33	6	2
1:A:432:HIS:O	1:A:436:GLN:HG3	0.42	2.14	2	1
1:A:423:MET:HA	1:A:427:THR:CG2	0.42	2.45	10	1
1:A:397:TYR:CE1	1:A:430:LEU:HD22	0.42	2.50	13	1
1:A:406:GLU:OE1	1:A:414:ARG:HB2	0.42	2.14	15	1
1:A:345:LEU:HB3	1:A:356:TRP:CE2	0.42	2.50	19	2
1:A:404:ARG:HD2	1:A:406:GLU:OE2	0.42	2.14	3	1
1:A:397:TYR:N	1:A:397:TYR:HD1	0.42	2.11	6	1
1:A:363:ILE:HD12	1:A:414:ARG:HG3	0.42	1.91	10	1
1:A:338:TRP:CD1	1:A:397:TYR:CZ	0.42	3.08	17	1
1:A:365:ARG:HG3	1:A:412:LEU:HD22	0.41	1.91	15	1
1:A:336:LEU:HD21	1:A:431:GLU:CG	0.41	2.46	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:395:ARG:HA	1:A:398:TYR:CD2	0.41	2.50	6	2
1:A:363:ILE:N	1:A:363:ILE:CD1	0.41	2.83	14	2
1:A:369:PRO:CG	1:A:411:LEU:HD13	0.41	2.45	15	2
1:A:411:LEU:HA	1:A:413:PHE:CE1	0.41	2.50	12	2
1:A:340:TYR:OH	1:A:375:LEU:HB3	0.41	2.16	10	2
1:A:345:LEU:HD13	1:A:356:TRP:CZ2	0.41	2.51	9	1
1:A:409:GLN:HB3	1:A:412:LEU:HB2	0.41	1.91	16	3
1:A:347:ASP:CB	1:A:349:ARG:NH1	0.41	2.83	13	1
1:A:347:ASP:HB3	1:A:350:TYR:CE2	0.41	2.50	10	1
1:A:409:GLN:HB3	1:A:412:LEU:CB	0.41	2.45	13	1
1:A:337:LEU:HA	1:A:376:TRP:NE1	0.41	2.31	17	1
1:A:337:LEU:HD21	1:A:394:LEU:HG	0.41	1.93	4	1
1:A:357:GLU:HB3	1:A:363:ILE:HG22	0.41	1.92	14	2
1:A:410:ARG:H	1:A:410:ARG:CD	0.41	2.29	9	1
1:A:363:ILE:HG23	1:A:412:LEU:HD12	0.41	1.92	18	1
1:A:386:THR:HG22	1:A:387:TYR:N	0.41	2.31	15	1
1:A:409:GLN:OE1	1:A:412:LEU:HG	0.41	2.16	2	1
1:A:427:THR:HA	1:A:430:LEU:HD23	0.40	1.93	18	1
1:A:361:SER:OG	1:A:363:ILE:HD13	0.40	2.16	15	1
1:A:430:LEU:O	1:A:434:GLU:HG3	0.40	2.17	4	1
1:A:358:ASP:HB2	1:A:361:SER:OG	0.40	2.17	12	1
1:A:349:ARG:CD	1:A:349:ARG:H	0.40	2.30	13	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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	100/128 (78%)	94±1 (94±1%)	5±2 (5±2%)	1±1 (1±1%)	15	64
All	All	1900/2432 (78%)	1791 (94%)	88 (5%)	21 (1%)	15	64

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	410	ARG	17
1	A	425	GLY	4

### 6.3.2 Protein sidechains ⓘ

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	94/119 (79%)	84±1 (89±1%)	10±1 (11±1%)	8	53
All	All	1786/2261 (79%)	1596 (89%)	190 (11%)	8	53

All 34 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	372	LEU	19
1	A	390	MET	19
1	A	410	ARG	19
1	A	412	LEU	19
1	A	433	LEU	19
1	A	411	LEU	13
1	A	352	ASN	12
1	A	435	SER	9
1	A	363	ILE	7
1	A	437	VAL	6
1	A	404	ARG	5
1	A	399	LYS	5
1	A	428	ASP	4
1	A	417	LYS	4
1	A	401	ASN	4
1	A	381	ASN	3
1	A	349	ARG	3
1	A	395	ARG	2
1	A	351	GLU	2
1	A	382	ARG	2
1	A	347	ASP	1
1	A	396	HIS	1
1	A	426	ARG	1
1	A	436	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	397	TYR	1
1	A	370	ASN	1
1	A	343	GLN	1
1	A	339	ASP	1
1	A	355	ARG	1
1	A	374	ARG	1
1	A	409	GLN	1
1	A	380	LYS	1
1	A	430	LEU	1
1	A	406	GLU	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

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 86% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

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

Total number of shifts	1630
Number of shifts mapped to atoms	1630
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	122	$-0.31 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	117	$0.23 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	111	$-0.22 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	115	$0.41 \pm 0.23$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 89%, i.e. 1367 atoms were assigned a chemical shift out of a possible 1530. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	483/498 (97%)	197/201 (98%)	192/200 (96%)	94/97 (97%)
Sidechain	744/878 (85%)	504/563 (90%)	227/264 (86%)	13/51 (25%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	140/154 (91%)	67/74 (91%)	64/71 (90%)	9/9 (100%)
Overall	1367/1530 (89%)	768/838 (92%)	483/535 (90%)	116/157 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1630 atoms were assigned a chemical shift out of a possible 1894. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	591/634 (93%)	243/256 (95%)	233/256 (91%)	115/122 (94%)
Sidechain	879/1077 (82%)	595/690 (86%)	268/327 (82%)	16/60 (27%)
Aromatic	160/183 (87%)	77/88 (88%)	73/83 (88%)	10/12 (83%)
Overall	1630/1894 (86%)	915/1034 (88%)	574/666 (86%)	141/194 (73%)

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

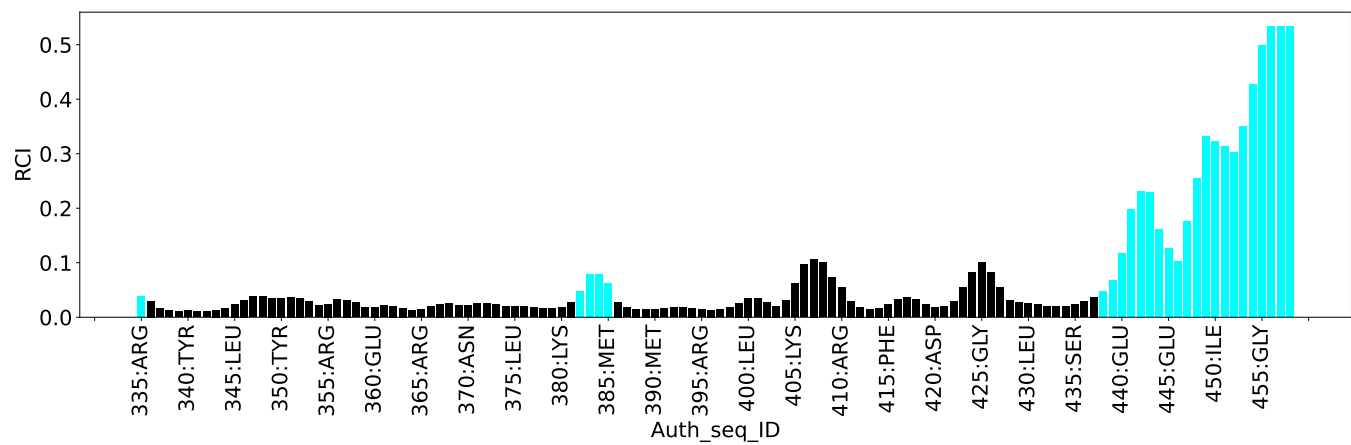
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	413	PHE	HB2	0.66	1.20 – 4.80	-6.5
1	A	345	LEU	HD11	-0.96	-0.61 – 2.12	-6.3
1	A	345	LEU	HD12	-0.96	-0.61 – 2.12	-6.3
1	A	345	LEU	HD13	-0.96	-0.61 – 2.12	-6.3

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2992
Intra-residue ( $ i-j =0$ )	1448
Sequential ( $ i-j =1$ )	525
Medium range ( $ i-j >1$ and $ i-j <5$ )	388
Long range ( $ i-j \geq 5$ )	631
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	190
Number of unmapped restraints	0
Number of restraints per residue	24.9
Number of long range restraints per residue <sup>1</sup>	4.9

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

### 8.2 Residual restraint violations

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

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

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	126.6	0.2
0.2-0.5 (Medium)	246.9	0.5
>0.5 (Large)	266.5	7.03

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	12.4	6.38
10.0-20.0 (Medium)	0.1	12.33
>20.0 (Large)	None	None



## 9 Distance violation analysis ⓘ

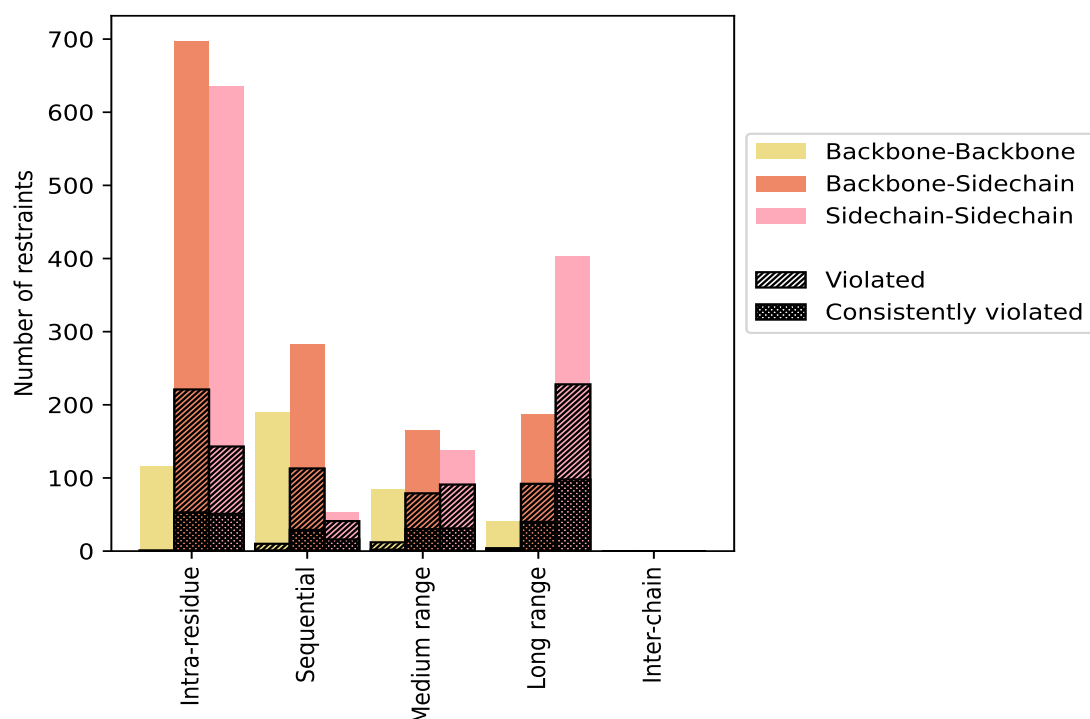
### 9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<a href="#">Intra-residue ( i-j =0)</a>	<a href="#">1448</a>	<a href="#">48.4</a>	<a href="#">365</a>	<a href="#">25.2</a>	<a href="#">12.2</a>	<a href="#">104</a>	<a href="#">7.2</a>	<a href="#">3.5</a>
Backbone-Backbone	116	3.9	1	0.9	0.0	0	0.0	0.0
Backbone-Sidechain	697	23.3	221	31.7	7.4	53	7.6	1.8
Sidechain-Sidechain	635	21.2	143	22.5	4.8	51	8.0	1.7
<a href="#">Sequential ( i-j =1)</a>	<a href="#">525</a>	<a href="#">17.5</a>	<a href="#">164</a>	<a href="#">31.2</a>	<a href="#">5.5</a>	<a href="#">46</a>	<a href="#">8.8</a>	<a href="#">1.5</a>
Backbone-Backbone	190	6.4	10	5.3	0.3	1	0.5	0.0
Backbone-Sidechain	282	9.4	113	40.1	3.8	29	10.3	1.0
Sidechain-Sidechain	53	1.8	41	77.4	1.4	16	30.2	0.5
<a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a>	<a href="#">388</a>	<a href="#">13.0</a>	<a href="#">182</a>	<a href="#">46.9</a>	<a href="#">6.1</a>	<a href="#">63</a>	<a href="#">16.2</a>	<a href="#">2.1</a>
Backbone-Backbone	85	2.8	12	14.1	0.4	2	2.4	0.1
Backbone-Sidechain	165	5.5	79	47.9	2.6	30	18.2	1.0
Sidechain-Sidechain	138	4.6	91	65.9	3.0	31	22.5	1.0
<a href="#">Long range ( i-j ≥5)</a>	<a href="#">631</a>	<a href="#">21.1</a>	<a href="#">324</a>	<a href="#">51.3</a>	<a href="#">10.8</a>	<a href="#">140</a>	<a href="#">22.2</a>	<a href="#">4.7</a>
Backbone-Backbone	41	1.4	4	9.8	0.1	2	4.9	0.1
Backbone-Sidechain	187	6.2	92	49.2	3.1	40	21.4	1.3
Sidechain-Sidechain	403	13.5	228	56.6	7.6	98	24.3	3.3
<a href="#">Inter-chain</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
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
<a href="#">Hydrogen bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Disulfide bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Total</a>	<a href="#">2992</a>	<a href="#">100.0</a>	<a href="#">1035</a>	<a href="#">34.6</a>	<a href="#">34.6</a>	<a href="#">353</a>	<a href="#">11.8</a>	<a href="#">11.8</a>
Backbone-Backbone	432	14.4	27	6.2	0.9	5	1.2	0.2
Backbone-Sidechain	1331	44.5	505	37.9	16.9	152	11.4	5.1
Sidechain-Sidechain	1229	41.1	503	40.9	16.8	196	15.9	6.6

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

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



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and 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 <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	202	110	119	221	0	652	0.67	4.26	0.7	0.42
2	210	94	122	220	0	646	0.68	4.57	0.71	0.42
3	208	105	117	217	0	647	0.63	4.52	0.64	0.41
4	211	107	115	219	0	652	0.69	4.2	0.72	0.42
5	217	102	113	209	0	641	0.67	4.18	0.7	0.42
6	196	97	121	220	0	634	0.68	4.26	0.72	0.41
7	205	104	115	223	0	647	0.67	4.14	0.69	0.43
8	214	101	119	228	0	662	0.67	4.5	0.69	0.41
9	213	103	116	225	0	657	0.66	4.08	0.67	0.41
10	227	97	113	210	0	647	0.68	4.25	0.69	0.43

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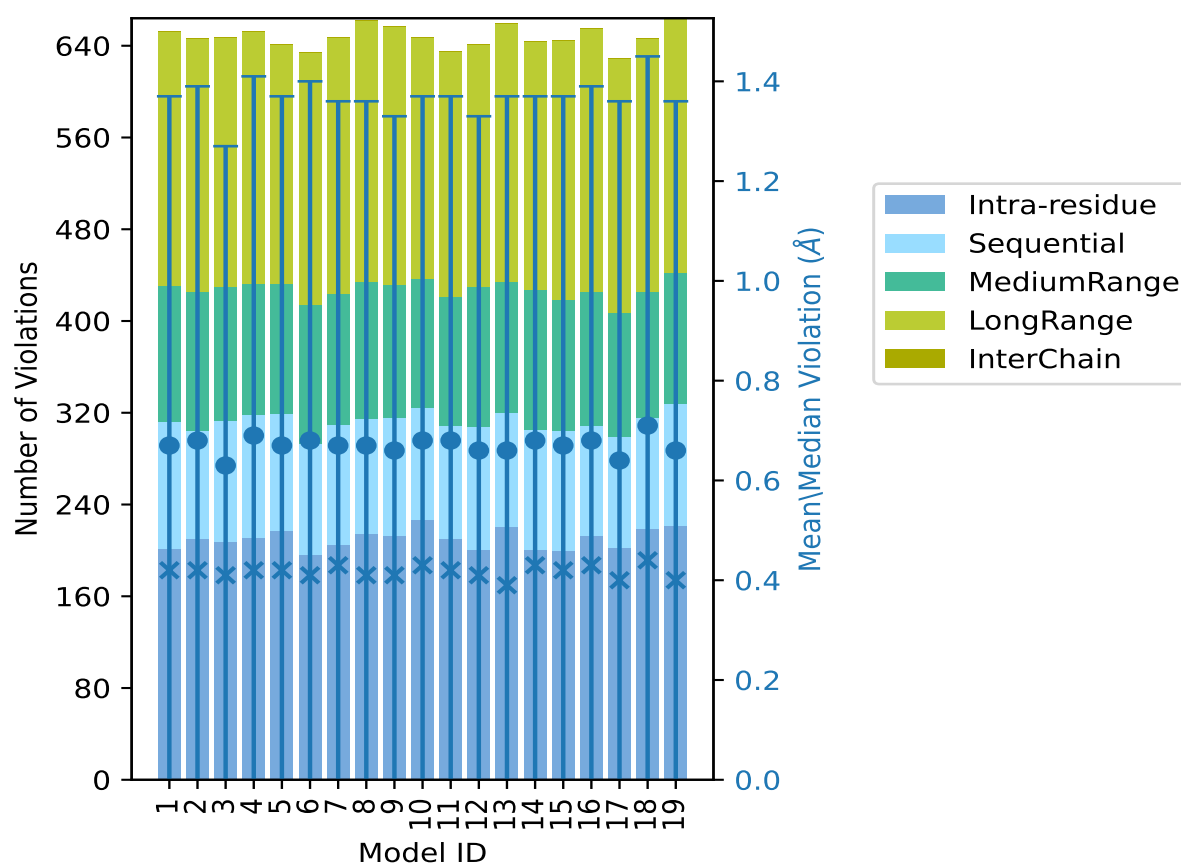
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	210	99	112	214	0	635	0.68	4.0	0.69	0.42
12	200	108	122	211	0	641	0.66	4.4	0.67	0.41
13	221	99	114	225	0	659	0.66	4.6	0.71	0.39
14	201	104	122	217	0	644	0.68	3.94	0.69	0.43
15	200	104	115	226	0	645	0.67	4.21	0.7	0.42
16	213	96	116	230	0	655	0.68	4.48	0.71	0.43
17	202	97	108	222	0	629	0.64	7.03	0.72	0.4
18	219	97	110	220	0	646	0.71	4.06	0.74	0.44
19	221	107	114	222	0	664	0.66	4.32	0.7	0.4

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

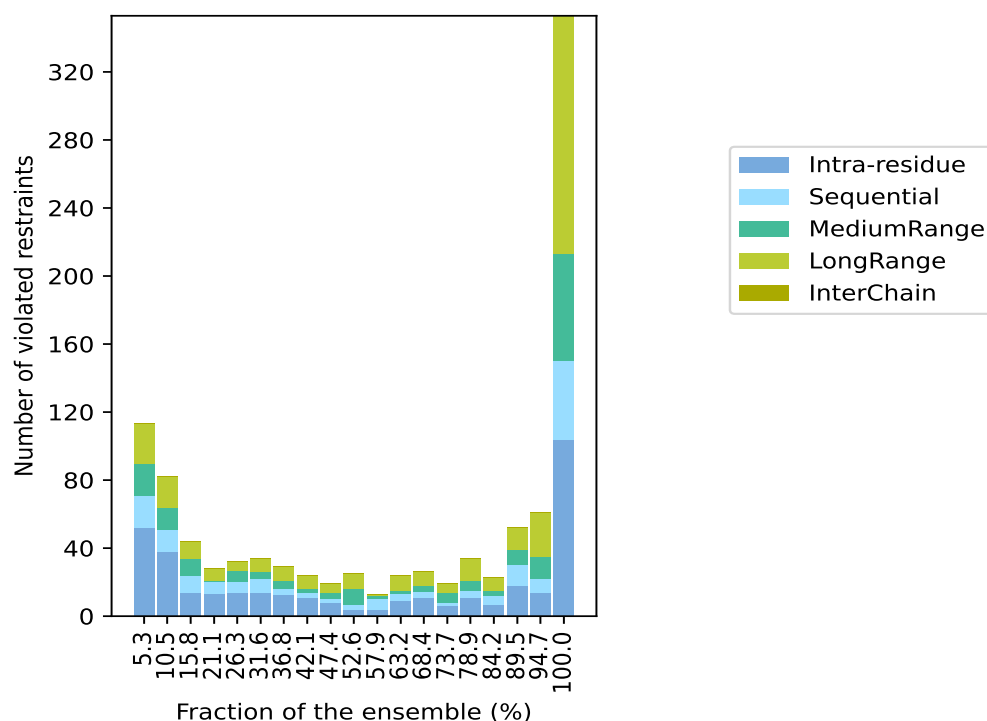
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1957(IR:1083, SQ:361, MR:206, LR:307, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
52	19	19	23	0	113	1	5.3
38	13	13	18	0	82	2	10.5
14	10	10	10	0	44	3	15.8
13	7	1	7	0	28	4	21.1
14	6	7	5	0	32	5	26.3
14	8	4	8	0	34	6	31.6
13	3	5	8	0	29	7	36.8
11	3	2	8	0	24	8	42.1
8	2	4	5	0	19	9	47.4
4	3	9	9	0	25	10	52.6
4	6	2	1	0	13	11	57.9
9	4	2	9	0	24	12	63.2
11	3	4	8	0	26	13	68.4
6	2	6	5	0	19	14	73.7
11	4	6	13	0	34	15	78.9
7	5	3	8	0	23	16	84.2
18	12	9	13	0	52	17	89.5
14	8	13	26	0	61	18	94.7
104	46	63	140	0	353	19	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

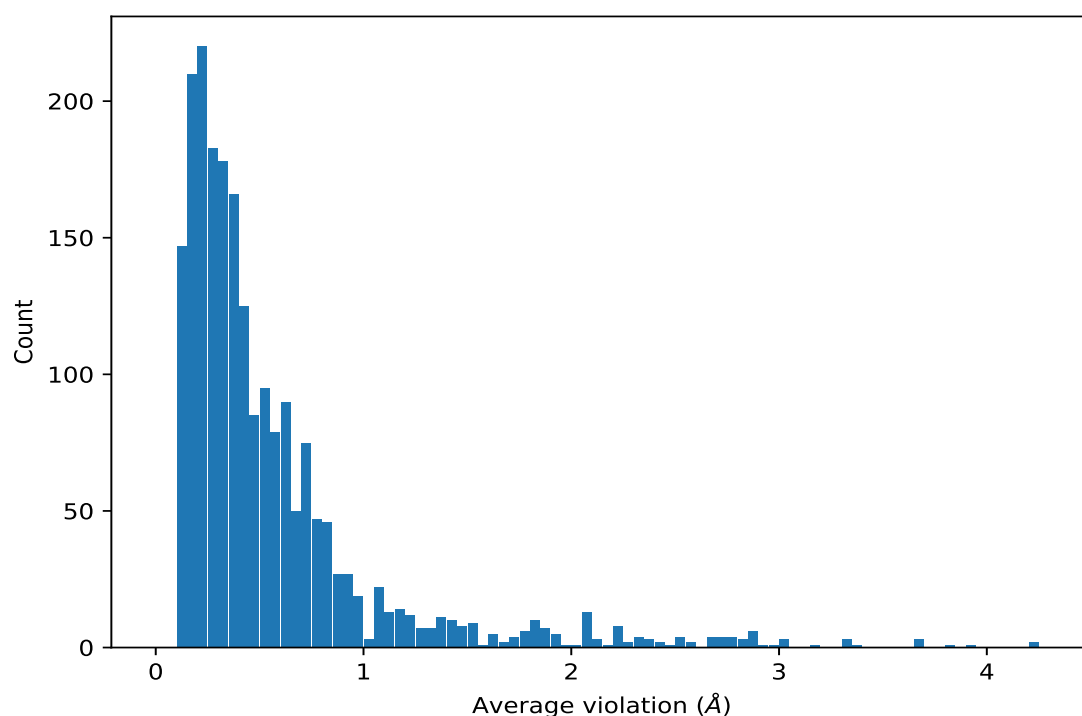
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB2	19	4.22	0.23	4.21
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB3	19	4.22	0.23	4.21
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	19	3.91	0.08	3.91
(1,1264)	1:354:A:ILE:HG21	1:364:A:PHE:HD1	19	3.67	0.07	3.65
(1,1264)	1:354:A:ILE:HG23	1:364:A:PHE:HD1	19	3.67	0.07	3.65
(1,1264)	1:354:A:ILE:HG22	1:364:A:PHE:HD1	19	3.67	0.07	3.65
(1,1004)	1:403:A:ILE:HG21	1:398:A:TYR:HE2	19	3.34	0.33	3.44
(1,1004)	1:403:A:ILE:HG23	1:398:A:TYR:HE2	19	3.34	0.33	3.44
(1,1004)	1:403:A:ILE:HG22	1:398:A:TYR:HE2	19	3.34	0.33	3.44
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	19	3.17	0.1	3.16
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	19	2.98	0.14	2.95
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG21	19	2.89	0.3	2.95
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG23	19	2.89	0.3	2.95
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG22	19	2.89	0.3	2.95
(1,1658)	1:395:A:ARG:HD3	1:398:A:TYR:HE1	19	2.79	0.48	2.65
(1,1658)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	19	2.79	0.48	2.65

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	19	2.71	0.26	2.68
(1,522)	1:394:A:LEU:HD12	1:413:A:PHE:HE1	19	2.7	0.21	2.72
(1,522)	1:394:A:LEU:HD11	1:413:A:PHE:HE1	19	2.7	0.21	2.72
(1,522)	1:394:A:LEU:HD13	1:413:A:PHE:HE1	19	2.7	0.21	2.72
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	19	2.69	0.16	2.66
(1,1173)	1:363:A:ILE:HG21	1:364:A:PHE:HD2	19	2.69	0.1	2.67
(1,1173)	1:363:A:ILE:HG22	1:364:A:PHE:HD2	19	2.69	0.1	2.67
(1,1173)	1:363:A:ILE:HG23	1:364:A:PHE:HD2	19	2.69	0.1	2.67
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	19	2.57	0.15	2.53
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	19	2.53	0.35	2.49
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD13	19	2.53	0.08	2.54
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD11	19	2.53	0.08	2.54
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD12	19	2.53	0.08	2.54
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	19	2.43	0.14	2.41
(1,2777)	1:387:A:TYR:HE2	1:394:A:LEU:HB2	19	2.43	0.14	2.41
(1,307)	1:366:A:ILE:HD13	1:413:A:PHE:HE1	19	2.37	0.09	2.35
(1,307)	1:366:A:ILE:HD11	1:413:A:PHE:HE1	19	2.37	0.09	2.35
(1,307)	1:366:A:ILE:HD12	1:413:A:PHE:HE1	19	2.37	0.09	2.35
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	19	2.33	0.1	2.32
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD11	19	2.33	0.23	2.31
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD12	19	2.33	0.23	2.31
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD13	19	2.33	0.23	2.31
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	19	2.27	0.51	2.19
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	19	2.25	0.41	2.2
(1,2634)	1:394:A:LEU:HD22	1:413:A:PHE:HZ	19	2.24	0.05	2.25
(1,2634)	1:394:A:LEU:HD21	1:413:A:PHE:HZ	19	2.24	0.05	2.25
(1,2634)	1:394:A:LEU:HD23	1:413:A:PHE:HZ	19	2.24	0.05	2.25
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	19	2.23	0.1	2.2
(1,302)	1:366:A:ILE:HG22	1:387:A:TYR:HE1	19	2.21	0.17	2.17
(1,302)	1:366:A:ILE:HG21	1:387:A:TYR:HE1	19	2.21	0.17	2.17
(1,302)	1:366:A:ILE:HG23	1:387:A:TYR:HE1	19	2.21	0.17	2.17
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	19	2.17	0.16	2.11
(1,2778)	1:366:A:ILE:HD13	1:387:A:TYR:HE1	19	2.13	0.13	2.13
(1,2778)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	19	2.13	0.13	2.13
(1,2778)	1:366:A:ILE:HD12	1:387:A:TYR:HE1	19	2.13	0.13	2.13
(1,381)	1:375:A:LEU:HD12	1:350:A:TYR:HE2	19	2.09	0.74	2.41
(1,381)	1:375:A:LEU:HD11	1:350:A:TYR:HE2	19	2.09	0.74	2.41
(1,381)	1:375:A:LEU:HD13	1:350:A:TYR:HE2	19	2.09	0.74	2.41
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	19	2.08	0.28	2.02
(1,2652)	1:405:A:LYS:HG3	1:398:A:TYR:HD2	19	2.06	0.25	2.08
(1,2652)	1:405:A:LYS:HG3	1:413:A:PHE:HE2	19	2.06	0.25	2.08
(1,308)	1:366:A:ILE:HD13	1:387:A:TYR:HE1	19	2.06	0.13	2.06

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,308)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	19	2.06	0.13	2.06
(1,308)	1:366:A:ILE:HD12	1:387:A:TYR:HE1	19	2.06	0.13	2.06
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	19	2.03	0.12	2.01
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	19	1.95	0.31	1.92
(1,1386)	1:373:A:ALA:HB3	1:387:A:TYR:HD1	19	1.94	0.15	1.92
(1,1386)	1:373:A:ALA:HB1	1:387:A:TYR:HD1	19	1.94	0.15	1.92
(1,1386)	1:373:A:ALA:HB2	1:387:A:TYR:HD1	19	1.94	0.15	1.92
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	19	1.93	0.1	1.92
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	19	1.89	0.39	1.89
(1,621)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	19	1.88	0.09	1.9
(1,621)	1:403:A:ILE:HG23	1:413:A:PHE:HD1	19	1.88	0.09	1.9
(1,621)	1:403:A:ILE:HG22	1:413:A:PHE:HD1	19	1.88	0.09	1.9
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	19	1.86	0.06	1.85
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	19	1.83	0.03	1.82
(1,1682)	1:402:A:ILE:HG23	1:415:A:PHE:HB2	19	1.82	0.03	1.83
(1,1682)	1:402:A:ILE:HG21	1:415:A:PHE:HB2	19	1.82	0.03	1.83
(1,1682)	1:402:A:ILE:HG22	1:415:A:PHE:HB2	19	1.82	0.03	1.83
(1,1080)	1:372:A:LEU:HD23	1:353:A:PHE:HD1	19	1.82	0.42	1.88
(1,1080)	1:372:A:LEU:HD21	1:353:A:PHE:HD1	19	1.82	0.42	1.88
(1,1080)	1:372:A:LEU:HD22	1:353:A:PHE:HD1	19	1.82	0.42	1.88
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	19	1.82	0.35	1.59
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	19	1.81	0.07	1.83
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	19	1.81	0.06	1.83
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	19	1.78	0.1	1.77
(1,2821)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	19	1.77	0.09	1.79
(1,2821)	1:403:A:ILE:HG23	1:413:A:PHE:HD1	19	1.77	0.09	1.79
(1,2821)	1:403:A:ILE:HG22	1:413:A:PHE:HD1	19	1.77	0.09	1.79
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	19	1.76	0.62	1.64
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	19	1.75	0.07	1.77
(1,1140)	1:366:A:ILE:HG22	1:387:A:TYR:HD1	19	1.73	0.1	1.72
(1,1140)	1:366:A:ILE:HG21	1:387:A:TYR:HD1	19	1.73	0.1	1.72
(1,1140)	1:366:A:ILE:HG23	1:387:A:TYR:HD1	19	1.73	0.1	1.72
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	19	1.67	0.11	1.68
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	19	1.65	0.33	1.75
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD11	19	1.61	0.14	1.61
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD12	19	1.61	0.14	1.61
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD22	19	1.61	0.14	1.61
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD13	19	1.61	0.14	1.61
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD23	19	1.61	0.14	1.61
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	19	1.58	0.03	1.57
(1,2790)	1:438:A:LEU:HD21	1:437:A:VAL:HB	19	1.54	0.17	1.6
(1,2790)	1:438:A:LEU:HD23	1:437:A:VAL:HB	19	1.54	0.17	1.6

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2790)	1:438:A:LEU:HD22	1:437:A:VAL:HB	19	1.54	0.17	1.6
(1,2790)	1:438:A:LEU:HD21	1:390:A:MET:HB2	19	1.54	0.17	1.6
(1,1684)	1:402:A:ILE:HG21	1:397:A:TYR:HB2	19	1.53	0.15	1.48
(1,1684)	1:402:A:ILE:HG22	1:397:A:TYR:HB2	19	1.53	0.15	1.48
(1,1684)	1:402:A:ILE:HG23	1:397:A:TYR:HB2	19	1.53	0.15	1.48
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	19	1.51	0.13	1.48
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	19	1.48	0.09	1.49
(1,387)	1:375:A:LEU:HD21	1:353:A:PHE:HE1	19	1.48	0.45	1.46
(1,387)	1:375:A:LEU:HD23	1:353:A:PHE:HE1	19	1.48	0.45	1.46
(1,387)	1:375:A:LEU:HD22	1:353:A:PHE:HE1	19	1.48	0.45	1.46
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	19	1.47	0.3	1.45
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	19	1.42	0.2	1.48
(1,900)	1:438:A:LEU:HD12	1:434:A:GLU:HB2	19	1.41	0.2	1.42
(1,900)	1:438:A:LEU:HD13	1:434:A:GLU:HB2	19	1.41	0.2	1.42
(1,900)	1:438:A:LEU:HD11	1:434:A:GLU:HB2	19	1.41	0.2	1.42
(1,1777)	1:337:A:LEU:HD13	1:340:A:TYR:HB2	19	1.41	0.08	1.43
(1,1777)	1:337:A:LEU:HD11	1:340:A:TYR:HB2	19	1.41	0.08	1.43
(1,1777)	1:337:A:LEU:HD12	1:340:A:TYR:HB2	19	1.41	0.08	1.43
(1,1158)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	19	1.39	0.14	1.34
(1,1158)	1:403:A:ILE:HG21	1:364:A:PHE:HE2	19	1.39	0.14	1.34
(1,1158)	1:403:A:ILE:HG23	1:364:A:PHE:HE2	19	1.39	0.14	1.34
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	19	1.37	0.01	1.37
(1,1183)	1:363:A:ILE:HD12	1:362:A:LYS:HG3	19	1.36	0.12	1.37
(1,1183)	1:363:A:ILE:HD13	1:362:A:LYS:HG3	19	1.36	0.12	1.37
(1,1183)	1:363:A:ILE:HD11	1:362:A:LYS:HG3	19	1.36	0.12	1.37
(1,2735)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	19	1.35	0.14	1.31
(1,2735)	1:403:A:ILE:HG21	1:364:A:PHE:HE2	19	1.35	0.14	1.31
(1,2735)	1:403:A:ILE:HG23	1:364:A:PHE:HE2	19	1.35	0.14	1.31
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	19	1.33	0.12	1.32
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	19	1.31	0.13	1.33
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	19	1.29	0.05	1.3
(1,1256)	1:410:A:ARG:HD3	1:412:A:LEU:HB3	19	1.27	0.32	1.26
(1,1256)	1:410:A:ARG:HD2	1:412:A:LEU:HB3	19	1.27	0.32	1.26
(1,1525)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	19	1.26	0.19	1.27
(1,1525)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	19	1.26	0.19	1.27
(1,1525)	1:422:A:ILE:HG22	1:417:A:LYS:HD3	19	1.26	0.19	1.27
(1,2687)	1:430:A:LEU:HD22	1:396:A:HIS:H	19	1.24	0.17	1.24
(1,2687)	1:430:A:LEU:HD21	1:396:A:HIS:H	19	1.24	0.17	1.24
(1,2687)	1:400:A:LEU:H	1:430:A:LEU:HD21	19	1.24	0.17	1.24
(1,2687)	1:430:A:LEU:HD23	1:396:A:HIS:H	19	1.24	0.17	1.24
(1,2687)	1:400:A:LEU:H	1:430:A:LEU:HD22	19	1.24	0.17	1.24
(1,2687)	1:400:A:LEU:H	1:430:A:LEU:HD23	19	1.24	0.17	1.24

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2851)	1:344:A:LEU:HD12	1:372:A:LEU:HB3	19	1.19	0.06	1.21
(1,2851)	1:344:A:LEU:HD13	1:372:A:LEU:HB3	19	1.19	0.06	1.21
(1,2851)	1:344:A:LEU:HD11	1:372:A:LEU:HB3	19	1.19	0.06	1.21
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	19	1.19	0.12	1.16
(1,172)	1:354:A:ILE:HG23	1:350:A:TYR:HD1	19	1.19	0.32	1.15
(1,172)	1:354:A:ILE:HG22	1:350:A:TYR:HD1	19	1.19	0.32	1.15
(1,172)	1:354:A:ILE:HG21	1:350:A:TYR:HD1	19	1.19	0.32	1.15
(1,1392)	1:386:A:THR:HG22	1:389:A:LYS:HG2	19	1.18	0.39	1.28
(1,1392)	1:386:A:THR:HG21	1:389:A:LYS:HG2	19	1.18	0.39	1.28
(1,1392)	1:386:A:THR:HG23	1:389:A:LYS:HG2	19	1.18	0.39	1.28
(1,383)	1:375:A:LEU:HD11	1:353:A:PHE:HE1	19	1.15	0.33	1.17
(1,383)	1:375:A:LEU:HD13	1:353:A:PHE:HE1	19	1.15	0.33	1.17
(1,383)	1:375:A:LEU:HD12	1:353:A:PHE:HE1	19	1.15	0.33	1.17
(1,2878)	1:403:A:ILE:HG23	1:414:A:ARG:HB3	19	1.14	0.13	1.13
(1,2878)	1:403:A:ILE:HG22	1:414:A:ARG:HB3	19	1.14	0.13	1.13
(1,2878)	1:403:A:ILE:HG21	1:414:A:ARG:HB3	19	1.14	0.13	1.13
(1,2806)	1:430:A:LEU:HD13	1:431:A:GLU:HG2	19	1.13	0.61	0.76
(1,2806)	1:430:A:LEU:HD12	1:431:A:GLU:HG2	19	1.13	0.61	0.76
(1,2806)	1:430:A:LEU:HD11	1:431:A:GLU:HG2	19	1.13	0.61	0.76
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	19	1.09	0.11	1.11
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG22	19	1.07	0.33	0.89
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG23	19	1.07	0.33	0.89
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG21	19	1.07	0.33	0.89
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB3	19	1.07	0.16	1.06
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB1	19	1.07	0.16	1.06
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB2	19	1.07	0.16	1.06
(1,2873)	1:418:A:THR:HG21	1:417:A:LYS:H	19	1.06	0.12	1.05
(1,2873)	1:418:A:THR:HG22	1:417:A:LYS:H	19	1.06	0.12	1.05
(1,2873)	1:418:A:THR:HG23	1:417:A:LYS:H	19	1.06	0.12	1.05
(1,2873)	1:430:A:LEU:H	1:427:A:THR:HG23	19	1.06	0.12	1.05
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	19	1.06	0.11	1.05
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	19	1.05	0.11	1.04
(1,2831)	1:411:A:LEU:HD13	1:413:A:PHE:HZ	19	1.05	0.06	1.06
(1,2831)	1:411:A:LEU:HD11	1:413:A:PHE:HZ	19	1.05	0.06	1.06
(1,2831)	1:411:A:LEU:HD12	1:413:A:PHE:HZ	19	1.05	0.06	1.06
(1,2831)	1:411:A:LEU:HD13	1:368:A:ASP:H	19	1.05	0.06	1.06
(1,2816)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	19	1.05	0.2	1.05
(1,2816)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	19	1.05	0.2	1.05
(1,2816)	1:422:A:ILE:HG22	1:417:A:LYS:HD3	19	1.05	0.2	1.05
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	19	0.98	0.03	0.98
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	19	0.98	0.13	0.98
(1,2760)	1:400:A:LEU:HD23	1:401:A:ASN:H	19	0.97	0.05	0.96

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2760)	1:400:A:LEU:HD22	1:401:A:ASN:H	19	0.97	0.05	0.96
(1,2760)	1:400:A:LEU:HD21	1:401:A:ASN:H	19	0.97	0.05	0.96
(1,2879)	1:344:A:LEU:HD12	1:350:A:TYR:HE1	19	0.95	0.15	1.0
(1,2879)	1:344:A:LEU:HD12	1:350:A:TYR:HE2	19	0.95	0.15	1.0
(1,2879)	1:344:A:LEU:HD13	1:350:A:TYR:HE1	19	0.95	0.15	1.0
(1,2879)	1:344:A:LEU:HD11	1:350:A:TYR:HE1	19	0.95	0.15	1.0
(1,2879)	1:344:A:LEU:HD11	1:350:A:TYR:HE2	19	0.95	0.15	1.0
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	19	0.95	0.55	1.27
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG12	19	0.95	0.12	0.94
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG11	19	0.95	0.12	0.94
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG13	19	0.95	0.12	0.94
(1,298)	1:366:A:ILE:HG21	1:369:A:PRO:HD2	19	0.94	0.03	0.95
(1,298)	1:366:A:ILE:HG23	1:369:A:PRO:HD2	19	0.94	0.03	0.95
(1,298)	1:366:A:ILE:HG22	1:369:A:PRO:HD2	19	0.94	0.03	0.95
(1,687)	1:411:A:LEU:HD23	1:369:A:PRO:HD2	19	0.92	0.02	0.92
(1,687)	1:411:A:LEU:HD21	1:369:A:PRO:HD2	19	0.92	0.02	0.92
(1,687)	1:411:A:LEU:HD22	1:369:A:PRO:HD2	19	0.92	0.02	0.92
(1,1331)	1:400:A:LEU:HD21	1:397:A:TYR:HA	19	0.9	0.04	0.9
(1,1331)	1:400:A:LEU:HD22	1:397:A:TYR:HA	19	0.9	0.04	0.9
(1,1331)	1:400:A:LEU:HD23	1:397:A:TYR:HA	19	0.9	0.04	0.9
(1,2694)	1:438:A:LEU:HD12	1:434:A:GLU:HA	19	0.89	0.17	0.81
(1,2694)	1:438:A:LEU:HD13	1:434:A:GLU:HA	19	0.89	0.17	0.81
(1,2694)	1:438:A:LEU:HD11	1:434:A:GLU:HA	19	0.89	0.17	0.81
(1,2694)	1:438:A:LEU:HD13	1:435:A:SER:HB2	19	0.89	0.17	0.81
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	19	0.89	0.1	0.89
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	19	0.88	0.09	0.9
(1,1495)	1:430:A:LEU:HD22	1:396:A:HIS:HA	19	0.87	0.38	0.77
(1,1495)	1:430:A:LEU:HD23	1:396:A:HIS:HA	19	0.87	0.38	0.77
(1,1495)	1:430:A:LEU:HD21	1:396:A:HIS:HA	19	0.87	0.38	0.77
(1,354)	1:393:A:ALA:HB1	1:438:A:LEU:HD23	19	0.87	0.09	0.87
(1,354)	1:393:A:ALA:HB3	1:438:A:LEU:HD22	19	0.87	0.09	0.87
(1,354)	1:393:A:ALA:HB1	1:438:A:LEU:HD22	19	0.87	0.09	0.87
(1,354)	1:393:A:ALA:HB2	1:438:A:LEU:HD23	19	0.87	0.09	0.87
(1,354)	1:393:A:ALA:HB3	1:438:A:LEU:HD23	19	0.87	0.09	0.87
(1,354)	1:393:A:ALA:HB2	1:438:A:LEU:HD21	19	0.87	0.09	0.87
(1,354)	1:393:A:ALA:HB3	1:438:A:LEU:HD21	19	0.87	0.09	0.87
(1,354)	1:393:A:ALA:HB2	1:438:A:LEU:HD22	19	0.87	0.09	0.87
(1,354)	1:393:A:ALA:HB1	1:438:A:LEU:HD21	19	0.87	0.09	0.87
(1,2840)	1:403:A:ILE:HG23	1:416:A:MET:H	19	0.86	0.11	0.87
(1,2840)	1:403:A:ILE:HG22	1:416:A:MET:H	19	0.86	0.11	0.87
(1,2840)	1:403:A:ILE:HG21	1:416:A:MET:H	19	0.86	0.11	0.87
(1,1024)	1:336:A:LEU:HD22	1:338:A:TRP:HZ2	19	0.84	0.09	0.86

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1024)	1:336:A:LEU:HD21	1:338:A:TRP:HZ2	19	0.84	0.09	0.86
(1,1024)	1:336:A:LEU:HD23	1:338:A:TRP:HZ2	19	0.84	0.09	0.86
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	19	0.84	0.11	0.83
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB1	19	0.84	0.43	0.74
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB2	19	0.84	0.43	0.74
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB3	19	0.84	0.43	0.74
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	19	0.84	0.05	0.85
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HG21	19	0.84	0.02	0.83
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HD11	19	0.84	0.02	0.83
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HD12	19	0.84	0.02	0.83
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HG22	19	0.84	0.02	0.83
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HG23	19	0.84	0.02	0.83
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HD13	19	0.84	0.02	0.83
(1,384)	1:344:A:LEU:HD11	1:375:A:LEU:HD23	19	0.83	0.13	0.87
(1,384)	1:344:A:LEU:HD12	1:375:A:LEU:HD23	19	0.83	0.13	0.87
(1,384)	1:344:A:LEU:HD12	1:375:A:LEU:HD22	19	0.83	0.13	0.87
(1,384)	1:344:A:LEU:HD13	1:375:A:LEU:HD22	19	0.83	0.13	0.87
(1,384)	1:344:A:LEU:HD11	1:375:A:LEU:HD21	19	0.83	0.13	0.87
(1,384)	1:344:A:LEU:HD12	1:375:A:LEU:HD21	19	0.83	0.13	0.87
(1,384)	1:344:A:LEU:HD13	1:375:A:LEU:HD23	19	0.83	0.13	0.87
(1,384)	1:344:A:LEU:HD11	1:375:A:LEU:HD22	19	0.83	0.13	0.87
(1,2984)	1:410:A:ARG:HE	1:366:A:ILE:HG21	19	0.83	0.16	0.79
(1,2984)	1:410:A:ARG:HE	1:367:A:VAL:HG22	19	0.83	0.16	0.79
(1,2984)	1:410:A:ARG:HE	1:367:A:VAL:HG23	19	0.83	0.16	0.79
(1,2984)	1:410:A:ARG:HE	1:367:A:VAL:HG21	19	0.83	0.16	0.79
(1,2984)	1:410:A:ARG:HE	1:366:A:ILE:HG23	19	0.83	0.16	0.79
(1,2984)	1:410:A:ARG:HE	1:366:A:ILE:HG22	19	0.83	0.16	0.79
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	19	0.82	0.05	0.82
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	19	0.82	0.05	0.82
(1,1723)	1:341:A:VAL:HG11	1:338:A:TRP:HE3	19	0.82	0.04	0.83
(1,1723)	1:341:A:VAL:HG13	1:338:A:TRP:HE3	19	0.82	0.04	0.83
(1,1723)	1:341:A:VAL:HG12	1:338:A:TRP:HE3	19	0.82	0.04	0.83
(1,2826)	1:413:A:PHE:H	1:412:A:LEU:HD23	19	0.81	0.04	0.82
(1,2826)	1:413:A:PHE:H	1:412:A:LEU:HD22	19	0.81	0.04	0.82
(1,2826)	1:413:A:PHE:H	1:412:A:LEU:HD21	19	0.81	0.04	0.82
(1,2826)	1:366:A:ILE:H	1:412:A:LEU:HD21	19	0.81	0.04	0.82
(1,2826)	1:366:A:ILE:H	1:412:A:LEU:HD23	19	0.81	0.04	0.82
(1,2826)	1:366:A:ILE:H	1:412:A:LEU:HD22	19	0.81	0.04	0.82
(1,624)	1:403:A:ILE:HG22	1:397:A:TYR:HB3	19	0.8	0.1	0.83
(1,624)	1:403:A:ILE:HG21	1:397:A:TYR:HB3	19	0.8	0.1	0.83
(1,624)	1:403:A:ILE:HG23	1:397:A:TYR:HB3	19	0.8	0.1	0.83
(1,2841)	1:403:A:ILE:HD12	1:397:A:TYR:HA	19	0.79	0.04	0.78

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2841)	1:403:A:ILE:HD11	1:397:A:TYR:HA	19	0.79	0.04	0.78
(1,2841)	1:403:A:ILE:HD13	1:397:A:TYR:HA	19	0.79	0.04	0.78
(1,1782)	1:337:A:LEU:HD13	1:397:A:TYR:HE2	19	0.79	0.05	0.79
(1,1782)	1:337:A:LEU:HD11	1:397:A:TYR:HE2	19	0.79	0.05	0.79
(1,1782)	1:337:A:LEU:HD12	1:397:A:TYR:HE2	19	0.79	0.05	0.79
(1,1599)	1:412:A:LEU:HD23	1:364:A:PHE:H	19	0.78	0.02	0.78
(1,1599)	1:412:A:LEU:HD22	1:364:A:PHE:H	19	0.78	0.02	0.78
(1,1599)	1:412:A:LEU:HD21	1:364:A:PHE:H	19	0.78	0.02	0.78
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	19	0.78	0.16	0.71
(1,2633)	1:394:A:LEU:HD11	1:366:A:ILE:HD11	19	0.78	0.11	0.76
(1,2633)	1:394:A:LEU:HD13	1:366:A:ILE:HD12	19	0.78	0.11	0.76
(1,2633)	1:394:A:LEU:HD13	1:366:A:ILE:HD13	19	0.78	0.11	0.76
(1,2633)	1:394:A:LEU:HD11	1:366:A:ILE:HD13	19	0.78	0.11	0.76
(1,2633)	1:394:A:LEU:HD12	1:366:A:ILE:HD11	19	0.78	0.11	0.76
(1,2633)	1:394:A:LEU:HD13	1:366:A:ILE:HD11	19	0.78	0.11	0.76
(1,2633)	1:394:A:LEU:HD11	1:366:A:ILE:HD12	19	0.78	0.11	0.76
(1,2633)	1:394:A:LEU:HD12	1:366:A:ILE:HD12	19	0.78	0.11	0.76
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	19	0.77	0.01	0.77
(1,2932)	1:420:A:ASP:H	1:422:A:ILE:HB	19	0.77	0.09	0.76
(1,2932)	1:420:A:ASP:H	1:418:A:THR:HG22	19	0.77	0.09	0.76
(1,2932)	1:420:A:ASP:H	1:418:A:THR:HG23	19	0.77	0.09	0.76
(1,2932)	1:420:A:ASP:H	1:418:A:THR:HG21	19	0.77	0.09	0.76
(1,2862)	1:376:A:TRP:HB3	1:340:A:TYR:HE2	19	0.77	0.2	0.84
(1,2862)	1:379:A:HIS:HB3	1:340:A:TYR:HE1	19	0.77	0.2	0.84
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	19	0.76	0.04	0.77
(1,1609)	1:411:A:LEU:HD21	1:387:A:TYR:HB2	19	0.75	0.12	0.76
(1,1609)	1:411:A:LEU:HD22	1:387:A:TYR:HB2	19	0.75	0.12	0.76
(1,1609)	1:411:A:LEU:HD23	1:387:A:TYR:HB2	19	0.75	0.12	0.76
(1,1804)	1:422:A:ILE:HD12	1:336:A:LEU:HD12	19	0.74	0.13	0.73
(1,1804)	1:422:A:ILE:HD13	1:336:A:LEU:HD12	19	0.74	0.13	0.73
(1,1804)	1:422:A:ILE:HD11	1:336:A:LEU:HD13	19	0.74	0.13	0.73
(1,1804)	1:422:A:ILE:HD12	1:336:A:LEU:HD13	19	0.74	0.13	0.73
(1,1804)	1:422:A:ILE:HD12	1:336:A:LEU:HD11	19	0.74	0.13	0.73
(1,1804)	1:422:A:ILE:HD13	1:336:A:LEU:HD11	19	0.74	0.13	0.73
(1,1804)	1:422:A:ILE:HD13	1:336:A:LEU:HD13	19	0.74	0.13	0.73
(1,1804)	1:422:A:ILE:HD11	1:336:A:LEU:HD11	19	0.74	0.13	0.73
(1,1804)	1:422:A:ILE:HD11	1:336:A:LEU:HD12	19	0.74	0.13	0.73
(1,2726)	1:367:A:VAL:HG13	1:355:A:ARG:HD3	19	0.74	0.23	0.69
(1,2726)	1:367:A:VAL:HG13	1:365:A:ARG:HD2	19	0.74	0.23	0.69
(1,2726)	1:367:A:VAL:HG12	1:355:A:ARG:HD3	19	0.74	0.23	0.69
(1,2726)	1:367:A:VAL:HG12	1:365:A:ARG:HD2	19	0.74	0.23	0.69
(1,2726)	1:367:A:VAL:HG13	1:355:A:ARG:HD2	19	0.74	0.23	0.69

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2726)	1:367:A:VAL:HG11	1:355:A:ARG:HD2	19	0.74	0.23	0.69
(1,2726)	1:367:A:VAL:HG11	1:365:A:ARG:HD2	19	0.74	0.23	0.69
(1,2726)	1:367:A:VAL:HG11	1:355:A:ARG:HD3	19	0.74	0.23	0.69
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	19	0.74	0.04	0.75
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	19	0.73	0.38	0.96
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD23	19	0.72	0.26	0.75
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD21	19	0.72	0.26	0.75
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD22	19	0.72	0.26	0.75
(1,2941)	1:411:A:LEU:H	1:412:A:LEU:HD11	19	0.72	0.26	0.75
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD13	19	0.72	0.05	0.71
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD11	19	0.72	0.05	0.71
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD12	19	0.72	0.05	0.71
(1,1917)	1:394:A:LEU:HD11	1:366:A:ILE:HD11	19	0.72	0.11	0.7
(1,1917)	1:394:A:LEU:HD13	1:366:A:ILE:HD12	19	0.72	0.11	0.7
(1,1917)	1:394:A:LEU:HD13	1:366:A:ILE:HD13	19	0.72	0.11	0.7
(1,1917)	1:394:A:LEU:HD11	1:366:A:ILE:HD13	19	0.72	0.11	0.7
(1,1917)	1:394:A:LEU:HD12	1:366:A:ILE:HD11	19	0.72	0.11	0.7
(1,1917)	1:394:A:LEU:HD13	1:366:A:ILE:HD11	19	0.72	0.11	0.7
(1,1917)	1:394:A:LEU:HD11	1:366:A:ILE:HD12	19	0.72	0.11	0.7
(1,1917)	1:394:A:LEU:HD12	1:366:A:ILE:HD12	19	0.72	0.11	0.7
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	19	0.71	0.55	0.56
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD12	19	0.7	0.07	0.71
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD13	19	0.7	0.07	0.71
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD11	19	0.7	0.07	0.71
(1,1774)	1:337:A:LEU:HD12	1:393:A:ALA:HB3	19	0.7	0.05	0.7
(1,1774)	1:337:A:LEU:HD13	1:393:A:ALA:HB2	19	0.7	0.05	0.7
(1,1774)	1:337:A:LEU:HD11	1:393:A:ALA:HB3	19	0.7	0.05	0.7
(1,1774)	1:337:A:LEU:HD13	1:393:A:ALA:HB1	19	0.7	0.05	0.7
(1,1774)	1:337:A:LEU:HD11	1:393:A:ALA:HB2	19	0.7	0.05	0.7
(1,1774)	1:337:A:LEU:HD12	1:393:A:ALA:HB1	19	0.7	0.05	0.7
(1,1774)	1:337:A:LEU:HD13	1:393:A:ALA:HB3	19	0.7	0.05	0.7
(1,1774)	1:337:A:LEU:HD11	1:393:A:ALA:HB1	19	0.7	0.05	0.7
(1,1774)	1:337:A:LEU:HD12	1:393:A:ALA:HB2	19	0.7	0.05	0.7
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	19	0.7	0.03	0.7
(1,2876)	1:372:A:LEU:HD13	1:374:A:ARG:H	19	0.7	0.09	0.71
(1,2876)	1:372:A:LEU:HD12	1:374:A:ARG:H	19	0.7	0.09	0.71
(1,2876)	1:372:A:LEU:HD11	1:374:A:ARG:H	19	0.7	0.09	0.71
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	19	0.69	0.27	0.64
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	19	0.69	0.1	0.68
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD13	19	0.68	0.03	0.66
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD11	19	0.68	0.03	0.66
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD12	19	0.68	0.03	0.66

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD12	19	0.67	0.02	0.67
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD11	19	0.67	0.02	0.67
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD13	19	0.67	0.02	0.67
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD12	19	0.67	0.02	0.66
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD13	19	0.67	0.02	0.66
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD11	19	0.67	0.02	0.66
(1,2644)	1:402:A:ILE:HD11	1:397:A:TYR:HE1	19	0.66	0.14	0.66
(1,2644)	1:402:A:ILE:HD12	1:397:A:TYR:HE1	19	0.66	0.14	0.66
(1,2644)	1:402:A:ILE:HD13	1:397:A:TYR:HE1	19	0.66	0.14	0.66
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	19	0.66	0.0	0.66
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD23	19	0.66	0.11	0.66
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD22	19	0.66	0.11	0.66
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD21	19	0.66	0.11	0.66
(1,1113)	1:411:A:LEU:HD13	1:369:A:PRO:HB2	19	0.66	0.05	0.68
(1,1113)	1:411:A:LEU:HD11	1:369:A:PRO:HB2	19	0.66	0.05	0.68
(1,1113)	1:411:A:LEU:HD12	1:369:A:PRO:HB2	19	0.66	0.05	0.68
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	19	0.65	0.02	0.65
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG21	19	0.65	0.02	0.65
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG23	19	0.65	0.02	0.65
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG22	19	0.65	0.02	0.65
(1,2805)	1:372:A:LEU:HD21	1:373:A:ALA:H	19	0.64	0.1	0.66
(1,2805)	1:372:A:LEU:HD22	1:373:A:ALA:H	19	0.64	0.1	0.66
(1,2805)	1:372:A:LEU:HD23	1:373:A:ALA:H	19	0.64	0.1	0.66
(1,2805)	1:430:A:LEU:HD13	1:433:A:LEU:H	19	0.64	0.1	0.66
(1,1923)	1:344:A:LEU:HD21	1:375:A:LEU:HD23	19	0.64	0.04	0.63
(1,1923)	1:344:A:LEU:HD21	1:375:A:LEU:HD22	19	0.64	0.04	0.63
(1,1923)	1:344:A:LEU:HD22	1:375:A:LEU:HD21	19	0.64	0.04	0.63
(1,1923)	1:344:A:LEU:HD22	1:375:A:LEU:HD22	19	0.64	0.04	0.63
(1,1923)	1:344:A:LEU:HD23	1:375:A:LEU:HD21	19	0.64	0.04	0.63
(1,1923)	1:344:A:LEU:HD23	1:375:A:LEU:HD23	19	0.64	0.04	0.63
(1,1923)	1:344:A:LEU:HD23	1:375:A:LEU:HD22	19	0.64	0.04	0.63
(1,1923)	1:344:A:LEU:HD22	1:375:A:LEU:HD23	19	0.64	0.04	0.63
(1,1923)	1:344:A:LEU:HD21	1:375:A:LEU:HD21	19	0.64	0.04	0.63
(1,2799)	1:412:A:LEU:HD23	1:365:A:ARG:HD3	19	0.64	0.21	0.6
(1,2799)	1:412:A:LEU:HD22	1:365:A:ARG:HD3	19	0.64	0.21	0.6
(1,2799)	1:412:A:LEU:HD21	1:365:A:ARG:HD3	19	0.64	0.21	0.6
(1,2799)	1:433:A:LEU:HD11	1:396:A:HIS:HB3	19	0.64	0.21	0.6
(1,1357)	1:394:A:LEU:HD23	1:390:A:MET:HG3	19	0.64	0.16	0.65
(1,1357)	1:394:A:LEU:HD22	1:390:A:MET:HG3	19	0.64	0.16	0.65
(1,1357)	1:394:A:LEU:HD21	1:390:A:MET:HG3	19	0.64	0.16	0.65
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	19	0.64	0.02	0.64
(1,267)	1:363:A:ILE:HG23	1:412:A:LEU:HG	19	0.63	0.03	0.63

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,267)	1:363:A:ILE:HG22	1:412:A:LEU:HG	19	0.63	0.03	0.63
(1,267)	1:363:A:ILE:HG21	1:412:A:LEU:HG	19	0.63	0.03	0.63
(1,1330)	1:400:A:LEU:HD12	1:399:A:LYS:HB2	19	0.63	0.05	0.63
(1,1330)	1:400:A:LEU:HD11	1:399:A:LYS:HB2	19	0.63	0.05	0.63
(1,1330)	1:400:A:LEU:HD13	1:399:A:LYS:HB2	19	0.63	0.05	0.63
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG21	19	0.63	0.09	0.64
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG23	19	0.63	0.09	0.64
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG22	19	0.63	0.09	0.64
(1,2768)	1:394:A:LEU:HD13	1:387:A:TYR:HD1	19	0.63	0.12	0.66
(1,2768)	1:394:A:LEU:HD12	1:387:A:TYR:HD1	19	0.63	0.12	0.66
(1,2768)	1:394:A:LEU:HD11	1:387:A:TYR:HD1	19	0.63	0.12	0.66
(1,35)	1:341:A:VAL:HG13	1:345:A:LEU:HD11	19	0.62	0.1	0.64
(1,35)	1:341:A:VAL:HG11	1:345:A:LEU:HD12	19	0.62	0.1	0.64
(1,35)	1:341:A:VAL:HG12	1:345:A:LEU:HD12	19	0.62	0.1	0.64
(1,35)	1:341:A:VAL:HG12	1:345:A:LEU:HD11	19	0.62	0.1	0.64
(1,35)	1:341:A:VAL:HG13	1:345:A:LEU:HD13	19	0.62	0.1	0.64
(1,35)	1:341:A:VAL:HG12	1:345:A:LEU:HD13	19	0.62	0.1	0.64
(1,35)	1:341:A:VAL:HG11	1:345:A:LEU:HD11	19	0.62	0.1	0.64
(1,35)	1:341:A:VAL:HG13	1:345:A:LEU:HD12	19	0.62	0.1	0.64
(1,35)	1:341:A:VAL:HG11	1:345:A:LEU:HD13	19	0.62	0.1	0.64
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG22	19	0.62	0.01	0.62
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG23	19	0.62	0.01	0.62
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG21	19	0.62	0.01	0.62
(1,2981)	1:428:A:ASP:H	1:427:A:THR:HG22	19	0.61	0.04	0.62
(1,2981)	1:413:A:PHE:H	1:412:A:LEU:HG	19	0.61	0.04	0.62
(1,2981)	1:428:A:ASP:H	1:427:A:THR:HG23	19	0.61	0.04	0.62
(1,2981)	1:428:A:ASP:H	1:427:A:THR:HG21	19	0.61	0.04	0.62
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	19	0.61	0.08	0.63
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	19	0.6	0.02	0.61
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD12	19	0.6	0.02	0.6
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD13	19	0.6	0.02	0.6
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD11	19	0.6	0.02	0.6
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	19	0.6	0.03	0.6
(1,266)	1:363:A:ILE:HG23	1:406:A:GLU:HG2	19	0.59	0.52	0.17
(1,266)	1:363:A:ILE:HG21	1:406:A:GLU:HG2	19	0.59	0.52	0.17
(1,266)	1:363:A:ILE:HG22	1:406:A:GLU:HG2	19	0.59	0.52	0.17
(1,1690)	1:402:A:ILE:HD12	1:400:A:LEU:HA	19	0.58	0.14	0.64
(1,1690)	1:402:A:ILE:HD13	1:400:A:LEU:HA	19	0.58	0.14	0.64
(1,1690)	1:402:A:ILE:HD11	1:400:A:LEU:HA	19	0.58	0.14	0.64
(1,2880)	1:402:A:ILE:HG21	1:397:A:TYR:HE2	19	0.58	0.07	0.57
(1,2880)	1:402:A:ILE:HG22	1:397:A:TYR:HE2	19	0.58	0.07	0.57
(1,2880)	1:402:A:ILE:HG23	1:397:A:TYR:HE2	19	0.58	0.07	0.57

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD22	19	0.58	0.14	0.61
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD23	19	0.58	0.14	0.61
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD21	19	0.58	0.14	0.61
(1,2770)	1:373:A:ALA:HB2	1:371:A:GLY:H	19	0.58	0.04	0.57
(1,2770)	1:373:A:ALA:HB3	1:371:A:GLY:H	19	0.58	0.04	0.57
(1,2770)	1:373:A:ALA:HB1	1:371:A:GLY:H	19	0.58	0.04	0.57
(1,1182)	1:363:A:ILE:HD12	1:406:A:GLU:HG2	19	0.57	0.2	0.62
(1,1182)	1:363:A:ILE:HD11	1:406:A:GLU:HG2	19	0.57	0.2	0.62
(1,1182)	1:363:A:ILE:HD13	1:406:A:GLU:HG2	19	0.57	0.2	0.62
(1,265)	1:363:A:ILE:HG23	1:412:A:LEU:HA	19	0.57	0.07	0.54
(1,265)	1:363:A:ILE:HG21	1:412:A:LEU:HA	19	0.57	0.07	0.54
(1,265)	1:363:A:ILE:HG22	1:412:A:LEU:HA	19	0.57	0.07	0.54
(1,1356)	1:394:A:LEU:HD21	1:338:A:TRP:HB3	19	0.56	0.05	0.55
(1,1356)	1:394:A:LEU:HD23	1:338:A:TRP:HB3	19	0.56	0.05	0.55
(1,1356)	1:394:A:LEU:HD22	1:338:A:TRP:HB3	19	0.56	0.05	0.55
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	19	0.56	0.11	0.59
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	19	0.56	0.02	0.56
(1,2884)	1:397:A:TYR:HE1	1:393:A:ALA:HA	19	0.56	0.06	0.55
(1,2884)	1:397:A:TYR:HE1	1:397:A:TYR:HA	19	0.56	0.06	0.55
(1,1119)	1:367:A:VAL:HG22	1:355:A:ARG:HA	19	0.55	0.08	0.58
(1,1119)	1:367:A:VAL:HG21	1:355:A:ARG:HA	19	0.55	0.08	0.58
(1,1119)	1:367:A:VAL:HG23	1:355:A:ARG:HA	19	0.55	0.08	0.58
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	19	0.55	0.1	0.57
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG3	19	0.55	0.1	0.57
(1,1776)	1:337:A:LEU:HD11	1:390:A:MET:HG3	19	0.54	0.19	0.53
(1,1776)	1:337:A:LEU:HD13	1:390:A:MET:HG3	19	0.54	0.19	0.53
(1,1776)	1:337:A:LEU:HD12	1:390:A:MET:HG3	19	0.54	0.19	0.53
(1,1776)	1:337:A:LEU:HD11	1:390:A:MET:HG2	19	0.54	0.19	0.53
(1,1776)	1:337:A:LEU:HD12	1:390:A:MET:HG2	19	0.54	0.19	0.53
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG22	19	0.54	0.12	0.58
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG21	19	0.54	0.12	0.58
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG23	19	0.54	0.12	0.58
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD13	19	0.54	0.02	0.53
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD11	19	0.54	0.02	0.53
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD12	19	0.54	0.02	0.53
(1,1918)	1:354:A:ILE:HD11	1:366:A:ILE:HD11	19	0.53	0.03	0.53
(1,1918)	1:354:A:ILE:HD12	1:366:A:ILE:HD12	19	0.53	0.03	0.53
(1,1918)	1:354:A:ILE:HD12	1:366:A:ILE:HD13	19	0.53	0.03	0.53
(1,1918)	1:354:A:ILE:HD11	1:366:A:ILE:HD13	19	0.53	0.03	0.53
(1,1918)	1:354:A:ILE:HD13	1:366:A:ILE:HD12	19	0.53	0.03	0.53
(1,1918)	1:354:A:ILE:HD13	1:366:A:ILE:HD11	19	0.53	0.03	0.53
(1,1918)	1:354:A:ILE:HD11	1:366:A:ILE:HD12	19	0.53	0.03	0.53

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1918)	1:354:A:ILE:HD13	1:366:A:ILE:HD13	19	0.53	0.03	0.53
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	19	0.53	0.04	0.52
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD22	19	0.53	0.24	0.46
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD23	19	0.53	0.24	0.46
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD21	19	0.53	0.24	0.46
(1,2828)	1:412:A:LEU:HD11	1:413:A:PHE:HD1	19	0.53	0.05	0.53
(1,2828)	1:412:A:LEU:HD12	1:413:A:PHE:HD1	19	0.53	0.05	0.53
(1,2828)	1:412:A:LEU:HD13	1:413:A:PHE:HD1	19	0.53	0.05	0.53
(1,908)	1:411:A:LEU:HD23	1:366:A:ILE:H	19	0.53	0.02	0.53
(1,908)	1:411:A:LEU:HD21	1:366:A:ILE:H	19	0.53	0.02	0.53
(1,908)	1:411:A:LEU:HD22	1:366:A:ILE:H	19	0.53	0.02	0.53
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG21	19	0.52	0.07	0.52
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG22	19	0.52	0.07	0.52
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG23	19	0.52	0.07	0.52
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	19	0.52	0.06	0.53
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD11	19	0.51	0.03	0.52
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD12	19	0.51	0.03	0.52
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD13	19	0.51	0.03	0.52
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	19	0.51	0.01	0.51
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD11	19	0.51	0.14	0.49
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD13	19	0.51	0.14	0.49
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD12	19	0.51	0.14	0.49
(1,2683)	1:429:A:ARG:HG3	1:429:A:ARG:H	19	0.51	0.08	0.54
(1,2683)	1:429:A:ARG:HG2	1:429:A:ARG:H	19	0.51	0.08	0.54
(1,457)	1:386:A:THR:HG22	1:389:A:LYS:HB2	19	0.51	0.1	0.5
(1,457)	1:386:A:THR:HG21	1:389:A:LYS:HB2	19	0.51	0.1	0.5
(1,457)	1:386:A:THR:HG23	1:389:A:LYS:HB2	19	0.51	0.1	0.5
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD11	19	0.5	0.01	0.5
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD13	19	0.5	0.01	0.5
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD12	19	0.5	0.01	0.5
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	19	0.5	0.29	0.72
(1,1484)	1:432:A:HIS:HB3	1:430:A:LEU:H	19	0.5	0.1	0.52
(1,1484)	1:432:A:HIS:HB2	1:430:A:LEU:H	19	0.5	0.1	0.52
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD21	19	0.5	0.09	0.5
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD22	19	0.5	0.09	0.5
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD23	19	0.5	0.09	0.5
(1,2858)	1:341:A:VAL:HG11	1:340:A:TYR:HD2	19	0.5	0.05	0.49
(1,2858)	1:341:A:VAL:HG12	1:340:A:TYR:HD2	19	0.5	0.05	0.49
(1,2858)	1:341:A:VAL:HG13	1:340:A:TYR:HD2	19	0.5	0.05	0.49
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD13	19	0.49	0.05	0.5
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD11	19	0.49	0.05	0.5
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD12	19	0.49	0.05	0.5

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	19	0.49	0.15	0.47
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD21	19	0.48	0.06	0.49
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD23	19	0.48	0.06	0.49
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD22	19	0.48	0.06	0.49
(1,1671)	1:403:A:ILE:HG21	1:405:A:LYS:HA	19	0.48	0.09	0.51
(1,1671)	1:403:A:ILE:HG23	1:405:A:LYS:HA	19	0.48	0.09	0.51
(1,1671)	1:403:A:ILE:HG22	1:405:A:LYS:HA	19	0.48	0.09	0.51
(1,2645)	1:402:A:ILE:HD13	1:338:A:TRP:HB3	19	0.48	0.16	0.47
(1,2645)	1:402:A:ILE:HD11	1:338:A:TRP:HB3	19	0.48	0.16	0.47
(1,2645)	1:402:A:ILE:HD12	1:338:A:TRP:HB3	19	0.48	0.16	0.47
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	19	0.48	0.03	0.48
(1,2860)	1:340:A:TYR:H	1:340:A:TYR:HD2	19	0.48	0.02	0.48
(1,2860)	1:340:A:TYR:HD1	1:340:A:TYR:H	19	0.48	0.02	0.48
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD12	19	0.47	0.02	0.48
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD13	19	0.47	0.02	0.48
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD11	19	0.47	0.02	0.48
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	19	0.47	0.11	0.42
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	19	0.46	0.04	0.48
(1,1025)	1:336:A:LEU:HD22	1:430:A:LEU:H	19	0.46	0.16	0.49
(1,1025)	1:336:A:LEU:HD21	1:430:A:LEU:H	19	0.46	0.16	0.49
(1,1025)	1:336:A:LEU:HD23	1:430:A:LEU:H	19	0.46	0.16	0.49
(1,1135)	1:367:A:VAL:HG13	1:352:A:ASN:H	19	0.46	0.04	0.46
(1,1135)	1:367:A:VAL:HG12	1:352:A:ASN:H	19	0.46	0.04	0.46
(1,1135)	1:367:A:VAL:HG11	1:352:A:ASN:H	19	0.46	0.04	0.46
(1,2688)	1:431:A:GLU:HG2	1:431:A:GLU:HB3	19	0.45	0.07	0.46
(1,2688)	1:440:A:GLU:HG2	1:440:A:GLU:HB3	19	0.45	0.07	0.46
(1,2688)	1:431:A:GLU:HG2	1:431:A:GLU:HB2	19	0.45	0.07	0.46
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD22	19	0.45	0.02	0.44
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD21	19	0.45	0.02	0.44
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD23	19	0.45	0.02	0.44
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	19	0.45	0.02	0.45
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	19	0.45	0.01	0.45
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB3	19	0.45	0.05	0.46
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB2	19	0.45	0.05	0.46
(1,620)	1:403:A:ILE:HG21	1:403:A:ILE:H	19	0.44	0.02	0.44
(1,620)	1:403:A:ILE:HG23	1:403:A:ILE:H	19	0.44	0.02	0.44
(1,620)	1:403:A:ILE:HG22	1:403:A:ILE:H	19	0.44	0.02	0.44
(1,1686)	1:402:A:ILE:HG23	1:403:A:ILE:HG12	19	0.44	0.07	0.42
(1,1686)	1:402:A:ILE:HG21	1:403:A:ILE:HG12	19	0.44	0.07	0.42
(1,1686)	1:402:A:ILE:HG22	1:403:A:ILE:HG12	19	0.44	0.07	0.42
(1,1771)	1:341:A:VAL:HG11	1:337:A:LEU:HD13	19	0.44	0.04	0.44
(1,1771)	1:341:A:VAL:HG12	1:337:A:LEU:HD11	19	0.44	0.04	0.44

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1771)	1:341:A:VAL:HG13	1:337:A:LEU:HD12	19	0.44	0.04	0.44
(1,1771)	1:341:A:VAL:HG13	1:337:A:LEU:HD11	19	0.44	0.04	0.44
(1,1771)	1:341:A:VAL:HG11	1:337:A:LEU:HD11	19	0.44	0.04	0.44
(1,1771)	1:341:A:VAL:HG12	1:337:A:LEU:HD13	19	0.44	0.04	0.44
(1,1771)	1:341:A:VAL:HG13	1:337:A:LEU:HD13	19	0.44	0.04	0.44
(1,1771)	1:341:A:VAL:HG11	1:337:A:LEU:HD12	19	0.44	0.04	0.44
(1,297)	1:366:A:ILE:HG21	1:368:A:ASP:HA	19	0.44	0.02	0.44
(1,297)	1:366:A:ILE:HG23	1:368:A:ASP:HA	19	0.44	0.02	0.44
(1,297)	1:366:A:ILE:HG22	1:368:A:ASP:HA	19	0.44	0.02	0.44
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	19	0.44	0.13	0.46
(1,1709)	1:344:A:LEU:HD23	1:345:A:LEU:H	19	0.44	0.08	0.46
(1,1709)	1:344:A:LEU:HD21	1:345:A:LEU:H	19	0.44	0.08	0.46
(1,1709)	1:344:A:LEU:HD22	1:345:A:LEU:H	19	0.44	0.08	0.46
(1,1266)	1:354:A:ILE:HD12	1:365:A:ARG:H	19	0.44	0.02	0.43
(1,1266)	1:354:A:ILE:HD13	1:365:A:ARG:H	19	0.44	0.02	0.43
(1,1266)	1:354:A:ILE:HD11	1:365:A:ARG:H	19	0.44	0.02	0.43
(1,1919)	1:367:A:VAL:HG21	1:367:A:VAL:HG13	19	0.43	0.02	0.44
(1,1919)	1:367:A:VAL:HG22	1:367:A:VAL:HG13	19	0.43	0.02	0.44
(1,1919)	1:367:A:VAL:HG23	1:367:A:VAL:HG13	19	0.43	0.02	0.44
(1,1919)	1:367:A:VAL:HG21	1:367:A:VAL:HG12	19	0.43	0.02	0.44
(1,1919)	1:367:A:VAL:HG22	1:367:A:VAL:HG11	19	0.43	0.02	0.44
(1,1919)	1:367:A:VAL:HG23	1:367:A:VAL:HG12	19	0.43	0.02	0.44
(1,1919)	1:367:A:VAL:HG21	1:367:A:VAL:HG11	19	0.43	0.02	0.44
(1,1919)	1:367:A:VAL:HG22	1:367:A:VAL:HG12	19	0.43	0.02	0.44
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG22	19	0.43	0.06	0.45
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG23	19	0.43	0.06	0.45
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG21	19	0.43	0.06	0.45
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	19	0.43	0.06	0.42
(1,456)	1:386:A:THR:HG21	1:387:A:TYR:HB2	19	0.43	0.11	0.45
(1,456)	1:386:A:THR:HG22	1:387:A:TYR:HB2	19	0.43	0.11	0.45
(1,456)	1:386:A:THR:HG23	1:387:A:TYR:HB2	19	0.43	0.11	0.45
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	19	0.43	0.01	0.43
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	19	0.42	0.01	0.42
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG23	19	0.41	0.03	0.42
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG21	19	0.41	0.03	0.42
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG22	19	0.41	0.03	0.42
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	19	0.41	0.0	0.41
(1,2784)	1:457:A:PRO:HB3	1:457:A:PRO:HD2	19	0.41	0.01	0.4
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	19	0.41	0.01	0.4
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD13	19	0.4	0.04	0.4
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD11	19	0.4	0.04	0.4
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD12	19	0.4	0.04	0.4

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2658)	1:366:A:ILE:HG21	1:411:A:LEU:HB2	19	0.4	0.05	0.39
(1,2658)	1:366:A:ILE:HG23	1:411:A:LEU:HB2	19	0.4	0.05	0.39
(1,2658)	1:366:A:ILE:HG22	1:411:A:LEU:HB2	19	0.4	0.05	0.39
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	19	0.4	0.02	0.4
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG22	19	0.4	0.13	0.42
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG21	19	0.4	0.13	0.42
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG23	19	0.4	0.13	0.42
(1,1800)	1:336:A:LEU:HD11	1:338:A:TRP:HD1	19	0.4	0.08	0.43
(1,1800)	1:336:A:LEU:HD12	1:338:A:TRP:HD1	19	0.4	0.08	0.43
(1,1800)	1:336:A:LEU:HD13	1:338:A:TRP:HD1	19	0.4	0.08	0.43
(1,1904)	1:437:A:VAL:HG11	1:438:A:LEU:HD21	19	0.39	0.04	0.39
(1,1904)	1:437:A:VAL:HG13	1:438:A:LEU:HD23	19	0.39	0.04	0.39
(1,1904)	1:437:A:VAL:HG12	1:438:A:LEU:HD23	19	0.39	0.04	0.39
(1,1904)	1:437:A:VAL:HG13	1:438:A:LEU:HD21	19	0.39	0.04	0.39
(1,1904)	1:437:A:VAL:HG12	1:438:A:LEU:HD21	19	0.39	0.04	0.39
(1,1904)	1:437:A:VAL:HG12	1:438:A:LEU:HD22	19	0.39	0.04	0.39
(1,1904)	1:437:A:VAL:HG11	1:438:A:LEU:HD23	19	0.39	0.04	0.39
(1,1904)	1:437:A:VAL:HG11	1:438:A:LEU:HD22	19	0.39	0.04	0.39
(1,1904)	1:437:A:VAL:HG13	1:438:A:LEU:HD22	19	0.39	0.04	0.39
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	19	0.39	0.01	0.39
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD23	19	0.39	0.11	0.4
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD22	19	0.39	0.11	0.4
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD21	19	0.39	0.11	0.4
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	19	0.39	0.12	0.4
(1,836)	1:430:A:LEU:HD13	1:427:A:THR:HB	19	0.39	0.64	0.24
(1,836)	1:430:A:LEU:HD12	1:427:A:THR:HB	19	0.39	0.64	0.24
(1,836)	1:430:A:LEU:HD11	1:427:A:THR:HB	19	0.39	0.64	0.24
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	19	0.39	0.05	0.4
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	19	0.39	0.1	0.38
(1,690)	1:411:A:LEU:HD21	1:369:A:PRO:HB2	19	0.39	0.05	0.4
(1,690)	1:411:A:LEU:HD22	1:369:A:PRO:HB2	19	0.39	0.05	0.4
(1,690)	1:411:A:LEU:HD23	1:369:A:PRO:HB2	19	0.39	0.05	0.4
(1,300)	1:366:A:ILE:HG21	1:411:A:LEU:HB3	19	0.39	0.06	0.39
(1,300)	1:366:A:ILE:HG23	1:411:A:LEU:HB3	19	0.39	0.06	0.39
(1,300)	1:366:A:ILE:HG22	1:411:A:LEU:HB3	19	0.39	0.06	0.39
(1,2643)	1:402:A:ILE:HD11	1:397:A:TYR:HD1	19	0.39	0.1	0.4
(1,2643)	1:402:A:ILE:HD12	1:397:A:TYR:HD1	19	0.39	0.1	0.4
(1,2643)	1:402:A:ILE:HD13	1:397:A:TYR:HD1	19	0.39	0.1	0.4
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD23	19	0.39	0.07	0.39
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD21	19	0.39	0.07	0.39
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD22	19	0.39	0.07	0.39
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD21	19	0.38	0.03	0.38

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD22	19	0.38	0.03	0.38
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD23	19	0.38	0.03	0.38
(1,2844)	1:402:A:ILE:HG21	1:397:A:TYR:HD2	19	0.38	0.13	0.37
(1,2844)	1:402:A:ILE:HG22	1:397:A:TYR:HD2	19	0.38	0.13	0.37
(1,2844)	1:402:A:ILE:HG23	1:397:A:TYR:HD2	19	0.38	0.13	0.37
(1,2844)	1:403:A:ILE:H	1:402:A:ILE:HG22	19	0.38	0.13	0.37
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	19	0.37	0.02	0.38
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG2	19	0.37	0.04	0.37
(1,2689)	1:436:A:GLN:HB3	1:436:A:GLN:HG2	19	0.37	0.04	0.37
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG3	19	0.37	0.04	0.37
(1,2872)	1:447:A:GLU:HG3	1:447:A:GLU:HB2	19	0.37	0.07	0.37
(1,2872)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	19	0.37	0.07	0.37
(1,2872)	1:444:A:GLN:HG2	1:444:A:GLN:HB3	19	0.37	0.07	0.37
(1,2872)	1:445:A:GLU:HB2	1:445:A:GLU:HG2	19	0.37	0.07	0.37
(1,2556)	1:341:A:VAL:HG12	1:364:A:PHE:HZ	19	0.37	0.07	0.39
(1,2556)	1:341:A:VAL:HG13	1:364:A:PHE:HZ	19	0.37	0.07	0.39
(1,2556)	1:341:A:VAL:HG11	1:364:A:PHE:HZ	19	0.37	0.07	0.39
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD11	19	0.37	0.02	0.36
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD12	19	0.37	0.02	0.36
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD13	19	0.37	0.02	0.36
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	19	0.36	0.01	0.37
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	19	0.36	0.13	0.34
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD21	19	0.36	0.06	0.37
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD23	19	0.36	0.06	0.37
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD22	19	0.36	0.06	0.37
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG3	19	0.36	0.02	0.37
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG2	19	0.36	0.02	0.37
(1,1897)	1:430:A:LEU:HD11	1:430:A:LEU:HD22	19	0.36	0.04	0.36
(1,1897)	1:430:A:LEU:HD13	1:430:A:LEU:HD21	19	0.36	0.04	0.36
(1,1897)	1:430:A:LEU:HD11	1:430:A:LEU:HD21	19	0.36	0.04	0.36
(1,1897)	1:430:A:LEU:HD11	1:430:A:LEU:HD23	19	0.36	0.04	0.36
(1,1897)	1:430:A:LEU:HD13	1:430:A:LEU:HD23	19	0.36	0.04	0.36
(1,1897)	1:430:A:LEU:HD12	1:430:A:LEU:HD23	19	0.36	0.04	0.36
(1,1897)	1:430:A:LEU:HD13	1:430:A:LEU:HD22	19	0.36	0.04	0.36
(1,1897)	1:430:A:LEU:HD12	1:430:A:LEU:HD22	19	0.36	0.04	0.36
(1,2697)	1:447:A:GLU:HG3	1:447:A:GLU:HB2	19	0.36	0.08	0.37
(1,2697)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	19	0.36	0.08	0.37
(1,2697)	1:445:A:GLU:HB2	1:445:A:GLU:HG2	19	0.36	0.08	0.37
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	19	0.36	0.01	0.36
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG21	19	0.36	0.05	0.35
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG22	19	0.36	0.05	0.35
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG23	19	0.36	0.05	0.35

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2618)	1:375:A:LEU:HD22	1:378:A:ASN:HB2	19	0.35	0.16	0.4
(1,2618)	1:375:A:LEU:HD21	1:378:A:ASN:HB2	19	0.35	0.16	0.4
(1,2618)	1:375:A:LEU:HD23	1:378:A:ASN:HB2	19	0.35	0.16	0.4
(1,2618)	1:433:A:LEU:HD21	1:396:A:HIS:HB3	19	0.35	0.16	0.4
(1,1921)	1:375:A:LEU:HD12	1:375:A:LEU:HD23	19	0.35	0.03	0.35
(1,1921)	1:375:A:LEU:HD12	1:375:A:LEU:HD22	19	0.35	0.03	0.35
(1,1921)	1:375:A:LEU:HD11	1:375:A:LEU:HD22	19	0.35	0.03	0.35
(1,1921)	1:375:A:LEU:HD11	1:375:A:LEU:HD21	19	0.35	0.03	0.35
(1,1921)	1:375:A:LEU:HD13	1:375:A:LEU:HD22	19	0.35	0.03	0.35
(1,1921)	1:375:A:LEU:HD13	1:375:A:LEU:HD21	19	0.35	0.03	0.35
(1,1921)	1:375:A:LEU:HD11	1:375:A:LEU:HD23	19	0.35	0.03	0.35
(1,1921)	1:375:A:LEU:HD12	1:375:A:LEU:HD21	19	0.35	0.03	0.35
(1,2527)	1:367:A:VAL:HG12	1:368:A:ASP:H	19	0.35	0.05	0.35
(1,2527)	1:367:A:VAL:HG11	1:368:A:ASP:H	19	0.35	0.05	0.35
(1,2527)	1:367:A:VAL:HG13	1:368:A:ASP:H	19	0.35	0.05	0.35
(1,1313)	1:375:A:LEU:HD13	1:376:A:TRP:H	19	0.35	0.09	0.34
(1,1313)	1:375:A:LEU:HD12	1:376:A:TRP:H	19	0.35	0.09	0.34
(1,1313)	1:375:A:LEU:HD11	1:376:A:TRP:H	19	0.35	0.09	0.34
(1,1121)	1:367:A:VAL:HG22	1:365:A:ARG:HA	19	0.35	0.13	0.32
(1,1121)	1:367:A:VAL:HG21	1:365:A:ARG:HA	19	0.35	0.13	0.32
(1,1121)	1:367:A:VAL:HG23	1:365:A:ARG:HA	19	0.35	0.13	0.32
(1,1315)	1:375:A:LEU:HD22	1:376:A:TRP:H	19	0.35	0.04	0.36
(1,1315)	1:375:A:LEU:HD21	1:376:A:TRP:H	19	0.35	0.04	0.36
(1,1315)	1:375:A:LEU:HD23	1:376:A:TRP:H	19	0.35	0.04	0.36
(1,1778)	1:337:A:LEU:HD12	1:376:A:TRP:HB3	19	0.35	0.1	0.37
(1,1778)	1:337:A:LEU:HD13	1:376:A:TRP:HB3	19	0.35	0.1	0.37
(1,1778)	1:337:A:LEU:HD11	1:376:A:TRP:HB3	19	0.35	0.1	0.37
(1,1726)	1:341:A:VAL:HG23	1:338:A:TRP:HA	19	0.35	0.03	0.34
(1,1726)	1:341:A:VAL:HG21	1:338:A:TRP:HA	19	0.35	0.03	0.34
(1,1726)	1:341:A:VAL:HG22	1:338:A:TRP:HA	19	0.35	0.03	0.34
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	19	0.35	0.01	0.35
(1,2956)	1:398:A:TYR:H	1:395:A:ARG:HA	19	0.35	0.01	0.35
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG23	19	0.34	0.04	0.35
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG22	19	0.34	0.04	0.35
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG21	19	0.34	0.04	0.35
(1,2611)	1:393:A:ALA:HB2	1:397:A:TYR:HE1	19	0.34	0.05	0.33
(1,2611)	1:393:A:ALA:HB1	1:397:A:TYR:HE1	19	0.34	0.05	0.33
(1,2611)	1:393:A:ALA:HB3	1:397:A:TYR:HE1	19	0.34	0.05	0.33
(1,108)	1:345:A:LEU:HD22	1:345:A:LEU:HB2	19	0.34	0.02	0.34
(1,108)	1:345:A:LEU:HD23	1:345:A:LEU:HB2	19	0.34	0.02	0.34
(1,108)	1:345:A:LEU:HD21	1:345:A:LEU:HB2	19	0.34	0.02	0.34
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD11	19	0.34	0.12	0.34

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD13	19	0.34	0.12	0.34
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD12	19	0.34	0.12	0.34
(1,2730)	1:366:A:ILE:HG21	1:370:A:ASN:H	19	0.34	0.05	0.32
(1,2730)	1:366:A:ILE:HG23	1:370:A:ASN:H	19	0.34	0.05	0.32
(1,2730)	1:366:A:ILE:HG23	1:373:A:ALA:H	19	0.34	0.05	0.32
(1,2730)	1:366:A:ILE:HG22	1:370:A:ASN:H	19	0.34	0.05	0.32
(1,2730)	1:366:A:ILE:HG22	1:373:A:ALA:H	19	0.34	0.05	0.32
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	19	0.33	0.02	0.34
(1,627)	1:403:A:ILE:HG23	1:413:A:PHE:HB2	19	0.33	0.05	0.34
(1,627)	1:403:A:ILE:HG22	1:413:A:PHE:HB2	19	0.33	0.05	0.34
(1,627)	1:403:A:ILE:HG21	1:413:A:PHE:HB2	19	0.33	0.05	0.34
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	19	0.33	0.05	0.33
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG21	19	0.33	0.02	0.33
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG22	19	0.33	0.02	0.33
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG23	19	0.33	0.02	0.33
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD11	19	0.33	0.06	0.33
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD12	19	0.33	0.06	0.33
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD13	19	0.33	0.06	0.33
(1,1670)	1:403:A:ILE:HG22	1:397:A:TYR:HB2	19	0.33	0.04	0.33
(1,1670)	1:403:A:ILE:HG21	1:397:A:TYR:HB2	19	0.33	0.04	0.33
(1,1670)	1:403:A:ILE:HG23	1:397:A:TYR:HB2	19	0.33	0.04	0.33
(1,2587)	1:362:A:LYS:HA	1:415:A:PHE:HD2	19	0.33	0.09	0.34
(1,2587)	1:361:A:SER:H	1:362:A:LYS:HA	19	0.33	0.09	0.34
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB3	19	0.32	0.07	0.33
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB2	19	0.32	0.07	0.33
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB1	19	0.32	0.07	0.33
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG23	19	0.32	0.04	0.32
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG22	19	0.32	0.04	0.32
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG21	19	0.32	0.04	0.32
(1,884)	1:437:A:VAL:HG23	1:392:A:ARG:HG3	19	0.32	0.3	0.18
(1,884)	1:437:A:VAL:HG22	1:392:A:ARG:HG3	19	0.32	0.3	0.18
(1,884)	1:437:A:VAL:HG21	1:392:A:ARG:HG3	19	0.32	0.3	0.18
(1,168)	1:354:A:ILE:HG22	1:354:A:ILE:HG13	19	0.32	0.01	0.32
(1,168)	1:354:A:ILE:HG21	1:354:A:ILE:HG13	19	0.32	0.01	0.32
(1,168)	1:354:A:ILE:HG23	1:354:A:ILE:HG13	19	0.32	0.01	0.32
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD22	19	0.32	0.04	0.31
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD23	19	0.32	0.04	0.31
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD21	19	0.32	0.04	0.31
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	19	0.32	0.0	0.32
(1,1912)	1:354:A:ILE:HD11	1:372:A:LEU:HD12	19	0.32	0.03	0.32
(1,1912)	1:354:A:ILE:HD12	1:372:A:LEU:HD11	19	0.32	0.03	0.32
(1,1912)	1:354:A:ILE:HD12	1:372:A:LEU:HD13	19	0.32	0.03	0.32

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1912)	1:354:A:ILE:HD11	1:372:A:LEU:HD13	19	0.32	0.03	0.32
(1,1912)	1:354:A:ILE:HD11	1:372:A:LEU:HD11	19	0.32	0.03	0.32
(1,1912)	1:354:A:ILE:HD13	1:372:A:LEU:HD13	19	0.32	0.03	0.32
(1,1912)	1:354:A:ILE:HD13	1:372:A:LEU:HD11	19	0.32	0.03	0.32
(1,1912)	1:354:A:ILE:HD13	1:372:A:LEU:HD12	19	0.32	0.03	0.32
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	19	0.32	0.02	0.32
(1,1887)	1:400:A:LEU:HD22	1:400:A:LEU:HD13	19	0.31	0.04	0.32
(1,1887)	1:400:A:LEU:HD21	1:400:A:LEU:HD11	19	0.31	0.04	0.32
(1,1887)	1:400:A:LEU:HD23	1:400:A:LEU:HD12	19	0.31	0.04	0.32
(1,1887)	1:400:A:LEU:HD23	1:400:A:LEU:HD13	19	0.31	0.04	0.32
(1,1887)	1:400:A:LEU:HD23	1:400:A:LEU:HD11	19	0.31	0.04	0.32
(1,1887)	1:400:A:LEU:HD21	1:400:A:LEU:HD13	19	0.31	0.04	0.32
(1,1887)	1:400:A:LEU:HD21	1:400:A:LEU:HD12	19	0.31	0.04	0.32
(1,1887)	1:400:A:LEU:HD22	1:400:A:LEU:HD11	19	0.31	0.04	0.32
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	19	0.31	0.12	0.28
(1,453)	1:386:A:THR:HG22	1:386:A:THR:HB	19	0.31	0.03	0.31
(1,453)	1:386:A:THR:HG21	1:386:A:THR:HB	19	0.31	0.03	0.31
(1,453)	1:386:A:THR:HG23	1:386:A:THR:HB	19	0.31	0.03	0.31
(1,1725)	1:341:A:VAL:HG22	1:342:A:TYR:HB2	19	0.31	0.02	0.3
(1,1725)	1:341:A:VAL:HG23	1:342:A:TYR:HB2	19	0.31	0.02	0.3
(1,1725)	1:341:A:VAL:HG21	1:342:A:TYR:HB2	19	0.31	0.02	0.3
(1,1497)	1:429:A:ARG:HG3	1:429:A:ARG:HB2	19	0.31	0.04	0.33
(1,1497)	1:429:A:ARG:HG2	1:429:A:ARG:HB3	19	0.31	0.04	0.33
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG23	19	0.31	0.05	0.29
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG21	19	0.31	0.05	0.29
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG22	19	0.31	0.05	0.29
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB2	19	0.3	0.03	0.3
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB3	19	0.3	0.03	0.3
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	19	0.3	0.04	0.3
(1,1600)	1:412:A:LEU:HD23	1:412:A:LEU:H	19	0.3	0.09	0.31
(1,1600)	1:412:A:LEU:HD22	1:412:A:LEU:H	19	0.3	0.09	0.31
(1,1600)	1:412:A:LEU:HD21	1:412:A:LEU:H	19	0.3	0.09	0.31
(1,1355)	1:395:A:ARG:HB3	1:395:A:ARG:HG2	19	0.29	0.03	0.3
(1,1355)	1:395:A:ARG:HB2	1:395:A:ARG:HG3	19	0.29	0.03	0.3
(1,1908)	1:341:A:VAL:HG22	1:345:A:LEU:HD12	19	0.29	0.02	0.29
(1,1908)	1:341:A:VAL:HG23	1:345:A:LEU:HD12	19	0.29	0.02	0.29
(1,1908)	1:341:A:VAL:HG22	1:345:A:LEU:HD13	19	0.29	0.02	0.29
(1,1908)	1:341:A:VAL:HG21	1:345:A:LEU:HD12	19	0.29	0.02	0.29
(1,1908)	1:341:A:VAL:HG21	1:345:A:LEU:HD11	19	0.29	0.02	0.29
(1,1908)	1:341:A:VAL:HG21	1:345:A:LEU:HD13	19	0.29	0.02	0.29
(1,1908)	1:341:A:VAL:HG23	1:345:A:LEU:HD13	19	0.29	0.02	0.29
(1,1908)	1:341:A:VAL:HG22	1:345:A:LEU:HD11	19	0.29	0.02	0.29

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1894)	1:411:A:LEU:HD23	1:411:A:LEU:HD13	19	0.29	0.02	0.3
(1,1894)	1:411:A:LEU:HD23	1:411:A:LEU:HD11	19	0.29	0.02	0.3
(1,1894)	1:411:A:LEU:HD21	1:411:A:LEU:HD12	19	0.29	0.02	0.3
(1,1894)	1:411:A:LEU:HD21	1:411:A:LEU:HD13	19	0.29	0.02	0.3
(1,1894)	1:411:A:LEU:HD22	1:411:A:LEU:HD11	19	0.29	0.02	0.3
(1,1894)	1:411:A:LEU:HD21	1:411:A:LEU:HD11	19	0.29	0.02	0.3
(1,1894)	1:411:A:LEU:HD23	1:411:A:LEU:HD12	19	0.29	0.02	0.3
(1,1084)	1:372:A:LEU:HD12	1:344:A:LEU:HD13	19	0.29	0.09	0.27
(1,1084)	1:372:A:LEU:HD11	1:344:A:LEU:HD13	19	0.29	0.09	0.27
(1,1084)	1:372:A:LEU:HD13	1:344:A:LEU:HD13	19	0.29	0.09	0.27
(1,1084)	1:372:A:LEU:HD13	1:344:A:LEU:HD11	19	0.29	0.09	0.27
(1,1084)	1:372:A:LEU:HD11	1:344:A:LEU:HD12	19	0.29	0.09	0.27
(1,1084)	1:372:A:LEU:HD11	1:344:A:LEU:HD11	19	0.29	0.09	0.27
(1,1084)	1:372:A:LEU:HD12	1:344:A:LEU:HD12	19	0.29	0.09	0.27
(1,1084)	1:372:A:LEU:HD13	1:344:A:LEU:HD12	19	0.29	0.09	0.27
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	19	0.28	0.01	0.29
(1,1884)	1:394:A:LEU:HD11	1:394:A:LEU:HD23	19	0.28	0.02	0.29
(1,1884)	1:394:A:LEU:HD11	1:394:A:LEU:HD21	19	0.28	0.02	0.29
(1,1884)	1:394:A:LEU:HD13	1:394:A:LEU:HD22	19	0.28	0.02	0.29
(1,1884)	1:394:A:LEU:HD12	1:394:A:LEU:HD22	19	0.28	0.02	0.29
(1,1884)	1:394:A:LEU:HD11	1:394:A:LEU:HD22	19	0.28	0.02	0.29
(1,1884)	1:394:A:LEU:HD13	1:394:A:LEU:HD21	19	0.28	0.02	0.29
(1,1884)	1:394:A:LEU:HD12	1:394:A:LEU:HD23	19	0.28	0.02	0.29
(1,1884)	1:394:A:LEU:HD12	1:394:A:LEU:HD21	19	0.28	0.02	0.29
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG12	19	0.27	0.03	0.28
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG11	19	0.27	0.03	0.28
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG13	19	0.27	0.03	0.28
(1,2557)	1:341:A:VAL:HG12	1:403:A:ILE:HD13	19	0.27	0.09	0.27
(1,2557)	1:341:A:VAL:HG13	1:403:A:ILE:HD13	19	0.27	0.09	0.27
(1,2557)	1:341:A:VAL:HG11	1:403:A:ILE:HD12	19	0.27	0.09	0.27
(1,2557)	1:341:A:VAL:HG11	1:403:A:ILE:HD11	19	0.27	0.09	0.27
(1,2557)	1:341:A:VAL:HG12	1:403:A:ILE:HD12	19	0.27	0.09	0.27
(1,2557)	1:341:A:VAL:HG13	1:403:A:ILE:HD11	19	0.27	0.09	0.27
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	19	0.27	0.0	0.27
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	19	0.27	0.02	0.27
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	19	0.27	0.02	0.26
(1,1916)	1:366:A:ILE:HG21	1:411:A:LEU:HD13	19	0.26	0.03	0.26
(1,1916)	1:366:A:ILE:HG23	1:411:A:LEU:HD11	19	0.26	0.03	0.26
(1,1916)	1:366:A:ILE:HG22	1:411:A:LEU:HD13	19	0.26	0.03	0.26
(1,1916)	1:366:A:ILE:HG23	1:411:A:LEU:HD12	19	0.26	0.03	0.26
(1,1916)	1:366:A:ILE:HG21	1:411:A:LEU:HD12	19	0.26	0.03	0.26
(1,1916)	1:366:A:ILE:HG23	1:411:A:LEU:HD13	19	0.26	0.03	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1916)	1:366:A:ILE:HG22	1:411:A:LEU:HD11	19	0.26	0.03	0.26
(1,1916)	1:366:A:ILE:HG22	1:411:A:LEU:HD12	19	0.26	0.03	0.26
(1,309)	1:366:A:ILE:HD11	1:364:A:PHE:HZ	19	0.26	0.02	0.26
(1,309)	1:366:A:ILE:HD12	1:364:A:PHE:HZ	19	0.26	0.02	0.26
(1,309)	1:366:A:ILE:HD13	1:364:A:PHE:HZ	19	0.26	0.02	0.26
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD13	19	0.26	0.04	0.25
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD11	19	0.26	0.04	0.25
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD12	19	0.26	0.04	0.25
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	19	0.25	0.17	0.22
(1,454)	1:386:A:THR:HG21	1:370:A:ASN:HA	19	0.25	0.07	0.25
(1,454)	1:386:A:THR:HG23	1:370:A:ASN:HA	19	0.25	0.07	0.25
(1,454)	1:386:A:THR:HG22	1:370:A:ASN:HA	19	0.25	0.07	0.25
(1,1903)	1:438:A:LEU:HD23	1:438:A:LEU:HD12	19	0.25	0.04	0.26
(1,1903)	1:438:A:LEU:HD22	1:438:A:LEU:HD12	19	0.25	0.04	0.26
(1,1903)	1:438:A:LEU:HD22	1:438:A:LEU:HD11	19	0.25	0.04	0.26
(1,1903)	1:438:A:LEU:HD21	1:438:A:LEU:HD11	19	0.25	0.04	0.26
(1,1903)	1:438:A:LEU:HD23	1:438:A:LEU:HD13	19	0.25	0.04	0.26
(1,1903)	1:438:A:LEU:HD23	1:438:A:LEU:HD11	19	0.25	0.04	0.26
(1,1903)	1:438:A:LEU:HD22	1:438:A:LEU:HD13	19	0.25	0.04	0.26
(1,1903)	1:438:A:LEU:HD21	1:438:A:LEU:HD13	19	0.25	0.04	0.26
(1,1903)	1:438:A:LEU:HD21	1:438:A:LEU:HD12	19	0.25	0.04	0.26
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD2	19	0.25	0.04	0.24
(1,2656)	1:410:A:ARG:HB2	1:410:A:ARG:HD3	19	0.25	0.04	0.24
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD3	19	0.25	0.04	0.24
(1,1901)	1:433:A:LEU:HD23	1:433:A:LEU:HD11	19	0.25	0.04	0.26
(1,1901)	1:433:A:LEU:HD23	1:433:A:LEU:HD12	19	0.25	0.04	0.26
(1,1901)	1:433:A:LEU:HD21	1:433:A:LEU:HD12	19	0.25	0.04	0.26
(1,1901)	1:433:A:LEU:HD21	1:433:A:LEU:HD11	19	0.25	0.04	0.26
(1,1901)	1:433:A:LEU:HD23	1:433:A:LEU:HD13	19	0.25	0.04	0.26
(1,1901)	1:433:A:LEU:HD22	1:433:A:LEU:HD11	19	0.25	0.04	0.26
(1,1901)	1:433:A:LEU:HD21	1:433:A:LEU:HD13	19	0.25	0.04	0.26
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	19	0.25	0.01	0.25
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	19	0.24	0.01	0.25
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD22	19	0.24	0.05	0.25
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD21	19	0.24	0.05	0.25
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD23	19	0.24	0.05	0.25
(1,174)	1:354:A:ILE:HD13	1:341:A:VAL:HA	19	0.24	0.05	0.25
(1,174)	1:354:A:ILE:HD11	1:341:A:VAL:HA	19	0.24	0.05	0.25
(1,174)	1:354:A:ILE:HD12	1:341:A:VAL:HA	19	0.24	0.05	0.25
(1,2659)	1:366:A:ILE:HD13	1:411:A:LEU:HB3	19	0.24	0.06	0.25
(1,2659)	1:366:A:ILE:HD11	1:411:A:LEU:HB3	19	0.24	0.06	0.25
(1,2659)	1:366:A:ILE:HD12	1:411:A:LEU:HB3	19	0.24	0.06	0.25

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2659)	1:366:A:ILE:HG22	1:411:A:LEU:HB3	19	0.24	0.06	0.25
(1,2659)	1:366:A:ILE:HG21	1:411:A:LEU:HB3	19	0.24	0.06	0.25
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	19	0.24	0.03	0.24
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG22	19	0.24	0.01	0.24
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG21	19	0.24	0.01	0.24
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG23	19	0.24	0.01	0.24
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD13	19	0.23	0.04	0.23
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD11	19	0.23	0.04	0.23
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD12	19	0.23	0.04	0.23
(1,1892)	1:403:A:ILE:HD13	1:402:A:ILE:HG23	19	0.23	0.07	0.23
(1,1892)	1:403:A:ILE:HD13	1:402:A:ILE:HG21	19	0.23	0.07	0.23
(1,1892)	1:403:A:ILE:HD12	1:402:A:ILE:HG23	19	0.23	0.07	0.23
(1,1892)	1:403:A:ILE:HD12	1:402:A:ILE:HG22	19	0.23	0.07	0.23
(1,1892)	1:403:A:ILE:HD11	1:402:A:ILE:HG21	19	0.23	0.07	0.23
(1,1892)	1:403:A:ILE:HD13	1:402:A:ILE:HG22	19	0.23	0.07	0.23
(1,1892)	1:403:A:ILE:HD12	1:402:A:ILE:HG21	19	0.23	0.07	0.23
(1,1892)	1:403:A:ILE:HD11	1:402:A:ILE:HG22	19	0.23	0.07	0.23
(1,1078)	1:372:A:LEU:HD13	1:340:A:TYR:HE2	19	0.23	0.02	0.24
(1,1078)	1:372:A:LEU:HD12	1:340:A:TYR:HE2	19	0.23	0.02	0.24
(1,1078)	1:372:A:LEU:HD11	1:340:A:TYR:HE2	19	0.23	0.02	0.24
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	19	0.22	0.04	0.23
(1,1207)	1:360:A:GLU:HB3	1:360:A:GLU:HG2	19	0.22	0.04	0.23
(1,1207)	1:360:A:GLU:HB2	1:360:A:GLU:HG3	19	0.22	0.04	0.23
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD2	19	0.22	0.03	0.21
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD3	19	0.22	0.03	0.21
(1,2686)	1:430:A:LEU:HD11	1:430:A:LEU:HD22	19	0.22	0.04	0.22
(1,2686)	1:430:A:LEU:HD13	1:430:A:LEU:HD21	19	0.22	0.04	0.22
(1,2686)	1:430:A:LEU:HD11	1:430:A:LEU:HD21	19	0.22	0.04	0.22
(1,2686)	1:430:A:LEU:HD13	1:402:A:ILE:HD13	19	0.22	0.04	0.22
(1,2686)	1:430:A:LEU:HD13	1:430:A:LEU:HD23	19	0.22	0.04	0.22
(1,2686)	1:430:A:LEU:HD12	1:430:A:LEU:HD23	19	0.22	0.04	0.22
(1,2686)	1:430:A:LEU:HD13	1:430:A:LEU:HD22	19	0.22	0.04	0.22
(1,2686)	1:430:A:LEU:HD11	1:430:A:LEU:HD23	19	0.22	0.04	0.22
(1,2686)	1:430:A:LEU:HD12	1:430:A:LEU:HD22	19	0.22	0.04	0.22
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD21	19	0.21	0.01	0.22
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD23	19	0.21	0.01	0.22
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD22	19	0.21	0.01	0.22
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	19	0.21	0.01	0.21
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	19	0.21	0.01	0.21
(1,2610)	1:372:A:LEU:HA	1:375:A:LEU:HG	19	0.21	0.01	0.21
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	19	0.2	0.0	0.2
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG11	19	0.2	0.04	0.21

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG13	19	0.2	0.04	0.21
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG12	19	0.2	0.04	0.21
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG22	19	0.2	0.01	0.2
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG23	19	0.2	0.01	0.2
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG21	19	0.2	0.01	0.2
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	19	0.2	0.01	0.2
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB2	19	0.19	0.03	0.19
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB3	19	0.19	0.03	0.19
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB1	19	0.19	0.03	0.19
(1,42)	1:341:A:VAL:HG22	1:415:A:PHE:HE2	19	0.19	0.03	0.19
(1,42)	1:341:A:VAL:HG23	1:415:A:PHE:HE2	19	0.19	0.03	0.19
(1,42)	1:341:A:VAL:HG21	1:415:A:PHE:HE2	19	0.19	0.03	0.19
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD21	19	0.18	0.02	0.18
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD23	19	0.18	0.02	0.18
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD22	19	0.18	0.02	0.18
(1,49)	1:341:A:VAL:HG22	1:342:A:TYR:HA	19	0.17	0.01	0.17
(1,49)	1:341:A:VAL:HG23	1:342:A:TYR:HA	19	0.17	0.01	0.17
(1,49)	1:341:A:VAL:HG21	1:342:A:TYR:HA	19	0.17	0.01	0.17
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	19	0.17	0.0	0.17
(1,595)	1:400:A:LEU:HD23	1:400:A:LEU:HG	19	0.16	0.03	0.16
(1,595)	1:400:A:LEU:HD22	1:400:A:LEU:HG	19	0.16	0.03	0.16
(1,595)	1:400:A:LEU:HD21	1:400:A:LEU:HG	19	0.16	0.03	0.16
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG22	19	0.16	0.01	0.16
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG21	19	0.16	0.01	0.16
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG23	19	0.16	0.01	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	19	0.16	0.0	0.16
(1,37)	1:341:A:VAL:HG12	1:341:A:VAL:HG23	19	0.16	0.02	0.16
(1,37)	1:341:A:VAL:HG13	1:341:A:VAL:HG21	19	0.16	0.02	0.16
(1,37)	1:341:A:VAL:HG11	1:341:A:VAL:HG23	19	0.16	0.02	0.16
(1,37)	1:341:A:VAL:HG11	1:341:A:VAL:HG22	19	0.16	0.02	0.16
(1,37)	1:341:A:VAL:HG12	1:341:A:VAL:HG22	19	0.16	0.02	0.16
(1,37)	1:341:A:VAL:HG13	1:341:A:VAL:HG22	19	0.16	0.02	0.16
(1,37)	1:341:A:VAL:HG12	1:341:A:VAL:HG21	19	0.16	0.02	0.16
(1,37)	1:341:A:VAL:HG11	1:341:A:VAL:HG21	19	0.16	0.02	0.16
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	19	0.16	0.03	0.16
(1,959)	1:449:A:THR:HG22	1:449:A:THR:HB	19	0.15	0.01	0.15
(1,959)	1:449:A:THR:HG21	1:449:A:THR:HB	19	0.15	0.01	0.15
(1,959)	1:449:A:THR:HG23	1:449:A:THR:HB	19	0.15	0.01	0.15
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	19	0.15	0.02	0.15
(1,812)	1:418:A:THR:H	1:418:A:THR:HG21	19	0.14	0.02	0.14
(1,812)	1:418:A:THR:H	1:418:A:THR:HG22	19	0.14	0.02	0.14
(1,812)	1:418:A:THR:H	1:418:A:THR:HG23	19	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD12	19	0.14	0.01	0.14
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD13	19	0.14	0.01	0.14
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD11	19	0.14	0.01	0.14
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	19	0.14	0.02	0.14
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	19	0.13	0.01	0.13
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	18	3.82	0.88	4.0
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	18	2.77	0.16	2.8
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	18	2.76	0.12	2.73
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	18	2.46	0.19	2.46
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	18	2.05	0.16	2.05
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	18	1.88	0.11	1.88
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	18	1.28	0.47	1.16
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	18	1.24	0.05	1.23
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	18	1.11	0.18	1.14
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	18	0.91	0.04	0.92
(1,1496)	1:430:A:LEU:HD22	1:427:A:THR:HA	18	0.82	0.08	0.82
(1,1496)	1:430:A:LEU:HD23	1:427:A:THR:HA	18	0.82	0.08	0.82
(1,1496)	1:430:A:LEU:HD21	1:427:A:THR:HA	18	0.82	0.08	0.82
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	18	0.74	0.27	0.82
(1,1522)	1:422:A:ILE:HG22	1:430:A:LEU:HG	18	0.73	0.13	0.76
(1,1522)	1:422:A:ILE:HG21	1:430:A:LEU:HG	18	0.73	0.13	0.76
(1,1522)	1:422:A:ILE:HG23	1:430:A:LEU:HG	18	0.73	0.13	0.76
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG23	18	0.67	0.12	0.72
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG21	18	0.67	0.12	0.72
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG22	18	0.67	0.12	0.72
(1,843)	1:430:A:LEU:HD21	1:336:A:LEU:HD11	18	0.66	0.07	0.68
(1,843)	1:430:A:LEU:HD22	1:336:A:LEU:HD11	18	0.66	0.07	0.68
(1,843)	1:430:A:LEU:HD23	1:336:A:LEU:HD11	18	0.66	0.07	0.68
(1,843)	1:430:A:LEU:HD23	1:336:A:LEU:HD12	18	0.66	0.07	0.68
(1,843)	1:430:A:LEU:HD21	1:336:A:LEU:HD13	18	0.66	0.07	0.68
(1,843)	1:430:A:LEU:HD23	1:336:A:LEU:HD13	18	0.66	0.07	0.68
(1,843)	1:430:A:LEU:HD22	1:336:A:LEU:HD12	18	0.66	0.07	0.68
(1,843)	1:430:A:LEU:HD21	1:336:A:LEU:HD12	18	0.66	0.07	0.68
(1,458)	1:386:A:THR:HG23	1:389:A:LYS:HD2	18	0.65	0.11	0.65
(1,458)	1:386:A:THR:HG22	1:389:A:LYS:HD2	18	0.65	0.11	0.65
(1,458)	1:386:A:THR:HG21	1:389:A:LYS:HD2	18	0.65	0.11	0.65
(1,2797)	1:433:A:LEU:HD11	1:434:A:GLU:HA	18	0.59	0.27	0.55
(1,2797)	1:433:A:LEU:HD13	1:434:A:GLU:HA	18	0.59	0.27	0.55
(1,2797)	1:430:A:LEU:HA	1:433:A:LEU:HD11	18	0.59	0.27	0.55
(1,2797)	1:433:A:LEU:HD12	1:434:A:GLU:HA	18	0.59	0.27	0.55
(1,2640)	1:400:A:LEU:HD21	1:402:A:ILE:HD12	18	0.58	0.1	0.56
(1,2640)	1:400:A:LEU:HD21	1:430:A:LEU:HD23	18	0.58	0.1	0.56

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2640)	1:400:A:LEU:HD22	1:402:A:ILE:HD12	18	0.58	0.1	0.56
(1,2640)	1:400:A:LEU:HD21	1:430:A:LEU:HD22	18	0.58	0.1	0.56
(1,2640)	1:400:A:LEU:HD21	1:430:A:LEU:HD21	18	0.58	0.1	0.56
(1,2640)	1:400:A:LEU:HD22	1:402:A:ILE:HD11	18	0.58	0.1	0.56
(1,2640)	1:400:A:LEU:HD23	1:430:A:LEU:HD22	18	0.58	0.1	0.56
(1,2640)	1:400:A:LEU:HD23	1:402:A:ILE:HD11	18	0.58	0.1	0.56
(1,2640)	1:400:A:LEU:HD23	1:402:A:ILE:HD13	18	0.58	0.1	0.56
(1,2640)	1:400:A:LEU:HD22	1:430:A:LEU:HD21	18	0.58	0.1	0.56
(1,2640)	1:400:A:LEU:HD22	1:430:A:LEU:HD23	18	0.58	0.1	0.56
(1,2640)	1:400:A:LEU:HD21	1:402:A:ILE:HD13	18	0.58	0.1	0.56
(1,2748)	1:359:A:LYS:HA	1:358:A:ASP:HB3	18	0.54	0.15	0.57
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE2	18	0.54	0.15	0.57
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE3	18	0.54	0.15	0.57
(1,1133)	1:367:A:VAL:HG12	1:352:A:ASN:HB3	18	0.53	0.15	0.56
(1,1133)	1:367:A:VAL:HG13	1:352:A:ASN:HB3	18	0.53	0.15	0.56
(1,1133)	1:367:A:VAL:HG11	1:352:A:ASN:HB3	18	0.53	0.15	0.56
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD23	18	0.5	0.13	0.54
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD22	18	0.5	0.13	0.54
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD21	18	0.5	0.13	0.54
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	18	0.46	0.4	0.22
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD21	18	0.45	0.16	0.46
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD23	18	0.45	0.16	0.46
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD22	18	0.45	0.16	0.46
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD11	18	0.42	0.08	0.45
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD12	18	0.42	0.08	0.45
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD13	18	0.42	0.08	0.45
(1,834)	1:430:A:LEU:HD12	1:397:A:TYR:HD1	18	0.41	0.1	0.44
(1,834)	1:430:A:LEU:HD11	1:397:A:TYR:HD1	18	0.41	0.1	0.44
(1,834)	1:430:A:LEU:HD13	1:397:A:TYR:HD1	18	0.41	0.1	0.44
(1,1021)	1:437:A:VAL:HG13	1:396:A:HIS:HD2	18	0.4	0.06	0.4
(1,1021)	1:437:A:VAL:HG12	1:396:A:HIS:HD2	18	0.4	0.06	0.4
(1,1021)	1:437:A:VAL:HG11	1:396:A:HIS:HD2	18	0.4	0.06	0.4
(1,1899)	1:430:A:LEU:HD11	1:400:A:LEU:HD21	18	0.4	0.18	0.39
(1,1899)	1:430:A:LEU:HD13	1:400:A:LEU:HD23	18	0.4	0.18	0.39
(1,1899)	1:430:A:LEU:HD13	1:400:A:LEU:HD22	18	0.4	0.18	0.39
(1,1899)	1:430:A:LEU:HD12	1:400:A:LEU:HD22	18	0.4	0.18	0.39
(1,1899)	1:430:A:LEU:HD12	1:400:A:LEU:HD23	18	0.4	0.18	0.39
(1,1899)	1:430:A:LEU:HD11	1:400:A:LEU:HD23	18	0.4	0.18	0.39
(1,1899)	1:430:A:LEU:HD13	1:400:A:LEU:HD21	18	0.4	0.18	0.39
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	18	0.39	0.05	0.4
(1,2972)	1:435:A:SER:H	1:436:A:GLN:HG3	18	0.39	0.22	0.34
(1,2972)	1:435:A:SER:H	1:434:A:GLU:HG2	18	0.39	0.22	0.34

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1422)	1:451:A:ALA:HB1	1:450:A:ILE:HA	18	0.38	0.06	0.37
(1,1422)	1:451:A:ALA:HB3	1:450:A:ILE:HA	18	0.38	0.06	0.37
(1,1422)	1:451:A:ALA:HB2	1:450:A:ILE:HA	18	0.38	0.06	0.37
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD21	18	0.38	0.02	0.38
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD23	18	0.38	0.02	0.38
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD22	18	0.38	0.02	0.38
(1,2974)	1:433:A:LEU:H	1:431:A:GLU:HB2	18	0.38	0.13	0.38
(1,2974)	1:433:A:LEU:H	1:436:A:GLN:HB2	18	0.38	0.13	0.38
(1,2974)	1:433:A:LEU:H	1:436:A:GLN:HB3	18	0.38	0.13	0.38
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	18	0.38	0.13	0.32
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG22	18	0.37	0.26	0.24
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG23	18	0.37	0.26	0.24
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG21	18	0.37	0.26	0.24
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	18	0.35	0.11	0.35
(1,1802)	1:336:A:LEU:HD13	1:431:A:GLU:HA	18	0.35	0.12	0.4
(1,1802)	1:336:A:LEU:HD11	1:431:A:GLU:HA	18	0.35	0.12	0.4
(1,1802)	1:336:A:LEU:HD12	1:431:A:GLU:HA	18	0.35	0.12	0.4
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD3	18	0.34	0.08	0.34
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD2	18	0.34	0.08	0.34
(1,34)	1:341:A:VAL:HG11	1:337:A:LEU:HG	18	0.33	0.05	0.33
(1,34)	1:341:A:VAL:HG12	1:337:A:LEU:HG	18	0.33	0.05	0.33
(1,34)	1:341:A:VAL:HG13	1:337:A:LEU:HG	18	0.33	0.05	0.33
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD21	18	0.33	0.02	0.32
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD23	18	0.33	0.02	0.32
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD22	18	0.33	0.02	0.32
(1,1895)	1:411:A:LEU:HD22	1:366:A:ILE:HD13	18	0.33	0.08	0.31
(1,1895)	1:411:A:LEU:HD22	1:366:A:ILE:HD11	18	0.33	0.08	0.31
(1,1895)	1:411:A:LEU:HD22	1:366:A:ILE:HD12	18	0.33	0.08	0.31
(1,1895)	1:411:A:LEU:HD23	1:366:A:ILE:HD13	18	0.33	0.08	0.31
(1,1895)	1:411:A:LEU:HD23	1:366:A:ILE:HD11	18	0.33	0.08	0.31
(1,1895)	1:411:A:LEU:HD21	1:366:A:ILE:HD11	18	0.33	0.08	0.31
(1,1895)	1:411:A:LEU:HD23	1:366:A:ILE:HD12	18	0.33	0.08	0.31
(1,1895)	1:411:A:LEU:HD21	1:366:A:ILE:HD12	18	0.33	0.08	0.31
(1,2597)	1:358:A:ASP:HB3	1:363:A:ILE:HG22	18	0.32	0.18	0.28
(1,2597)	1:358:A:ASP:HB3	1:363:A:ILE:HG21	18	0.32	0.18	0.28
(1,2597)	1:358:A:ASP:HB2	1:363:A:ILE:HG22	18	0.32	0.18	0.28
(1,2597)	1:358:A:ASP:HB2	1:363:A:ILE:HG23	18	0.32	0.18	0.28
(1,2597)	1:358:A:ASP:HB2	1:363:A:ILE:HG21	18	0.32	0.18	0.28
(1,2597)	1:358:A:ASP:HB3	1:363:A:ILE:HG23	18	0.32	0.18	0.28
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD21	18	0.31	0.1	0.3
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD22	18	0.31	0.1	0.3
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD23	18	0.31	0.1	0.3

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD12	18	0.31	0.11	0.28
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD11	18	0.31	0.11	0.28
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD13	18	0.31	0.11	0.28
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB1	18	0.3	0.11	0.29
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB3	18	0.3	0.11	0.29
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB2	18	0.3	0.11	0.29
(1,306)	1:354:A:ILE:HD11	1:366:A:ILE:HG23	18	0.3	0.08	0.3
(1,306)	1:354:A:ILE:HD12	1:366:A:ILE:HG22	18	0.3	0.08	0.3
(1,306)	1:354:A:ILE:HD12	1:366:A:ILE:HG21	18	0.3	0.08	0.3
(1,306)	1:354:A:ILE:HD11	1:366:A:ILE:HG21	18	0.3	0.08	0.3
(1,306)	1:354:A:ILE:HD11	1:366:A:ILE:HG22	18	0.3	0.08	0.3
(1,306)	1:354:A:ILE:HD13	1:366:A:ILE:HG23	18	0.3	0.08	0.3
(1,306)	1:354:A:ILE:HD13	1:366:A:ILE:HG21	18	0.3	0.08	0.3
(1,306)	1:354:A:ILE:HD13	1:366:A:ILE:HG22	18	0.3	0.08	0.3
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD22	18	0.26	0.04	0.26
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD23	18	0.26	0.04	0.26
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD12	18	0.26	0.04	0.26
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD21	18	0.26	0.04	0.26
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	18	0.24	0.13	0.18
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG21	18	0.24	0.03	0.24
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG23	18	0.24	0.03	0.24
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG22	18	0.24	0.03	0.24
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD13	18	0.23	0.06	0.25
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD12	18	0.23	0.06	0.25
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD11	18	0.23	0.06	0.25
(1,902)	1:438:A:LEU:HD12	1:376:A:TRP:HZ2	18	0.23	0.04	0.22
(1,902)	1:438:A:LEU:HD13	1:376:A:TRP:HZ2	18	0.23	0.04	0.22
(1,902)	1:438:A:LEU:HD11	1:376:A:TRP:HZ2	18	0.23	0.04	0.22
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	18	0.22	0.03	0.2
(1,104)	1:345:A:LEU:HD22	1:356:A:TRP:HE3	18	0.21	0.06	0.24
(1,104)	1:345:A:LEU:HD23	1:356:A:TRP:HE3	18	0.21	0.06	0.24
(1,104)	1:345:A:LEU:HD21	1:356:A:TRP:HE3	18	0.21	0.06	0.24
(1,1267)	1:354:A:ILE:HD11	1:367:A:VAL:H	18	0.19	0.07	0.17
(1,1267)	1:354:A:ILE:HD12	1:367:A:VAL:H	18	0.19	0.07	0.17
(1,1267)	1:354:A:ILE:HD13	1:367:A:VAL:H	18	0.19	0.07	0.17
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	18	0.19	0.05	0.18
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	18	0.18	0.06	0.15
(1,903)	1:438:A:LEU:HD22	1:438:A:LEU:HB3	18	0.18	0.03	0.18
(1,903)	1:438:A:LEU:HD21	1:438:A:LEU:HB3	18	0.18	0.03	0.18
(1,903)	1:438:A:LEU:HD23	1:438:A:LEU:HB3	18	0.18	0.03	0.18
(1,41)	1:341:A:VAL:HG23	1:364:A:PHE:HZ	18	0.18	0.02	0.19
(1,41)	1:341:A:VAL:HG21	1:364:A:PHE:HZ	18	0.18	0.02	0.19

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,41)	1:341:A:VAL:HG22	1:364:A:PHE:HZ	18	0.18	0.02	0.19
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD21	18	0.15	0.01	0.15
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD23	18	0.15	0.01	0.15
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD22	18	0.15	0.01	0.15
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	18	0.14	0.02	0.14
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	18	0.14	0.01	0.14
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG12	18	0.13	0.01	0.13
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG13	18	0.13	0.01	0.13
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG11	18	0.13	0.01	0.13
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	17	3.37	0.38	3.33
(1,2629)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	17	3.0	0.36	2.95
(1,2629)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	17	3.0	0.36	2.95
(1,2629)	1:395:A:ARG:HD3	1:398:A:TYR:HE1	17	3.0	0.36	2.95
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD23	17	2.87	0.44	2.94
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD22	17	2.87	0.44	2.94
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD21	17	2.87	0.44	2.94
(1,388)	1:375:A:LEU:HD23	1:350:A:TYR:HE2	17	2.83	0.59	3.07
(1,388)	1:375:A:LEU:HD22	1:350:A:TYR:HE2	17	2.83	0.59	3.07
(1,388)	1:375:A:LEU:HD21	1:350:A:TYR:HE2	17	2.83	0.59	3.07
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	17	2.56	0.48	2.42
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	17	2.2	0.6	2.04
(1,382)	1:375:A:LEU:HD12	1:350:A:TYR:HD2	17	2.09	0.37	2.22
(1,382)	1:375:A:LEU:HD11	1:350:A:TYR:HD2	17	2.09	0.37	2.22
(1,382)	1:375:A:LEU:HD13	1:350:A:TYR:HD2	17	2.09	0.37	2.22
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	17	1.91	0.61	2.15
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	17	1.87	0.56	1.75
(1,2795)	1:433:A:LEU:HD23	1:440:A:GLU:HG2	17	1.42	0.32	1.46
(1,2795)	1:433:A:LEU:HD22	1:440:A:GLU:HG2	17	1.42	0.32	1.46
(1,2795)	1:433:A:LEU:HD21	1:440:A:GLU:HG2	17	1.42	0.32	1.46
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	17	1.37	0.05	1.38
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	17	1.33	0.65	1.08
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	17	1.21	0.27	1.21
(1,2793)	1:433:A:LEU:HD22	1:429:A:ARG:HA	17	0.79	0.15	0.76
(1,2793)	1:433:A:LEU:HD23	1:429:A:ARG:HA	17	0.79	0.15	0.76
(1,2793)	1:433:A:LEU:HD21	1:429:A:ARG:HA	17	0.79	0.15	0.76
(1,2793)	1:433:A:LEU:HD21	1:393:A:ALA:HA	17	0.79	0.15	0.76
(1,1424)	1:450:A:ILE:HG23	1:452:A:SER:HB2	17	0.74	0.26	0.66
(1,1424)	1:450:A:ILE:HG21	1:452:A:SER:HB2	17	0.74	0.26	0.66
(1,1424)	1:450:A:ILE:HG22	1:452:A:SER:HB2	17	0.74	0.26	0.66
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	17	0.74	0.22	0.84
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	17	0.67	0.13	0.72
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	17	0.67	0.08	0.66

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	17	0.66	0.31	0.71
(1,2813)	1:418:A:THR:HG22	1:362:A:LYS:HD3	17	0.63	0.21	0.59
(1,2813)	1:418:A:THR:HG21	1:362:A:LYS:HD2	17	0.63	0.21	0.59
(1,2813)	1:418:A:THR:HG22	1:362:A:LYS:HD2	17	0.63	0.21	0.59
(1,2813)	1:418:A:THR:HG23	1:362:A:LYS:HD2	17	0.63	0.21	0.59
(1,2813)	1:418:A:THR:HG21	1:362:A:LYS:HD3	17	0.63	0.21	0.59
(1,2813)	1:418:A:THR:HG23	1:362:A:LYS:HD3	17	0.63	0.21	0.59
(1,2681)	1:418:A:THR:HG23	1:342:A:TYR:HD1	17	0.62	0.15	0.62
(1,2681)	1:418:A:THR:HG21	1:342:A:TYR:HD1	17	0.62	0.15	0.62
(1,2681)	1:418:A:THR:HG22	1:342:A:TYR:HD1	17	0.62	0.15	0.62
(1,1393)	1:386:A:THR:HG22	1:388:A:GLU:HB3	17	0.62	0.26	0.63
(1,1393)	1:386:A:THR:HG21	1:388:A:GLU:HB3	17	0.62	0.26	0.63
(1,1393)	1:386:A:THR:HG23	1:388:A:GLU:HB3	17	0.62	0.26	0.63
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	17	0.61	0.08	0.6
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	17	0.6	0.08	0.59
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	17	0.6	0.06	0.6
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	17	0.53	0.15	0.5
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB3	17	0.51	0.07	0.5
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB2	17	0.51	0.07	0.5
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	17	0.5	0.02	0.5
(1,2555)	1:340:A:TYR:HA	1:339:A:ASP:HB3	17	0.44	0.17	0.39
(1,2555)	1:340:A:TYR:HA	1:343:A:GLN:HG2	17	0.44	0.17	0.39
(1,2555)	1:340:A:TYR:HA	1:339:A:ASP:HB2	17	0.44	0.17	0.39
(1,5)	1:337:A:LEU:HD22	1:390:A:MET:HG3	17	0.42	0.18	0.46
(1,5)	1:337:A:LEU:HD21	1:390:A:MET:HG3	17	0.42	0.18	0.46
(1,5)	1:337:A:LEU:HD23	1:390:A:MET:HG3	17	0.42	0.18	0.46
(1,1480)	1:412:A:LEU:HD21	1:357:A:GLU:HG2	17	0.39	0.1	0.41
(1,1480)	1:412:A:LEU:HD23	1:357:A:GLU:HG2	17	0.39	0.1	0.41
(1,1480)	1:412:A:LEU:HD22	1:357:A:GLU:HG2	17	0.39	0.1	0.41
(1,1607)	1:411:A:LEU:HD13	1:366:A:ILE:H	17	0.3	0.08	0.32
(1,1607)	1:411:A:LEU:HD11	1:366:A:ILE:H	17	0.3	0.08	0.32
(1,1607)	1:411:A:LEU:HD12	1:366:A:ILE:H	17	0.3	0.08	0.32
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB2	17	0.3	0.09	0.3
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB3	17	0.3	0.09	0.3
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	17	0.29	0.03	0.29
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	17	0.28	0.09	0.28
(1,1475)	1:433:A:LEU:HD23	1:434:A:GLU:H	17	0.28	0.08	0.26
(1,1475)	1:433:A:LEU:HD21	1:434:A:GLU:H	17	0.28	0.08	0.26
(1,1475)	1:433:A:LEU:HD22	1:434:A:GLU:H	17	0.28	0.08	0.26
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	17	0.27	0.08	0.26
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG21	17	0.27	0.09	0.26
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG22	17	0.27	0.09	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG23	17	0.27	0.09	0.26
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	17	0.26	0.03	0.27
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD12	17	0.24	0.03	0.25
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD13	17	0.24	0.03	0.25
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD11	17	0.24	0.03	0.25
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	17	0.23	0.02	0.23
(1,1217)	1:359:A:LYS:HD2	1:356:A:TRP:HZ2	17	0.23	0.04	0.23
(1,1217)	1:359:A:LYS:HD3	1:356:A:TRP:HZ2	17	0.23	0.04	0.23
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG23	17	0.22	0.05	0.22
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG22	17	0.22	0.05	0.22
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG21	17	0.22	0.05	0.22
(1,970)	1:450:A:ILE:HG22	1:450:A:ILE:HG12	17	0.21	0.02	0.22
(1,970)	1:450:A:ILE:HG23	1:450:A:ILE:HG12	17	0.21	0.02	0.22
(1,970)	1:450:A:ILE:HG21	1:450:A:ILE:HG12	17	0.21	0.02	0.22
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	17	0.21	0.01	0.21
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	17	0.19	0.06	0.17
(1,1175)	1:363:A:ILE:HG23	1:363:A:ILE:HG13	17	0.19	0.05	0.2
(1,1175)	1:363:A:ILE:HG22	1:363:A:ILE:HG13	17	0.19	0.05	0.2
(1,1175)	1:363:A:ILE:HG21	1:363:A:ILE:HG13	17	0.19	0.05	0.2
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	17	0.18	0.01	0.18
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	17	0.15	0.02	0.16
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	17	0.14	0.02	0.14
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG21	17	0.12	0.01	0.12
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG22	17	0.12	0.01	0.12
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG23	17	0.12	0.01	0.12
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD11	17	0.12	0.01	0.12
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD13	17	0.12	0.01	0.12
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD12	17	0.12	0.01	0.12
(1,2789)	1:438:A:LEU:HD13	1:381:A:ASN:HD22	16	0.9	0.64	0.66
(1,2789)	1:438:A:LEU:HD13	1:444:A:GLN:HE22	16	0.9	0.64	0.66
(1,2789)	1:438:A:LEU:HD12	1:381:A:ASN:HD22	16	0.9	0.64	0.66
(1,2789)	1:438:A:LEU:HD11	1:381:A:ASN:HD22	16	0.9	0.64	0.66
(1,1403)	1:383:A:THR:HG23	1:382:A:ARG:HD2	16	0.74	0.44	0.77
(1,1403)	1:383:A:THR:HG21	1:382:A:ARG:HD2	16	0.74	0.44	0.77
(1,1403)	1:383:A:THR:HG22	1:382:A:ARG:HD2	16	0.74	0.44	0.77
(1,2762)	1:394:A:LEU:HD22	1:398:A:TYR:HE1	16	0.55	0.29	0.57
(1,2762)	1:394:A:LEU:HD21	1:398:A:TYR:HE1	16	0.55	0.29	0.57
(1,2762)	1:394:A:LEU:HD23	1:398:A:TYR:HE1	16	0.55	0.29	0.57
(1,2762)	1:394:A:LEU:HD23	1:398:A:TYR:HE2	16	0.55	0.29	0.57
(1,2423)	1:441:A:GLN:H	1:441:A:GLN:HB2	16	0.53	0.05	0.52
(1,1006)	1:380:A:LYS:HA	1:380:A:LYS:HD3	16	0.49	0.08	0.48
(1,1906)	1:451:A:ALA:HB2	1:449:A:THR:HG23	16	0.46	0.12	0.44

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1906)	1:451:A:ALA:HB1	1:449:A:THR:HG21	16	0.46	0.12	0.44
(1,1906)	1:451:A:ALA:HB3	1:449:A:THR:HG22	16	0.46	0.12	0.44
(1,1906)	1:451:A:ALA:HB1	1:449:A:THR:HG23	16	0.46	0.12	0.44
(1,1906)	1:451:A:ALA:HB2	1:449:A:THR:HG21	16	0.46	0.12	0.44
(1,1906)	1:451:A:ALA:HB2	1:449:A:THR:HG22	16	0.46	0.12	0.44
(1,1906)	1:451:A:ALA:HB1	1:449:A:THR:HG22	16	0.46	0.12	0.44
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD13	16	0.44	0.08	0.44
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD11	16	0.44	0.08	0.44
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD12	16	0.44	0.08	0.44
(1,2661)	1:411:A:LEU:HD13	1:410:A:ARG:HD3	16	0.44	0.08	0.44
(1,2667)	1:414:A:ARG:HA	1:414:A:ARG:HD2	16	0.4	0.2	0.56
(1,2612)	1:393:A:ALA:HB1	1:376:A:TRP:HZ3	16	0.29	0.11	0.28
(1,2612)	1:393:A:ALA:HB3	1:376:A:TRP:HZ3	16	0.29	0.11	0.28
(1,2612)	1:393:A:ALA:HB2	1:376:A:TRP:HZ3	16	0.29	0.11	0.28
(1,890)	1:439:A:ASP:H	1:438:A:LEU:HB2	16	0.24	0.04	0.23
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG23	16	0.23	0.06	0.23
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG21	16	0.23	0.06	0.23
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG22	16	0.23	0.06	0.23
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG21	16	0.22	0.1	0.2
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG22	16	0.22	0.1	0.2
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG23	16	0.22	0.1	0.2
(1,2825)	1:413:A:PHE:HE2	1:366:A:ILE:HB	16	0.22	0.04	0.22
(1,1077)	1:372:A:LEU:HD13	1:340:A:TYR:HD2	16	0.21	0.05	0.21
(1,1077)	1:372:A:LEU:HD12	1:340:A:TYR:HD2	16	0.21	0.05	0.21
(1,1077)	1:372:A:LEU:HD11	1:340:A:TYR:HD2	16	0.21	0.05	0.21
(1,2931)	1:420:A:ASP:H	1:421:A:GLU:HG3	16	0.21	0.09	0.19
(1,1920)	1:372:A:LEU:HD11	1:366:A:ILE:HD12	16	0.19	0.07	0.18
(1,1920)	1:372:A:LEU:HD13	1:366:A:ILE:HD13	16	0.19	0.07	0.18
(1,1920)	1:372:A:LEU:HD12	1:366:A:ILE:HD11	16	0.19	0.07	0.18
(1,1920)	1:372:A:LEU:HD12	1:366:A:ILE:HD12	16	0.19	0.07	0.18
(1,1920)	1:372:A:LEU:HD13	1:366:A:ILE:HD11	16	0.19	0.07	0.18
(1,1920)	1:372:A:LEU:HD12	1:366:A:ILE:HD13	16	0.19	0.07	0.18
(1,1920)	1:372:A:LEU:HD13	1:366:A:ILE:HD12	16	0.19	0.07	0.18
(1,1920)	1:372:A:LEU:HD11	1:366:A:ILE:HD13	16	0.19	0.07	0.18
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD12	16	0.18	0.04	0.16
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD13	16	0.18	0.04	0.16
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD11	16	0.18	0.04	0.16
(1,760)	1:338:A:TRP:HZ2	1:419:A:PRO:HA	16	0.17	0.03	0.17
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD23	16	0.17	0.04	0.16
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD22	16	0.17	0.04	0.16
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD21	16	0.17	0.04	0.16
(1,2811)	1:428:A:ASP:HA	1:431:A:GLU:HB2	16	0.15	0.02	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2811)	1:423:A:MET:HA	1:423:A:MET:HB2	16	0.15	0.02	0.16
(1,1438)	1:444:A:GLN:HA	1:444:A:GLN:HB2	16	0.15	0.01	0.15
(1,58)	1:343:A:GLN:HG3	1:343:A:GLN:HB2	16	0.13	0.02	0.13
(1,58)	1:343:A:GLN:HG2	1:343:A:GLN:HB3	16	0.13	0.02	0.13
(1,58)	1:343:A:GLN:HG2	1:343:A:GLN:HB2	16	0.13	0.02	0.13
(1,2945)	1:364:A:PHE:H	1:412:A:LEU:HG	16	0.13	0.02	0.12
(1,52)	1:443:A:TYR:HE2	1:456:A:TRP:HD1	15	2.94	0.96	3.01
(1,1445)	1:442:A:THR:HG23	1:443:A:TYR:HE2	15	1.49	0.44	1.5
(1,1445)	1:442:A:THR:HG22	1:443:A:TYR:HE2	15	1.49	0.44	1.5
(1,1445)	1:442:A:THR:HG21	1:443:A:TYR:HE2	15	1.49	0.44	1.5
(1,1446)	1:442:A:THR:HG23	1:443:A:TYR:HD2	15	1.21	0.34	1.16
(1,1446)	1:442:A:THR:HG22	1:443:A:TYR:HD2	15	1.21	0.34	1.16
(1,1446)	1:442:A:THR:HG21	1:443:A:TYR:HD2	15	1.21	0.34	1.16
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD11	15	1.14	0.85	1.65
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD13	15	1.14	0.85	1.65
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD12	15	1.14	0.85	1.65
(1,2254)	1:443:A:TYR:H	1:443:A:TYR:HD2	15	1.06	0.35	0.91
(1,1430)	1:447:A:GLU:HB2	1:448:A:PRO:HD3	15	0.86	0.26	0.87
(1,2794)	1:433:A:LEU:HD22	1:429:A:ARG:HD3	15	0.77	0.39	0.84
(1,2794)	1:433:A:LEU:HD23	1:429:A:ARG:HD3	15	0.77	0.39	0.84
(1,2794)	1:375:A:LEU:HD23	1:353:A:PHE:HB2	15	0.77	0.39	0.84
(1,2794)	1:433:A:LEU:HD23	1:429:A:ARG:HD2	15	0.77	0.39	0.84
(1,2794)	1:433:A:LEU:HD21	1:429:A:ARG:HD3	15	0.77	0.39	0.84
(1,2794)	1:433:A:LEU:HD22	1:429:A:ARG:HD2	15	0.77	0.39	0.84
(1,2794)	1:433:A:LEU:HD21	1:429:A:ARG:HD2	15	0.77	0.39	0.84
(1,2794)	1:375:A:LEU:HD21	1:353:A:PHE:HB2	15	0.77	0.39	0.84
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB2	15	0.64	0.29	0.65
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB1	15	0.64	0.29	0.65
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB3	15	0.64	0.29	0.65
(1,2791)	1:438:A:LEU:HD23	1:385:A:MET:HG2	15	0.56	0.27	0.51
(1,2791)	1:438:A:LEU:HD21	1:385:A:MET:HG2	15	0.56	0.27	0.51
(1,2791)	1:380:A:LYS:HE3	1:438:A:LEU:HD23	15	0.56	0.27	0.51
(1,2791)	1:438:A:LEU:HD22	1:385:A:MET:HG2	15	0.56	0.27	0.51
(1,2791)	1:380:A:LYS:HE3	1:438:A:LEU:HD22	15	0.56	0.27	0.51
(1,1142)	1:450:A:ILE:HD12	1:454:A:VAL:HA	15	0.45	0.17	0.39
(1,1142)	1:450:A:ILE:HD11	1:454:A:VAL:HA	15	0.45	0.17	0.39
(1,1142)	1:450:A:ILE:HD13	1:454:A:VAL:HA	15	0.45	0.17	0.39
(1,2947)	1:362:A:LYS:H	1:363:A:ILE:HB	15	0.44	0.05	0.43
(1,2947)	1:362:A:LYS:H	1:362:A:LYS:HD2	15	0.44	0.05	0.43
(1,1316)	1:433:A:LEU:HD21	1:396:A:HIS:HD2	15	0.42	0.07	0.41
(1,1316)	1:433:A:LEU:HD22	1:396:A:HIS:HD2	15	0.42	0.07	0.41
(1,1316)	1:433:A:LEU:HD23	1:396:A:HIS:HD2	15	0.42	0.07	0.41

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2775)	1:387:A:TYR:HD1	1:390:A:MET:HG2	15	0.42	0.1	0.41
(1,2775)	1:387:A:TYR:HD2	1:390:A:MET:HG2	15	0.42	0.1	0.41
(1,2775)	1:443:A:TYR:HD2	1:445:A:GLU:HB2	15	0.42	0.1	0.41
(1,400)	1:377:A:GLY:HA3	1:382:A:ARG:HB3	15	0.4	0.26	0.3
(1,1872)	1:426:A:ARG:HG2	1:426:A:ARG:HD2	15	0.37	0.0	0.37
(1,1761)	1:340:A:TYR:HB2	1:337:A:LEU:HA	15	0.32	0.08	0.31
(1,2359)	1:382:A:ARG:H	1:382:A:ARG:HG3	15	0.29	0.11	0.28
(1,530)	1:394:A:LEU:HD21	1:397:A:TYR:HB3	15	0.28	0.17	0.22
(1,530)	1:394:A:LEU:HD23	1:397:A:TYR:HB3	15	0.28	0.17	0.22
(1,530)	1:394:A:LEU:HD22	1:397:A:TYR:HB3	15	0.28	0.17	0.22
(1,2850)	1:344:A:LEU:HD12	1:350:A:TYR:HD1	15	0.26	0.11	0.22
(1,2850)	1:344:A:LEU:HD11	1:350:A:TYR:HD1	15	0.26	0.11	0.22
(1,2850)	1:344:A:LEU:HD13	1:350:A:TYR:HD1	15	0.26	0.11	0.22
(1,2850)	1:344:A:LEU:HD11	1:350:A:TYR:HD2	15	0.26	0.11	0.22
(1,2850)	1:344:A:LEU:HD12	1:350:A:TYR:HD2	15	0.26	0.11	0.22
(1,2940)	1:411:A:LEU:H	1:410:A:ARG:HG3	15	0.25	0.05	0.24
(1,2940)	1:434:A:GLU:H	1:433:A:LEU:HB2	15	0.25	0.05	0.24
(1,594)	1:400:A:LEU:HD21	1:426:A:ARG:HG3	15	0.24	0.08	0.22
(1,594)	1:400:A:LEU:HD23	1:426:A:ARG:HG3	15	0.24	0.08	0.22
(1,594)	1:400:A:LEU:HD22	1:426:A:ARG:HG3	15	0.24	0.08	0.22
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD23	15	0.23	0.05	0.25
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD21	15	0.23	0.05	0.25
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD22	15	0.23	0.05	0.25
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD23	15	0.21	0.06	0.21
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD21	15	0.21	0.06	0.21
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD22	15	0.21	0.06	0.21
(1,2425)	1:440:A:GLU:H	1:440:A:GLU:HG2	15	0.21	0.02	0.2
(1,2567)	1:345:A:LEU:HD22	1:355:A:ARG:HA	15	0.2	0.06	0.2
(1,2567)	1:345:A:LEU:HD21	1:355:A:ARG:HA	15	0.2	0.06	0.2
(1,2567)	1:345:A:LEU:HD23	1:356:A:TRP:HA	15	0.2	0.06	0.2
(1,2567)	1:345:A:LEU:HD23	1:355:A:ARG:HA	15	0.2	0.06	0.2
(1,121)	1:349:A:ARG:H	1:349:A:ARG:HB3	15	0.18	0.03	0.19
(1,2871)	1:444:A:GLN:HB2	1:444:A:GLN:HG3	15	0.17	0.04	0.17
(1,2871)	1:445:A:GLU:HB3	1:445:A:GLU:HG2	15	0.17	0.04	0.17
(1,2871)	1:447:A:GLU:HG2	1:447:A:GLU:HB3	15	0.17	0.04	0.17
(1,2871)	1:445:A:GLU:HG3	1:445:A:GLU:HB3	15	0.17	0.04	0.17
(1,885)	1:437:A:VAL:HG11	1:393:A:ALA:HA	15	0.17	0.03	0.16
(1,885)	1:437:A:VAL:HG12	1:393:A:ALA:HA	15	0.17	0.03	0.16
(1,885)	1:437:A:VAL:HG13	1:393:A:ALA:HA	15	0.17	0.03	0.16
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD13	15	0.16	0.03	0.16
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD11	15	0.16	0.03	0.16
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD12	15	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,138)	1:351:A:GLU:HG3	1:351:A:GLU:HB2	15	0.15	0.03	0.15
(1,2662)	1:411:A:LEU:HD23	1:366:A:ILE:HB	15	0.15	0.03	0.15
(1,2662)	1:411:A:LEU:HD21	1:366:A:ILE:HB	15	0.15	0.03	0.15
(1,2662)	1:411:A:LEU:HD22	1:366:A:ILE:HB	15	0.15	0.03	0.15
(1,2295)	1:356:A:TRP:HE1	1:345:A:LEU:HG	15	0.13	0.02	0.13
(1,2599)	1:363:A:ILE:HG21	1:363:A:ILE:HB	15	0.12	0.01	0.12
(1,2599)	1:363:A:ILE:HG22	1:363:A:ILE:HB	15	0.12	0.01	0.12
(1,2599)	1:363:A:ILE:HG23	1:363:A:ILE:HB	15	0.12	0.01	0.12
(1,2763)	1:398:A:TYR:HD1	1:398:A:TYR:HE1	15	0.1	0.0	0.1
(1,1541)	1:445:A:GLU:HA	1:443:A:TYR:HD1	14	1.02	0.62	1.01
(1,547)	1:395:A:ARG:HD2	1:395:A:ARG:H	14	0.95	0.61	1.0
(1,1442)	1:443:A:TYR:HE2	1:445:A:GLU:HG2	14	0.92	0.43	1.0
(1,1045)	1:349:A:ARG:HG2	1:349:A:ARG:HD2	14	0.59	0.12	0.62
(1,455)	1:386:A:THR:HG23	1:389:A:LYS:HE2	14	0.48	0.26	0.52
(1,455)	1:386:A:THR:HG23	1:389:A:LYS:HE3	14	0.48	0.26	0.52
(1,455)	1:386:A:THR:HG22	1:389:A:LYS:HE3	14	0.48	0.26	0.52
(1,455)	1:386:A:THR:HG22	1:389:A:LYS:HE2	14	0.48	0.26	0.52
(1,455)	1:386:A:THR:HG21	1:389:A:LYS:HE3	14	0.48	0.26	0.52
(1,455)	1:386:A:THR:HG21	1:389:A:LYS:HE2	14	0.48	0.26	0.52
(1,2675)	1:417:A:LYS:HD2	1:402:A:ILE:HG13	14	0.45	0.1	0.45
(1,577)	1:399:A:LYS:HA	1:399:A:LYS:HG3	14	0.36	0.02	0.36
(1,1033)	1:348:A:SER:HB3	1:351:A:GLU:HB3	14	0.36	0.13	0.32
(1,1444)	1:442:A:THR:HG23	1:443:A:TYR:HA	14	0.35	0.21	0.28
(1,1444)	1:442:A:THR:HG22	1:443:A:TYR:HA	14	0.35	0.21	0.28
(1,1444)	1:442:A:THR:HG21	1:443:A:TYR:HA	14	0.35	0.21	0.28
(1,1427)	1:447:A:GLU:HA	1:448:A:PRO:HD3	14	0.31	0.12	0.3
(1,2824)	1:413:A:PHE:HE2	1:411:A:LEU:HD22	14	0.25	0.06	0.24
(1,2824)	1:413:A:PHE:HE2	1:411:A:LEU:HD23	14	0.25	0.06	0.24
(1,2824)	1:413:A:PHE:HE1	1:411:A:LEU:HD23	14	0.25	0.06	0.24
(1,2824)	1:413:A:PHE:HE2	1:411:A:LEU:HD21	14	0.25	0.06	0.24
(1,1909)	1:344:A:LEU:HD13	1:354:A:ILE:HG21	14	0.25	0.08	0.22
(1,1909)	1:344:A:LEU:HD13	1:354:A:ILE:HG23	14	0.25	0.08	0.22
(1,1909)	1:344:A:LEU:HD11	1:354:A:ILE:HG22	14	0.25	0.08	0.22
(1,1909)	1:344:A:LEU:HD12	1:354:A:ILE:HG21	14	0.25	0.08	0.22
(1,1909)	1:344:A:LEU:HD11	1:354:A:ILE:HG21	14	0.25	0.08	0.22
(1,1909)	1:344:A:LEU:HD12	1:354:A:ILE:HG23	14	0.25	0.08	0.22
(1,1909)	1:344:A:LEU:HD11	1:354:A:ILE:HG23	14	0.25	0.08	0.22
(1,1909)	1:344:A:LEU:HD12	1:354:A:ILE:HG22	14	0.25	0.08	0.22
(1,2655)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	14	0.25	0.08	0.26
(1,2655)	1:410:A:ARG:HB2	1:410:A:ARG:HD3	14	0.25	0.08	0.26
(1,2655)	1:395:A:ARG:HB3	1:395:A:ARG:HD2	14	0.25	0.08	0.26
(1,544)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	14	0.25	0.1	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,544)	1:395:A:ARG:HB3	1:395:A:ARG:HD2	14	0.25	0.1	0.2
(1,1488)	1:431:A:GLU:HB2	1:336:A:LEU:HD22	14	0.22	0.06	0.22
(1,1488)	1:431:A:GLU:HB2	1:336:A:LEU:HD21	14	0.22	0.06	0.22
(1,1488)	1:431:A:GLU:HB2	1:336:A:LEU:HD23	14	0.22	0.06	0.22
(1,528)	1:394:A:LEU:HD22	1:364:A:PHE:HZ	14	0.18	0.05	0.18
(1,528)	1:394:A:LEU:HD21	1:364:A:PHE:HZ	14	0.18	0.05	0.18
(1,528)	1:394:A:LEU:HD23	1:364:A:PHE:HZ	14	0.18	0.05	0.18
(1,301)	1:366:A:ILE:HG23	1:372:A:LEU:HB3	14	0.17	0.05	0.17
(1,301)	1:366:A:ILE:HG22	1:372:A:LEU:HB3	14	0.17	0.05	0.17
(1,301)	1:366:A:ILE:HG21	1:372:A:LEU:HB3	14	0.17	0.05	0.17
(1,1505)	1:385:A:MET:HA	1:389:A:LYS:HB2	14	0.17	0.04	0.17
(1,1645)	1:404:A:ARG:HB3	1:404:A:ARG:HG3	14	0.14	0.03	0.14
(1,1407)	1:456:A:TRP:HB3	1:456:A:TRP:HZ3	13	1.0	0.52	1.26
(1,127)	1:349:A:ARG:HD2	1:350:A:TYR:HE1	13	0.67	0.66	0.4
(1,2258)	1:450:A:ILE:H	1:450:A:ILE:HG13	13	0.56	0.19	0.63
(1,1201)	1:363:A:ILE:HG13	1:361:A:SER:HB2	13	0.55	0.06	0.56
(1,1200)	1:361:A:SER:HA	1:361:A:SER:HB2	13	0.55	0.01	0.55
(1,2774)	1:443:A:TYR:HD2	1:445:A:GLU:HB2	13	0.52	0.36	0.43
(1,2774)	1:443:A:TYR:HD1	1:445:A:GLU:HB2	13	0.52	0.36	0.43
(1,2774)	1:443:A:TYR:HD1	1:444:A:GLN:HB3	13	0.52	0.36	0.43
(1,2725)	1:367:A:VAL:HG22	1:365:A:ARG:HB3	13	0.45	0.21	0.4
(1,2725)	1:367:A:VAL:HG21	1:365:A:ARG:HB3	13	0.45	0.21	0.4
(1,2725)	1:354:A:ILE:HG13	1:367:A:VAL:HG23	13	0.45	0.21	0.4
(1,2725)	1:367:A:VAL:HG23	1:365:A:ARG:HB3	13	0.45	0.21	0.4
(1,1885)	1:400:A:LEU:HD23	1:402:A:ILE:HD13	13	0.42	0.11	0.44
(1,1885)	1:400:A:LEU:HD23	1:402:A:ILE:HD11	13	0.42	0.11	0.44
(1,1885)	1:400:A:LEU:HD22	1:402:A:ILE:HD11	13	0.42	0.11	0.44
(1,1885)	1:400:A:LEU:HD23	1:402:A:ILE:HD12	13	0.42	0.11	0.44
(1,1885)	1:400:A:LEU:HD21	1:402:A:ILE:HD11	13	0.42	0.11	0.44
(1,1885)	1:400:A:LEU:HD21	1:402:A:ILE:HD13	13	0.42	0.11	0.44
(1,1885)	1:400:A:LEU:HD22	1:402:A:ILE:HD12	13	0.42	0.11	0.44
(1,2693)	1:437:A:VAL:HG21	1:441:A:GLN:HE22	13	0.4	0.22	0.38
(1,2693)	1:437:A:VAL:HG23	1:441:A:GLN:HE22	13	0.4	0.22	0.38
(1,2693)	1:437:A:VAL:HG22	1:441:A:GLN:HE22	13	0.4	0.22	0.38
(1,2693)	1:437:A:VAL:HG11	1:396:A:HIS:HD2	13	0.4	0.22	0.38
(1,1659)	1:404:A:ARG:HB2	1:404:A:ARG:HD3	13	0.34	0.37	0.17
(1,2508)	1:434:A:GLU:H	1:434:A:GLU:HG2	13	0.29	0.09	0.27
(1,2882)	1:402:A:ILE:HB	1:397:A:TYR:HD2	13	0.27	0.07	0.24
(1,864)	1:433:A:LEU:HA	1:433:A:LEU:HD11	13	0.23	0.24	0.17
(1,864)	1:433:A:LEU:HA	1:433:A:LEU:HD12	13	0.23	0.24	0.17
(1,864)	1:433:A:LEU:HA	1:433:A:LEU:HD13	13	0.23	0.24	0.17
(1,1604)	1:365:A:ARG:HB2	1:412:A:LEU:HD13	13	0.22	0.06	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1604)	1:365:A:ARG:HB2	1:412:A:LEU:HD11	13	0.22	0.06	0.2
(1,1604)	1:365:A:ARG:HB2	1:412:A:LEU:HD12	13	0.22	0.06	0.2
(1,1827)	1:430:A:LEU:HB3	1:430:A:LEU:HD22	13	0.22	0.23	0.14
(1,1827)	1:430:A:LEU:HB3	1:430:A:LEU:HD21	13	0.22	0.23	0.14
(1,1827)	1:430:A:LEU:HB3	1:430:A:LEU:HD23	13	0.22	0.23	0.14
(1,1250)	1:345:A:LEU:HD22	1:355:A:ARG:HA	13	0.21	0.06	0.22
(1,1250)	1:345:A:LEU:HD21	1:355:A:ARG:HA	13	0.21	0.06	0.22
(1,1250)	1:345:A:LEU:HD23	1:355:A:ARG:HA	13	0.21	0.06	0.22
(1,2705)	1:394:A:LEU:HA	1:397:A:TYR:HD1	13	0.21	0.04	0.21
(1,2705)	1:394:A:LEU:HA	1:397:A:TYR:HD2	13	0.21	0.04	0.21
(1,203)	1:357:A:GLU:HB2	1:412:A:LEU:HD23	13	0.21	0.07	0.21
(1,203)	1:357:A:GLU:HB2	1:412:A:LEU:HD21	13	0.21	0.07	0.21
(1,203)	1:357:A:GLU:HB2	1:412:A:LEU:HD22	13	0.21	0.07	0.21
(1,1883)	1:393:A:ALA:HB1	1:437:A:VAL:HG22	13	0.2	0.05	0.2
(1,1883)	1:393:A:ALA:HB3	1:437:A:VAL:HG22	13	0.2	0.05	0.2
(1,1883)	1:393:A:ALA:HB1	1:437:A:VAL:HG21	13	0.2	0.05	0.2
(1,1883)	1:393:A:ALA:HB2	1:437:A:VAL:HG21	13	0.2	0.05	0.2
(1,1883)	1:393:A:ALA:HB2	1:437:A:VAL:HG22	13	0.2	0.05	0.2
(1,1883)	1:393:A:ALA:HB2	1:437:A:VAL:HG23	13	0.2	0.05	0.2
(1,1883)	1:393:A:ALA:HB3	1:437:A:VAL:HG21	13	0.2	0.05	0.2
(1,1883)	1:393:A:ALA:HB3	1:437:A:VAL:HG23	13	0.2	0.05	0.2
(1,2051)	1:361:A:SER:H	1:361:A:SER:HB3	13	0.2	0.01	0.2
(1,2126)	1:410:A:ARG:H	1:410:A:ARG:HB3	13	0.19	0.04	0.2
(1,2126)	1:410:A:ARG:H	1:410:A:ARG:HB2	13	0.19	0.04	0.2
(1,813)	1:427:A:THR:HG23	1:425:A:GLY:H	13	0.18	0.06	0.18
(1,813)	1:427:A:THR:HG21	1:425:A:GLY:H	13	0.18	0.06	0.18
(1,813)	1:427:A:THR:HG22	1:425:A:GLY:H	13	0.18	0.06	0.18
(1,1626)	1:406:A:GLU:H	1:406:A:GLU:HG3	13	0.18	0.04	0.18
(1,699)	1:413:A:PHE:HB2	1:364:A:PHE:HE2	13	0.17	0.05	0.15
(1,666)	1:352:A:ASN:HA	1:351:A:GLU:HG3	13	0.13	0.03	0.11
(1,666)	1:352:A:ASN:HA	1:351:A:GLU:HG2	13	0.13	0.03	0.11
(1,1865)	1:431:A:GLU:HA	1:431:A:GLU:HB2	13	0.12	0.01	0.12
(1,2447)	1:385:A:MET:H	1:444:A:GLN:HE21	12	1.51	1.73	1.08
(1,2696)	1:438:A:LEU:HD21	1:382:A:ARG:HD2	12	0.68	0.25	0.71
(1,2696)	1:438:A:LEU:HD22	1:382:A:ARG:HD2	12	0.68	0.25	0.71
(1,2696)	1:438:A:LEU:HD23	1:382:A:ARG:HD2	12	0.68	0.25	0.71
(1,1828)	1:398:A:TYR:HA	1:399:A:LYS:HD2	12	0.57	0.77	0.14
(1,1523)	1:422:A:ILE:HG23	1:426:A:ARG:HG2	12	0.51	0.35	0.42
(1,1523)	1:422:A:ILE:HG21	1:426:A:ARG:HG2	12	0.51	0.35	0.42
(1,1523)	1:422:A:ILE:HG22	1:426:A:ARG:HG2	12	0.51	0.35	0.42
(1,2550)	1:451:A:ALA:H	1:450:A:ILE:HG23	12	0.51	0.08	0.5
(1,2550)	1:451:A:ALA:H	1:450:A:ILE:HG21	12	0.51	0.08	0.5

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2550)	1:451:A:ALA:H	1:450:A:ILE:HG22	12	0.51	0.08	0.5
(1,1402)	1:383:A:THR:HG22	1:384:A:ASN:HD21	12	0.46	0.26	0.46
(1,1402)	1:383:A:THR:HG23	1:384:A:ASN:HD21	12	0.46	0.26	0.46
(1,1402)	1:383:A:THR:HG21	1:384:A:ASN:HD21	12	0.46	0.26	0.46
(1,2837)	1:410:A:ARG:HB2	1:410:A:ARG:HD3	12	0.38	0.1	0.42
(1,2837)	1:404:A:ARG:HD3	1:404:A:ARG:HB3	12	0.38	0.1	0.42
(1,2895)	1:353:A:PHE:H	1:367:A:VAL:HG21	12	0.31	0.14	0.32
(1,2895)	1:353:A:PHE:H	1:367:A:VAL:HG23	12	0.31	0.14	0.32
(1,2895)	1:353:A:PHE:H	1:367:A:VAL:HG22	12	0.31	0.14	0.32
(1,2724)	1:367:A:VAL:HG21	1:352:A:ASN:HA	12	0.31	0.12	0.34
(1,2724)	1:367:A:VAL:HG23	1:352:A:ASN:HA	12	0.31	0.12	0.34
(1,2724)	1:367:A:VAL:HG22	1:352:A:ASN:HA	12	0.31	0.12	0.34
(1,1432)	1:445:A:GLU:HG2	1:445:A:GLU:HA	12	0.28	0.09	0.26
(1,1224)	1:363:A:ILE:HG21	1:357:A:GLU:HG2	12	0.26	0.1	0.3
(1,1224)	1:363:A:ILE:HG23	1:357:A:GLU:HG2	12	0.26	0.1	0.3
(1,1224)	1:363:A:ILE:HG22	1:357:A:GLU:HG2	12	0.26	0.1	0.3
(1,2649)	1:403:A:ILE:HG21	1:364:A:PHE:HZ	12	0.25	0.12	0.22
(1,2649)	1:403:A:ILE:HG22	1:364:A:PHE:HZ	12	0.25	0.12	0.22
(1,2649)	1:403:A:ILE:HG23	1:364:A:PHE:HZ	12	0.25	0.12	0.22
(1,876)	1:436:A:GLN:HB2	1:437:A:VAL:HG13	12	0.22	0.11	0.22
(1,876)	1:436:A:GLN:HB3	1:437:A:VAL:HG11	12	0.22	0.11	0.22
(1,876)	1:436:A:GLN:HB2	1:437:A:VAL:HG12	12	0.22	0.11	0.22
(1,871)	1:435:A:SER:HB2	1:435:A:SER:HA	12	0.22	0.02	0.22
(1,2067)	1:365:A:ARG:H	1:355:A:ARG:HG2	12	0.21	0.08	0.2
(1,2637)	1:349:A:ARG:HB2	1:349:A:ARG:HA	12	0.21	0.01	0.21
(1,870)	1:435:A:SER:HB3	1:435:A:SER:H	12	0.21	0.01	0.21
(1,1603)	1:357:A:GLU:HG2	1:412:A:LEU:HD12	12	0.2	0.07	0.18
(1,1603)	1:357:A:GLU:HG2	1:412:A:LEU:HD13	12	0.2	0.07	0.18
(1,1603)	1:357:A:GLU:HG2	1:412:A:LEU:HD11	12	0.2	0.07	0.18
(1,556)	1:397:A:TYR:HA	1:400:A:LEU:HB3	12	0.19	0.06	0.17
(1,1756)	1:402:A:ILE:HB	1:397:A:TYR:HB2	12	0.18	0.07	0.16
(1,2537)	1:394:A:LEU:H	1:394:A:LEU:HD12	12	0.17	0.05	0.16
(1,2537)	1:394:A:LEU:H	1:394:A:LEU:HD13	12	0.17	0.05	0.16
(1,2537)	1:394:A:LEU:H	1:394:A:LEU:HD11	12	0.17	0.05	0.16
(1,960)	1:450:A:ILE:HA	1:450:A:ILE:HG13	12	0.14	0.02	0.15
(1,1311)	1:421:A:GLU:HA	1:421:A:GLU:HG3	12	0.13	0.01	0.14
(1,259)	1:362:A:LYS:HG2	1:362:A:LYS:HD2	12	0.11	0.0	0.11
(1,478)	1:389:A:LYS:HG3	1:389:A:LYS:HE2	11	0.5	0.24	0.42
(1,2569)	1:349:A:ARG:HD3	1:350:A:TYR:HE1	11	0.46	0.1	0.47
(1,2569)	1:349:A:ARG:HD3	1:350:A:TYR:HE2	11	0.46	0.1	0.47
(1,822)	1:429:A:ARG:HA	1:429:A:ARG:HG2	11	0.37	0.18	0.33
(1,1452)	1:361:A:SER:H	1:360:A:GLU:HG2	11	0.24	0.09	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1452)	1:361:A:SER:H	1:360:A:GLU:HG3	11	0.24	0.09	0.22
(1,88)	1:346:A:SER:HB2	1:346:A:SER:HA	11	0.23	0.19	0.15
(1,2964)	1:446:A:ASP:H	1:445:A:GLU:HB3	11	0.22	0.06	0.21
(1,1672)	1:403:A:ILE:HG21	1:405:A:LYS:H	11	0.18	0.04	0.17
(1,1672)	1:403:A:ILE:HG23	1:405:A:LYS:H	11	0.18	0.04	0.17
(1,1672)	1:403:A:ILE:HG22	1:405:A:LYS:H	11	0.18	0.04	0.17
(1,1533)	1:378:A:ASN:HB2	1:375:A:LEU:HA	11	0.16	0.03	0.16
(1,956)	1:450:A:ILE:H	1:449:A:THR:HB	11	0.15	0.04	0.14
(1,1118)	1:367:A:VAL:HG22	1:366:A:ILE:HA	11	0.14	0.03	0.14
(1,1118)	1:367:A:VAL:HG21	1:366:A:ILE:HA	11	0.14	0.03	0.14
(1,1118)	1:367:A:VAL:HG23	1:366:A:ILE:HA	11	0.14	0.03	0.14
(1,887)	1:437:A:VAL:HG22	1:393:A:ALA:HA	11	0.14	0.04	0.13
(1,887)	1:437:A:VAL:HG21	1:393:A:ALA:HA	11	0.14	0.04	0.13
(1,887)	1:437:A:VAL:HG23	1:393:A:ALA:HA	11	0.14	0.04	0.13
(1,947)	1:447:A:GLU:HG2	1:447:A:GLU:HA	11	0.14	0.02	0.14
(1,2516)	1:342:A:TYR:H	1:341:A:VAL:HG22	11	0.12	0.02	0.11
(1,2516)	1:342:A:TYR:H	1:341:A:VAL:HG21	11	0.12	0.02	0.11
(1,2516)	1:342:A:TYR:H	1:341:A:VAL:HG23	11	0.12	0.02	0.11
(1,734)	1:416:A:MET:HG2	1:403:A:ILE:HA	10	1.33	0.21	1.31
(1,1172)	1:363:A:ILE:HG22	1:409:A:GLN:HE22	10	1.32	0.37	1.38
(1,1172)	1:363:A:ILE:HG21	1:409:A:GLN:HE22	10	1.32	0.37	1.38
(1,1172)	1:363:A:ILE:HG23	1:409:A:GLN:HE22	10	1.32	0.37	1.38
(1,1003)	1:409:A:GLN:HG2	1:406:A:GLU:HB2	10	1.21	0.5	1.36
(1,888)	1:437:A:VAL:HG21	1:441:A:GLN:HE22	10	0.98	1.82	0.35
(1,888)	1:437:A:VAL:HG23	1:441:A:GLN:HE22	10	0.98	1.82	0.35
(1,888)	1:437:A:VAL:HG22	1:441:A:GLN:HE22	10	0.98	1.82	0.35
(1,715)	1:414:A:ARG:HD2	1:414:A:ARG:HH12	10	0.73	0.18	0.72
(1,2472)	1:409:A:GLN:HE22	1:412:A:LEU:HD12	10	0.71	0.2	0.8
(1,2472)	1:409:A:GLN:HE22	1:412:A:LEU:HD13	10	0.71	0.2	0.8
(1,2472)	1:409:A:GLN:HE22	1:412:A:LEU:HD11	10	0.71	0.2	0.8
(1,85)	1:344:A:LEU:HD21	1:350:A:TYR:HD1	10	0.54	0.53	0.31
(1,85)	1:344:A:LEU:HD23	1:350:A:TYR:HD1	10	0.54	0.53	0.31
(1,85)	1:344:A:LEU:HD22	1:350:A:TYR:HD1	10	0.54	0.53	0.31
(1,2684)	1:429:A:ARG:HG2	1:433:A:LEU:HD22	10	0.43	0.34	0.31
(1,2684)	1:429:A:ARG:HG2	1:433:A:LEU:HD23	10	0.43	0.34	0.31
(1,2684)	1:429:A:ARG:HG3	1:430:A:LEU:HD23	10	0.43	0.34	0.31
(1,2684)	1:429:A:ARG:HG2	1:433:A:LEU:HD21	10	0.43	0.34	0.31
(1,2684)	1:429:A:ARG:HG2	1:430:A:LEU:HD22	10	0.43	0.34	0.31
(1,2684)	1:429:A:ARG:HG3	1:433:A:LEU:HD21	10	0.43	0.34	0.31
(1,1304)	1:376:A:TRP:HZ2	1:380:A:LYS:HE3	10	0.42	0.28	0.3
(1,1193)	1:362:A:LYS:HE2	1:362:A:LYS:HA	10	0.37	0.11	0.4
(1,978)	1:453:A:PRO:HA	1:450:A:ILE:HD13	10	0.31	0.11	0.35

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,978)	1:453:A:PRO:HA	1:450:A:ILE:HD11	10	0.31	0.11	0.35
(1,978)	1:453:A:PRO:HA	1:450:A:ILE:HD12	10	0.31	0.11	0.35
(1,2418)	1:444:A:GLN:H	1:441:A:GLN:HG2	10	0.31	0.13	0.31
(1,2418)	1:444:A:GLN:H	1:441:A:GLN:HG3	10	0.31	0.13	0.31
(1,1128)	1:355:A:ARG:HB3	1:367:A:VAL:HG21	10	0.29	0.1	0.34
(1,1128)	1:355:A:ARG:HB3	1:367:A:VAL:HG22	10	0.29	0.1	0.34
(1,1128)	1:355:A:ARG:HB3	1:367:A:VAL:HG23	10	0.29	0.1	0.34
(1,1372)	1:390:A:MET:HG2	1:390:A:MET:H	10	0.27	0.23	0.18
(1,1780)	1:337:A:LEU:HD13	1:376:A:TRP:HA	10	0.25	0.1	0.22
(1,1780)	1:337:A:LEU:HD11	1:376:A:TRP:HA	10	0.25	0.1	0.22
(1,1026)	1:336:A:LEU:HD22	1:432:A:HIS:H	10	0.24	0.08	0.2
(1,1026)	1:336:A:LEU:HD21	1:432:A:HIS:H	10	0.24	0.08	0.2
(1,1026)	1:336:A:LEU:HD23	1:432:A:HIS:H	10	0.24	0.08	0.2
(1,533)	1:394:A:LEU:HD21	1:403:A:ILE:HG21	10	0.2	0.02	0.2
(1,533)	1:394:A:LEU:HD23	1:403:A:ILE:HG22	10	0.2	0.02	0.2
(1,533)	1:394:A:LEU:HD23	1:403:A:ILE:HG23	10	0.2	0.02	0.2
(1,533)	1:394:A:LEU:HD21	1:403:A:ILE:HG22	10	0.2	0.02	0.2
(1,533)	1:394:A:LEU:HD21	1:403:A:ILE:HG23	10	0.2	0.02	0.2
(1,533)	1:394:A:LEU:HD23	1:403:A:ILE:HG21	10	0.2	0.02	0.2
(1,1412)	1:454:A:VAL:HB	1:450:A:ILE:HA	10	0.18	0.04	0.18
(1,1795)	1:431:A:GLU:HG3	1:336:A:LEU:HD22	10	0.18	0.02	0.19
(1,1795)	1:431:A:GLU:HG3	1:336:A:LEU:HD23	10	0.18	0.02	0.19
(1,1795)	1:431:A:GLU:HG3	1:336:A:LEU:HD21	10	0.18	0.02	0.19
(1,2499)	1:421:A:GLU:H	1:420:A:ASP:HB2	10	0.16	0.04	0.15
(1,1784)	1:337:A:LEU:HD13	1:340:A:TYR:H	10	0.16	0.04	0.15
(1,1784)	1:337:A:LEU:HD12	1:340:A:TYR:H	10	0.16	0.04	0.15
(1,1784)	1:337:A:LEU:HD11	1:340:A:TYR:H	10	0.16	0.04	0.15
(1,2090)	1:371:A:GLY:H	1:370:A:ASN:HB2	10	0.14	0.01	0.15
(1,2199)	1:412:A:LEU:H	1:412:A:LEU:HD13	10	0.14	0.02	0.15
(1,2199)	1:412:A:LEU:H	1:412:A:LEU:HD11	10	0.14	0.02	0.15
(1,2199)	1:412:A:LEU:H	1:412:A:LEU:HD12	10	0.14	0.02	0.15
(1,859)	1:436:A:GLN:H	1:434:A:GLU:HA	10	0.13	0.02	0.13
(1,2682)	1:418:A:THR:HG22	1:419:A:PRO:HD2	10	0.12	0.02	0.12
(1,2682)	1:418:A:THR:HG23	1:419:A:PRO:HD2	10	0.12	0.02	0.12
(1,2682)	1:418:A:THR:HG21	1:362:A:LYS:HE2	10	0.12	0.02	0.12
(1,2682)	1:418:A:THR:HG21	1:419:A:PRO:HD2	10	0.12	0.02	0.12
(1,236)	1:361:A:SER:HB3	1:358:A:ASP:HB2	9	1.12	0.37	1.29
(1,718)	1:414:A:ARG:HB3	1:414:A:ARG:HD3	9	0.59	0.01	0.6
(1,718)	1:414:A:ARG:HB2	1:414:A:ARG:HD3	9	0.59	0.01	0.6
(1,1653)	1:404:A:ARG:HG2	1:414:A:ARG:HD3	9	0.49	0.21	0.44
(1,2552)	1:452:A:SER:H	1:451:A:ALA:HB2	9	0.38	0.14	0.44
(1,2552)	1:452:A:SER:H	1:451:A:ALA:HB3	9	0.38	0.14	0.44

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1130)	1:365:A:ARG:HG2	1:367:A:VAL:HG21	9	0.35	0.09	0.37
(1,1130)	1:365:A:ARG:HG2	1:367:A:VAL:HG23	9	0.35	0.09	0.37
(1,1130)	1:365:A:ARG:HG2	1:367:A:VAL:HG22	9	0.35	0.09	0.37
(1,432)	1:381:A:ASN:H	1:381:A:ASN:HB2	9	0.31	0.01	0.31
(1,1340)	1:399:A:LYS:HD3	1:396:A:HIS:HA	9	0.31	0.1	0.32
(1,347)	1:373:A:ALA:HA	1:376:A:TRP:HB2	9	0.3	0.08	0.32
(1,1344)	1:398:A:TYR:HD1	1:398:A:TYR:H	9	0.3	0.11	0.26
(1,2752)	1:392:A:ARG:H	1:392:A:ARG:HD3	9	0.25	0.06	0.22
(1,2752)	1:392:A:ARG:H	1:392:A:ARG:HD2	9	0.25	0.06	0.22
(1,204)	1:357:A:GLU:HB3	1:412:A:LEU:HD12	9	0.22	0.1	0.16
(1,204)	1:357:A:GLU:HB3	1:412:A:LEU:HD13	9	0.22	0.1	0.16
(1,204)	1:357:A:GLU:HB3	1:412:A:LEU:HD11	9	0.22	0.1	0.16
(1,1666)	1:403:A:ILE:HG13	1:364:A:PHE:HZ	9	0.2	0.06	0.18
(1,359)	1:374:A:ARG:HA	1:374:A:ARG:HB3	9	0.18	0.06	0.14
(1,359)	1:374:A:ARG:HA	1:374:A:ARG:HB2	9	0.18	0.06	0.14
(1,2663)	1:411:A:LEU:HD23	1:387:A:TYR:HE2	9	0.16	0.03	0.15
(1,2663)	1:411:A:LEU:HD21	1:387:A:TYR:HE2	9	0.16	0.03	0.15
(1,2663)	1:411:A:LEU:HD22	1:387:A:TYR:HE2	9	0.16	0.03	0.15
(1,2663)	1:411:A:LEU:HD23	1:387:A:TYR:HE1	9	0.16	0.03	0.15
(1,2406)	1:383:A:THR:H	1:382:A:ARG:HG2	9	0.15	0.04	0.14
(1,845)	1:431:A:GLU:HA	1:431:A:GLU:HG3	9	0.14	0.02	0.14
(1,1740)	1:339:A:ASP:HB2	1:419:A:PRO:HG3	9	0.13	0.01	0.14
(1,2812)	1:375:A:LEU:HB3	1:375:A:LEU:HA	9	0.11	0.01	0.11
(1,2812)	1:421:A:GLU:HB3	1:421:A:GLU:HA	9	0.11	0.01	0.11
(1,943)	1:446:A:ASP:HB3	1:446:A:ASP:HA	9	0.1	0.0	0.1
(1,234)	1:356:A:TRP:HE1	1:359:A:LYS:HE2	8	1.12	0.24	1.18
(1,2553)	1:454:A:VAL:H	1:454:A:VAL:HG22	8	0.94	0.61	1.32
(1,2553)	1:454:A:VAL:H	1:454:A:VAL:HG21	8	0.94	0.61	1.32
(1,2553)	1:454:A:VAL:H	1:454:A:VAL:HG23	8	0.94	0.61	1.32
(1,1164)	1:363:A:ILE:HG13	1:358:A:ASP:HB2	8	0.77	0.27	0.92
(1,1485)	1:432:A:HIS:HD2	1:433:A:LEU:HD23	8	0.75	0.8	0.42
(1,1485)	1:432:A:HIS:HD2	1:433:A:LEU:HD22	8	0.75	0.8	0.42
(1,1485)	1:432:A:HIS:HD2	1:433:A:LEU:HD21	8	0.75	0.8	0.42
(1,1448)	1:442:A:THR:HG22	1:456:A:TRP:HB3	8	0.5	0.18	0.48
(1,1448)	1:442:A:THR:HG21	1:456:A:TRP:HB3	8	0.5	0.18	0.48
(1,1448)	1:442:A:THR:HG23	1:456:A:TRP:HB3	8	0.5	0.18	0.48
(1,2058)	1:363:A:ILE:H	1:358:A:ASP:HB2	8	0.46	0.07	0.46
(1,445)	1:384:A:ASN:HD22	1:384:A:ASN:HB2	8	0.45	0.08	0.49
(1,1126)	1:355:A:ARG:HD2	1:367:A:VAL:HG23	8	0.39	0.17	0.5
(1,1126)	1:355:A:ARG:HD3	1:367:A:VAL:HG22	8	0.39	0.17	0.5
(1,1126)	1:355:A:ARG:HD2	1:367:A:VAL:HG21	8	0.39	0.17	0.5
(1,1126)	1:355:A:ARG:HD2	1:367:A:VAL:HG22	8	0.39	0.17	0.5

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1840)	1:374:A:ARG:HA	1:374:A:ARG:HD2	8	0.38	0.09	0.36
(1,1840)	1:374:A:ARG:HD3	1:374:A:ARG:HA	8	0.38	0.09	0.36
(1,1713)	1:343:A:GLN:HE21	1:343:A:GLN:HG2	8	0.37	0.01	0.37
(1,1873)	1:383:A:THR:HG22	1:384:A:ASN:HD22	8	0.3	0.16	0.25
(1,1873)	1:383:A:THR:HG21	1:384:A:ASN:HD22	8	0.3	0.16	0.25
(1,1873)	1:383:A:THR:HG23	1:384:A:ASN:HD22	8	0.3	0.16	0.25
(1,713)	1:414:A:ARG:HE	1:414:A:ARG:HB3	8	0.26	0.08	0.27
(1,713)	1:414:A:ARG:HE	1:414:A:ARG:HB2	8	0.26	0.08	0.27
(1,141)	1:352:A:ASN:HD22	1:352:A:ASN:HB3	8	0.25	0.02	0.26
(1,850)	1:431:A:GLU:HG3	1:431:A:GLU:HB2	8	0.2	0.05	0.23
(1,629)	1:403:A:ILE:HD13	1:415:A:PHE:HD1	8	0.18	0.04	0.18
(1,629)	1:403:A:ILE:HD12	1:415:A:PHE:HD1	8	0.18	0.04	0.18
(1,629)	1:403:A:ILE:HD11	1:415:A:PHE:HD1	8	0.18	0.04	0.18
(1,268)	1:364:A:PHE:HA	1:345:A:LEU:HD22	8	0.17	0.06	0.18
(1,268)	1:364:A:PHE:HA	1:345:A:LEU:HD23	8	0.17	0.06	0.18
(1,2596)	1:363:A:ILE:HG21	1:364:A:PHE:HA	8	0.16	0.07	0.14
(1,2596)	1:363:A:ILE:HG22	1:364:A:PHE:HA	8	0.16	0.07	0.14
(1,2596)	1:363:A:ILE:HG23	1:364:A:PHE:HA	8	0.16	0.07	0.14
(1,800)	1:426:A:ARG:HB2	1:426:A:ARG:HG2	8	0.16	0.04	0.16
(1,15)	1:339:A:ASP:HB2	1:336:A:LEU:HB2	8	0.15	0.04	0.16
(1,15)	1:339:A:ASP:HB3	1:336:A:LEU:HB2	8	0.15	0.04	0.16
(1,2728)	1:366:A:ILE:HB	1:413:A:PHE:HZ	8	0.15	0.05	0.14
(1,364)	1:374:A:ARG:HA	1:374:A:ARG:HG3	8	0.14	0.02	0.14
(1,2739)	1:362:A:LYS:HB2	1:356:A:TRP:HZ3	8	0.12	0.01	0.12
(1,1667)	1:403:A:ILE:HG12	1:403:A:ILE:H	8	0.12	0.01	0.11
(1,1203)	1:360:A:GLU:H	1:360:A:GLU:HA	8	0.11	0.01	0.11
(1,1349)	1:443:A:TYR:HE1	1:445:A:GLU:HA	7	0.88	0.6	0.69
(1,820)	1:429:A:ARG:HA	1:432:A:HIS:HB2	7	0.78	0.25	0.6
(1,599)	1:401:A:ASN:H	1:401:A:ASN:HB3	7	0.73	0.01	0.73
(1,2473)	1:409:A:GLN:HE21	1:412:A:LEU:HD12	7	0.54	0.2	0.6
(1,2473)	1:409:A:GLN:HE21	1:412:A:LEU:HD13	7	0.54	0.2	0.6
(1,2473)	1:409:A:GLN:HE21	1:412:A:LEU:HD11	7	0.54	0.2	0.6
(1,2579)	1:358:A:ASP:HB2	1:363:A:ILE:HG22	7	0.45	0.16	0.38
(1,2579)	1:358:A:ASP:HB2	1:363:A:ILE:HG23	7	0.45	0.16	0.38
(1,2579)	1:358:A:ASP:HB2	1:363:A:ILE:HG21	7	0.45	0.16	0.38
(1,444)	1:384:A:ASN:HD21	1:384:A:ASN:HB2	7	0.44	0.13	0.49
(1,2607)	1:367:A:VAL:HA	1:365:A:ARG:HD2	7	0.41	0.18	0.43
(1,2324)	1:352:A:ASN:HD21	1:367:A:VAL:HG21	7	0.39	0.22	0.27
(1,2324)	1:352:A:ASN:HD21	1:367:A:VAL:HG23	7	0.39	0.22	0.27
(1,2324)	1:352:A:ASN:HD21	1:367:A:VAL:HG22	7	0.39	0.22	0.27
(1,365)	1:374:A:ARG:H	1:374:A:ARG:HD2	7	0.36	0.08	0.35
(1,1821)	1:386:A:THR:H	1:389:A:LYS:HD2	7	0.32	0.11	0.27

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2786)	1:446:A:ASP:H	1:445:A:GLU:HG2	7	0.31	0.17	0.21
(1,2786)	1:431:A:GLU:H	1:431:A:GLU:HG2	7	0.31	0.17	0.21
(1,2786)	1:447:A:GLU:HG2	1:446:A:ASP:H	7	0.31	0.17	0.21
(1,2786)	1:445:A:GLU:HG3	1:446:A:ASP:H	7	0.31	0.17	0.21
(1,205)	1:357:A:GLU:HB3	1:363:A:ILE:HG23	7	0.3	0.11	0.27
(1,205)	1:357:A:GLU:HB3	1:363:A:ILE:HG22	7	0.3	0.11	0.27
(1,205)	1:357:A:GLU:HB3	1:363:A:ILE:HG21	7	0.3	0.11	0.27
(1,937)	1:444:A:GLN:HE22	1:444:A:GLN:HG2	7	0.29	0.12	0.22
(1,443)	1:384:A:ASN:H	1:384:A:ASN:HB2	7	0.26	0.13	0.19
(1,2669)	1:365:A:ARG:HB3	1:365:A:ARG:HD3	7	0.26	0.02	0.25
(1,2669)	1:414:A:ARG:HB3	1:414:A:ARG:HD3	7	0.26	0.02	0.25
(1,2669)	1:414:A:ARG:HB2	1:414:A:ARG:HD3	7	0.26	0.02	0.25
(1,602)	1:401:A:ASN:HD22	1:401:A:ASN:HB3	7	0.24	0.0	0.24
(1,941)	1:447:A:GLU:H	1:446:A:ASP:HB2	7	0.24	0.1	0.2
(1,166)	1:354:A:ILE:HG23	1:372:A:LEU:HD21	7	0.22	0.06	0.22
(1,166)	1:354:A:ILE:HG23	1:372:A:LEU:HD22	7	0.22	0.06	0.22
(1,166)	1:354:A:ILE:HG21	1:372:A:LEU:HD23	7	0.22	0.06	0.22
(1,166)	1:354:A:ILE:HG21	1:372:A:LEU:HD22	7	0.22	0.06	0.22
(1,231)	1:359:A:LYS:HG3	1:359:A:LYS:HE2	7	0.21	0.03	0.22
(1,929)	1:443:A:TYR:H	1:442:A:THR:HB	7	0.21	0.06	0.21
(1,1016)	1:338:A:TRP:HH2	1:422:A:ILE:HG23	7	0.2	0.05	0.2
(1,1016)	1:338:A:TRP:HH2	1:422:A:ILE:HG22	7	0.2	0.05	0.2
(1,1016)	1:338:A:TRP:HH2	1:422:A:ILE:HG21	7	0.2	0.05	0.2
(1,1635)	1:405:A:LYS:HG2	1:405:A:LYS:HD3	7	0.19	0.01	0.19
(1,1123)	1:354:A:ILE:H	1:367:A:VAL:HG21	7	0.19	0.08	0.15
(1,1123)	1:354:A:ILE:H	1:367:A:VAL:HG22	7	0.19	0.08	0.15
(1,1123)	1:354:A:ILE:H	1:367:A:VAL:HG23	7	0.19	0.08	0.15
(1,603)	1:401:A:ASN:HA	1:401:A:ASN:HB2	7	0.18	0.01	0.18
(1,1011)	1:356:A:TRP:HH2	1:418:A:THR:HG22	7	0.18	0.05	0.19
(1,1011)	1:356:A:TRP:HH2	1:418:A:THR:HG21	7	0.18	0.05	0.19
(1,1011)	1:356:A:TRP:HH2	1:418:A:THR:HG23	7	0.18	0.05	0.19
(1,678)	1:411:A:LEU:HA	1:411:A:LEU:HD22	7	0.16	0.03	0.16
(1,678)	1:411:A:LEU:HA	1:411:A:LEU:HD23	7	0.16	0.03	0.16
(1,678)	1:411:A:LEU:HA	1:411:A:LEU:HD21	7	0.16	0.03	0.16
(1,601)	1:401:A:ASN:HD21	1:401:A:ASN:HB3	7	0.15	0.01	0.15
(1,2758)	1:375:A:LEU:HD22	1:340:A:TYR:HE2	7	0.14	0.03	0.14
(1,2758)	1:375:A:LEU:HD21	1:340:A:TYR:HE2	7	0.14	0.03	0.14
(1,2758)	1:375:A:LEU:HD23	1:340:A:TYR:HE2	7	0.14	0.03	0.14
(1,2529)	1:373:A:ALA:H	1:373:A:ALA:HB3	7	0.12	0.01	0.11
(1,2529)	1:373:A:ALA:H	1:373:A:ALA:HB1	7	0.12	0.01	0.11
(1,2529)	1:373:A:ALA:H	1:373:A:ALA:HB2	7	0.12	0.01	0.11
(1,2547)	1:442:A:THR:H	1:442:A:THR:HG23	6	0.87	0.36	0.66

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2547)	1:442:A:THR:H	1:442:A:THR:HG21	6	0.87	0.36	0.66
(1,2547)	1:442:A:THR:H	1:442:A:THR:HG22	6	0.87	0.36	0.66
(1,180)	1:355:A:ARG:HB2	1:355:A:ARG:HD2	6	0.62	0.01	0.62
(1,649)	1:405:A:LYS:HD2	1:405:A:LYS:HG3	6	0.6	0.01	0.6
(1,865)	1:438:A:LEU:HD12	1:380:A:LYS:HE3	6	0.57	0.26	0.58
(1,865)	1:438:A:LEU:HD13	1:380:A:LYS:HE3	6	0.57	0.26	0.58
(1,865)	1:438:A:LEU:HD11	1:380:A:LYS:HE3	6	0.57	0.26	0.58
(1,57)	1:343:A:GLN:HG2	1:344:A:LEU:HD23	6	0.56	0.37	0.38
(1,57)	1:343:A:GLN:HG3	1:344:A:LEU:HD23	6	0.56	0.37	0.38
(1,57)	1:343:A:GLN:HG3	1:344:A:LEU:HD21	6	0.56	0.37	0.38
(1,852)	1:431:A:GLU:H	1:431:A:GLU:HG2	6	0.55	0.03	0.54
(1,471)	1:388:A:GLU:HB3	1:388:A:GLU:HG2	6	0.51	0.17	0.59
(1,1512)	1:424:A:SER:HA	1:424:A:SER:HB2	6	0.48	0.13	0.54
(1,2415)	1:447:A:GLU:H	1:448:A:PRO:HD3	6	0.41	0.14	0.47
(1,2551)	1:451:A:ALA:H	1:451:A:ALA:HB1	6	0.38	0.06	0.4
(1,2551)	1:451:A:ALA:H	1:451:A:ALA:HB2	6	0.38	0.06	0.4
(1,2551)	1:451:A:ALA:H	1:451:A:ALA:HB3	6	0.38	0.06	0.4
(1,1060)	1:351:A:GLU:HB2	1:355:A:ARG:HD3	6	0.33	0.05	0.33
(1,1060)	1:351:A:GLU:HB2	1:355:A:ARG:HD2	6	0.33	0.05	0.33
(1,926)	1:442:A:THR:H	1:441:A:GLN:HG2	6	0.32	0.33	0.18
(1,2129)	1:447:A:GLU:H	1:447:A:GLU:HB3	6	0.31	0.09	0.26
(1,358)	1:374:A:ARG:HA	1:374:A:ARG:HD2	6	0.31	0.21	0.19
(1,1874)	1:382:A:ARG:HD3	1:382:A:ARG:HA	6	0.3	0.37	0.15
(1,2906)	1:361:A:SER:H	1:360:A:GLU:HA	6	0.29	0.01	0.29
(1,999)	1:409:A:GLN:HE22	1:409:A:GLN:HG2	6	0.29	0.01	0.29
(1,237)	1:361:A:SER:HB3	1:363:A:ILE:HG12	6	0.29	0.02	0.29
(1,2598)	1:363:A:ILE:HG21	1:357:A:GLU:HG3	6	0.28	0.11	0.34
(1,2598)	1:363:A:ILE:HG22	1:357:A:GLU:HG2	6	0.28	0.11	0.34
(1,2598)	1:363:A:ILE:HG22	1:357:A:GLU:HG3	6	0.28	0.11	0.34
(1,1502)	1:422:A:ILE:HA	1:427:A:THR:HG22	6	0.27	0.15	0.24
(1,1502)	1:422:A:ILE:HA	1:427:A:THR:HG21	6	0.27	0.15	0.24
(1,1502)	1:422:A:ILE:HA	1:427:A:THR:HG23	6	0.27	0.15	0.24
(1,2048)	1:361:A:SER:H	1:358:A:ASP:HB2	6	0.25	0.1	0.22
(1,2539)	1:404:A:ARG:H	1:403:A:ILE:HG22	6	0.25	0.05	0.26
(1,2539)	1:404:A:ARG:H	1:403:A:ILE:HG21	6	0.25	0.05	0.26
(1,2539)	1:404:A:ARG:H	1:403:A:ILE:HG23	6	0.25	0.05	0.26
(1,2798)	1:412:A:LEU:HD22	1:410:A:ARG:HD3	6	0.24	0.16	0.2
(1,2798)	1:412:A:LEU:HD23	1:410:A:ARG:HD2	6	0.24	0.16	0.2
(1,2798)	1:412:A:LEU:HD22	1:365:A:ARG:HD2	6	0.24	0.16	0.2
(1,2798)	1:412:A:LEU:HD22	1:410:A:ARG:HD2	6	0.24	0.16	0.2
(1,2798)	1:412:A:LEU:HD21	1:410:A:ARG:HD2	6	0.24	0.16	0.2
(1,1179)	1:361:A:SER:HB3	1:363:A:ILE:HD13	6	0.22	0.01	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1179)	1:361:A:SER:HB3	1:363:A:ILE:HD12	6	0.22	0.01	0.22
(1,2650)	1:403:A:ILE:HD12	1:338:A:TRP:HA	6	0.22	0.09	0.2
(1,2650)	1:403:A:ILE:HD11	1:338:A:TRP:HA	6	0.22	0.09	0.2
(1,2650)	1:403:A:ILE:HD13	1:338:A:TRP:HA	6	0.22	0.09	0.2
(1,1462)	1:435:A:SER:H	1:434:A:GLU:HB3	6	0.21	0.06	0.2
(1,1000)	1:409:A:GLN:HE21	1:409:A:GLN:HG2	6	0.17	0.02	0.18
(1,1882)	1:393:A:ALA:HB2	1:437:A:VAL:HG12	6	0.16	0.01	0.16
(1,1882)	1:393:A:ALA:HB3	1:437:A:VAL:HG11	6	0.16	0.01	0.16
(1,1882)	1:393:A:ALA:HB1	1:437:A:VAL:HG13	6	0.16	0.01	0.16
(1,1882)	1:393:A:ALA:HB3	1:437:A:VAL:HG13	6	0.16	0.01	0.16
(1,1882)	1:393:A:ALA:HB2	1:437:A:VAL:HG11	6	0.16	0.01	0.16
(1,2836)	1:404:A:ARG:HG3	1:405:A:LYS:H	6	0.15	0.05	0.15
(1,2836)	1:414:A:ARG:HG3	1:363:A:ILE:H	6	0.15	0.05	0.15
(1,2122)	1:410:A:ARG:H	1:409:A:GLN:HG3	6	0.14	0.02	0.14
(1,2122)	1:410:A:ARG:H	1:409:A:GLN:HG2	6	0.14	0.02	0.14
(1,93)	1:345:A:LEU:HA	1:354:A:ILE:HG23	6	0.14	0.04	0.12
(1,93)	1:345:A:LEU:HA	1:354:A:ILE:HG21	6	0.14	0.04	0.12
(1,93)	1:345:A:LEU:HA	1:354:A:ILE:HG22	6	0.14	0.04	0.12
(1,2276)	1:410:A:ARG:HE	1:365:A:ARG:HE	6	0.14	0.04	0.14
(1,1044)	1:349:A:ARG:HB2	1:349:A:ARG:HG3	6	0.13	0.04	0.12
(1,1044)	1:349:A:ARG:HB2	1:349:A:ARG:HG2	6	0.13	0.04	0.12
(1,1580)	1:413:A:PHE:HB2	1:413:A:PHE:HD1	6	0.11	0.0	0.11
(1,946)	1:447:A:GLU:HG2	1:446:A:ASP:H	5	0.96	0.67	1.37
(1,1479)	1:433:A:LEU:HD13	1:393:A:ALA:HA	5	0.92	1.17	0.19
(1,1479)	1:433:A:LEU:HD11	1:393:A:ALA:HA	5	0.92	1.17	0.19
(1,1479)	1:433:A:LEU:HD12	1:393:A:ALA:HA	5	0.92	1.17	0.19
(1,1898)	1:427:A:THR:HG23	1:430:A:LEU:HD13	5	0.9	1.44	0.19
(1,1898)	1:427:A:THR:HG21	1:430:A:LEU:HD12	5	0.9	1.44	0.19
(1,1898)	1:427:A:THR:HG23	1:430:A:LEU:HD12	5	0.9	1.44	0.19
(1,1898)	1:427:A:THR:HG21	1:430:A:LEU:HD13	5	0.9	1.44	0.19
(1,964)	1:451:A:ALA:H	1:450:A:ILE:HA	5	0.87	0.01	0.88
(1,1871)	1:426:A:ARG:HD2	1:426:A:ARG:HB3	5	0.62	0.22	0.46
(1,958)	1:449:A:THR:H	1:449:A:THR:HG23	5	0.59	0.21	0.63
(1,958)	1:449:A:THR:H	1:449:A:THR:HG22	5	0.59	0.21	0.63
(1,958)	1:449:A:THR:H	1:449:A:THR:HG21	5	0.59	0.21	0.63
(1,1798)	1:336:A:LEU:H	1:336:A:LEU:HD11	5	0.58	0.07	0.55
(1,1798)	1:336:A:LEU:H	1:336:A:LEU:HD13	5	0.58	0.07	0.55
(1,2887)	1:336:A:LEU:H	1:336:A:LEU:HD11	5	0.54	0.07	0.51
(1,2887)	1:336:A:LEU:H	1:336:A:LEU:HD13	5	0.54	0.07	0.51
(1,1509)	1:426:A:ARG:HG3	1:426:A:ARG:HB2	5	0.45	0.01	0.46
(1,1507)	1:426:A:ARG:HG2	1:426:A:ARG:HA	5	0.37	0.08	0.34
(1,803)	1:426:A:ARG:H	1:426:A:ARG:HG2	5	0.35	0.15	0.31

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2252)	1:442:A:THR:H	1:441:A:GLN:HB3	5	0.31	0.09	0.31
(1,1453)	1:438:A:LEU:HD11	1:435:A:SER:H	5	0.23	0.08	0.21
(1,1453)	1:438:A:LEU:HD12	1:435:A:SER:H	5	0.23	0.08	0.21
(1,1453)	1:438:A:LEU:HD13	1:435:A:SER:H	5	0.23	0.08	0.21
(1,2852)	1:343:A:GLN:HB3	1:340:A:TYR:HD1	5	0.23	0.06	0.23
(1,2852)	1:343:A:GLN:HB2	1:340:A:TYR:HD1	5	0.23	0.06	0.23
(1,1954)	1:399:A:LYS:H	1:399:A:LYS:HG2	5	0.19	0.03	0.2
(1,590)	1:400:A:LEU:HD12	1:397:A:TYR:HE1	5	0.19	0.09	0.14
(1,590)	1:400:A:LEU:HD11	1:397:A:TYR:HE1	5	0.19	0.09	0.14
(1,979)	1:453:A:PRO:HG2	1:453:A:PRO:HB3	5	0.19	0.03	0.2
(1,2952)	1:382:A:ARG:H	1:381:A:ASN:HB2	5	0.18	0.02	0.17
(1,2952)	1:382:A:ARG:H	1:382:A:ARG:HD3	5	0.18	0.02	0.17
(1,2918)	1:374:A:ARG:H	1:376:A:TRP:H	5	0.17	0.07	0.15
(1,1086)	1:371:A:GLY:HA3	1:374:A:ARG:HB3	5	0.17	0.03	0.15
(1,1086)	1:371:A:GLY:HA3	1:374:A:ARG:HB2	5	0.17	0.03	0.15
(1,1931)	1:335:A:ARG:H	1:336:A:LEU:HB2	5	0.17	0.04	0.19
(1,1910)	1:354:A:ILE:HG22	1:345:A:LEU:HD21	5	0.17	0.03	0.18
(1,1910)	1:354:A:ILE:HG22	1:345:A:LEU:HD22	5	0.17	0.03	0.18
(1,1910)	1:354:A:ILE:HG23	1:345:A:LEU:HD23	5	0.17	0.03	0.18
(1,898)	1:438:A:LEU:HD13	1:382:A:ARG:HG2	5	0.16	0.06	0.15
(1,898)	1:438:A:LEU:HD11	1:382:A:ARG:HG2	5	0.16	0.06	0.15
(1,898)	1:438:A:LEU:HD12	1:382:A:ARG:HG2	5	0.16	0.06	0.15
(1,1461)	1:435:A:SER:H	1:435:A:SER:HB2	5	0.15	0.02	0.16
(1,1332)	1:399:A:LYS:HA	1:399:A:LYS:HE2	5	0.15	0.02	0.16
(1,2603)	1:368:A:ASP:H	1:366:A:ILE:HA	5	0.15	0.02	0.13
(1,872)	1:436:A:GLN:H	1:435:A:SER:HB2	5	0.14	0.03	0.15
(1,2721)	1:354:A:ILE:HD11	1:372:A:LEU:HD23	5	0.14	0.03	0.15
(1,2721)	1:354:A:ILE:HD13	1:372:A:LEU:HD21	5	0.14	0.03	0.15
(1,2721)	1:354:A:ILE:HD13	1:372:A:LEU:HD23	5	0.14	0.03	0.15
(1,2721)	1:354:A:ILE:HD13	1:372:A:LEU:HD22	5	0.14	0.03	0.15
(1,1265)	1:354:A:ILE:HG22	1:355:A:ARG:H	5	0.13	0.03	0.12
(1,1265)	1:354:A:ILE:HG23	1:355:A:ARG:H	5	0.13	0.03	0.12
(1,1429)	1:447:A:GLU:HA	1:447:A:GLU:HB2	5	0.13	0.0	0.13
(1,27)	1:341:A:VAL:HA	1:372:A:LEU:HD13	5	0.12	0.02	0.12
(1,27)	1:341:A:VAL:HA	1:372:A:LEU:HD11	5	0.12	0.02	0.12
(1,27)	1:341:A:VAL:HA	1:372:A:LEU:HD12	5	0.12	0.02	0.12
(1,855)	1:432:A:HIS:HB2	1:432:A:HIS:HD2	5	0.12	0.01	0.12
(1,1834)	1:361:A:SER:HB2	1:358:A:ASP:HB2	4	1.06	0.08	1.04
(1,933)	1:443:A:TYR:HB3	1:443:A:TYR:HD1	4	0.68	0.01	0.68
(1,87)	1:346:A:SER:H	1:346:A:SER:HB2	4	0.64	0.02	0.64
(1,932)	1:443:A:TYR:HB2	1:443:A:TYR:HD2	4	0.63	0.02	0.62
(1,2708)	1:349:A:ARG:HD2	1:350:A:TYR:HE1	4	0.56	0.22	0.54

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2708)	1:349:A:ARG:HD2	1:350:A:TYR:HE2	4	0.56	0.22	0.54
(1,927)	1:441:A:GLN:H	1:441:A:GLN:HG2	4	0.54	0.3	0.54
(1,1661)	1:404:A:ARG:HG2	1:404:A:ARG:HD3	4	0.46	0.2	0.57
(1,495)	1:392:A:ARG:HA	1:392:A:ARG:HG2	4	0.3	0.13	0.33
(1,2216)	1:408:A:GLY:H	1:409:A:GLN:HG2	4	0.3	0.26	0.16
(1,2216)	1:408:A:GLY:H	1:409:A:GLN:HG3	4	0.3	0.26	0.16
(1,232)	1:359:A:LYS:HG2	1:359:A:LYS:HE2	4	0.26	0.24	0.12
(1,232)	1:359:A:LYS:HG2	1:359:A:LYS:HE3	4	0.26	0.24	0.12
(1,2548)	1:443:A:TYR:H	1:442:A:THR:HG23	4	0.25	0.09	0.2
(1,2548)	1:443:A:TYR:H	1:442:A:THR:HG22	4	0.25	0.09	0.2
(1,1498)	1:429:A:ARG:HD2	1:429:A:ARG:HB2	4	0.24	0.03	0.22
(1,924)	1:441:A:GLN:HE22	1:441:A:GLN:HG2	4	0.23	0.12	0.22
(1,1328)	1:399:A:LYS:H	1:400:A:LEU:HD12	4	0.22	0.06	0.24
(1,1328)	1:399:A:LYS:H	1:400:A:LEU:HD13	4	0.22	0.06	0.24
(1,1328)	1:399:A:LYS:H	1:400:A:LEU:HD11	4	0.22	0.06	0.24
(1,2493)	1:440:A:GLU:H	1:439:A:ASP:HB3	4	0.2	0.15	0.12
(1,1787)	1:376:A:TRP:HZ2	1:337:A:LEU:HD21	4	0.18	0.06	0.16
(1,1787)	1:376:A:TRP:HZ2	1:337:A:LEU:HD22	4	0.18	0.06	0.16
(1,1787)	1:376:A:TRP:HZ2	1:337:A:LEU:HD23	4	0.18	0.06	0.16
(1,1825)	1:418:A:THR:HB	1:419:A:PRO:HD2	4	0.18	0.03	0.19
(1,1606)	1:411:A:LEU:HD13	1:369:A:PRO:HA	4	0.15	0.02	0.14
(1,1606)	1:411:A:LEU:HD12	1:369:A:PRO:HA	4	0.15	0.02	0.14
(1,791)	1:428:A:ASP:HA	1:428:A:ASP:HB3	4	0.15	0.03	0.15
(1,2845)	1:402:A:ILE:HD13	1:338:A:TRP:HB2	4	0.14	0.02	0.14
(1,2845)	1:402:A:ILE:HD12	1:338:A:TRP:HB2	4	0.14	0.02	0.14
(1,1180)	1:363:A:ILE:HD13	1:414:A:ARG:HD2	4	0.14	0.06	0.12
(1,2707)	1:349:A:ARG:HG3	1:350:A:TYR:HD2	4	0.14	0.03	0.14
(1,2412)	1:451:A:ALA:H	1:456:A:TRP:HZ2	4	0.14	0.02	0.14
(1,1647)	1:404:A:ARG:HB2	1:404:A:ARG:HG2	4	0.14	0.02	0.15
(1,2284)	1:414:A:ARG:HE	1:404:A:ARG:HE	4	0.13	0.02	0.13
(1,2867)	1:372:A:LEU:HD11	1:340:A:TYR:HE2	4	0.11	0.01	0.11
(1,2867)	1:372:A:LEU:HD12	1:340:A:TYR:HE2	4	0.11	0.01	0.11
(1,2867)	1:372:A:LEU:HD13	1:340:A:TYR:HE2	4	0.11	0.01	0.11
(1,433)	1:381:A:ASN:HA	1:381:A:ASN:HB3	4	0.11	0.0	0.11
(1,842)	1:430:A:LEU:HG	1:430:A:LEU:HD22	4	0.11	0.01	0.11
(1,842)	1:430:A:LEU:HG	1:430:A:LEU:HD21	4	0.11	0.01	0.11
(1,1397)	1:385:A:MET:HB2	1:374:A:ARG:HA	3	0.92	0.43	1.22
(1,2167)	1:392:A:ARG:H	1:392:A:ARG:HG2	3	0.78	0.13	0.69
(1,1360)	1:392:A:ARG:HD2	1:392:A:ARG:HB3	3	0.74	0.07	0.78
(1,1341)	1:399:A:LYS:HD2	1:400:A:LEU:H	3	0.7	0.01	0.69
(1,1456)	1:436:A:GLN:HB2	1:433:A:LEU:HD12	3	0.68	0.36	0.89
(1,1456)	1:436:A:GLN:HB2	1:433:A:LEU:HD11	3	0.68	0.36	0.89

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1450)	1:442:A:THR:HG21	1:445:A:GLU:HB3	3	0.62	0.18	0.62
(1,1450)	1:442:A:THR:HG23	1:445:A:GLU:HB3	3	0.62	0.18	0.62
(1,1450)	1:442:A:THR:HG22	1:445:A:GLU:HB3	3	0.62	0.18	0.62
(1,2745)	1:360:A:GLU:HA	1:359:A:LYS:HG2	3	0.6	0.45	0.36
(1,2275)	1:365:A:ARG:HE	1:412:A:LEU:HD11	3	0.51	0.05	0.49
(1,549)	1:396:A:HIS:HB3	1:430:A:LEU:HD22	3	0.49	0.23	0.46
(1,549)	1:396:A:HIS:HB3	1:430:A:LEU:HD21	3	0.49	0.23	0.46
(1,549)	1:396:A:HIS:HB3	1:430:A:LEU:HD23	3	0.49	0.23	0.46
(1,2706)	1:349:A:ARG:HB3	1:350:A:TYR:HE2	3	0.48	0.11	0.55
(1,2706)	1:349:A:ARG:HB3	1:350:A:TYR:HE1	3	0.48	0.11	0.55
(1,2159)	1:389:A:LYS:H	1:388:A:GLU:HG2	3	0.47	0.05	0.49
(1,973)	1:452:A:SER:H	1:452:A:SER:HB2	3	0.44	0.05	0.47
(1,1974)	1:349:A:ARG:H	1:349:A:ARG:HB2	3	0.42	0.08	0.42
(1,1969)	1:347:A:ASP:H	1:346:A:SER:HB2	3	0.38	0.01	0.37
(1,921)	1:441:A:GLN:HA	1:441:A:GLN:HB2	3	0.35	0.04	0.38
(1,790)	1:428:A:ASP:HA	1:428:A:ASP:HB2	3	0.34	0.02	0.35
(1,1449)	1:442:A:THR:HG22	1:445:A:GLU:HB2	3	0.33	0.09	0.35
(1,1449)	1:442:A:THR:HG23	1:445:A:GLU:HB2	3	0.33	0.09	0.35
(1,1486)	1:432:A:HIS:HD2	1:436:A:GLN:HB2	3	0.33	0.1	0.36
(1,2549)	1:450:A:ILE:H	1:449:A:THR:HG23	3	0.29	0.03	0.27
(1,2549)	1:450:A:ILE:H	1:449:A:THR:HG21	3	0.29	0.03	0.27
(1,2549)	1:450:A:ILE:H	1:449:A:THR:HG22	3	0.29	0.03	0.27
(1,954)	1:450:A:ILE:H	1:449:A:THR:HA	3	0.29	0.15	0.25
(1,367)	1:374:A:ARG:HB3	1:374:A:ARG:HD2	3	0.27	0.04	0.26
(1,2133)	1:383:A:THR:H	1:384:A:ASN:H	3	0.24	0.03	0.26
(1,16)	1:340:A:TYR:HA	1:343:A:GLN:HB2	3	0.23	0.03	0.22
(1,429)	1:381:A:ASN:HA	1:381:A:ASN:HB2	3	0.23	0.0	0.23
(1,1820)	1:392:A:ARG:HB3	1:392:A:ARG:HA	3	0.23	0.1	0.17
(1,2158)	1:382:A:ARG:H	1:377:A:GLY:HA3	3	0.22	0.11	0.18
(1,923)	1:441:A:GLN:HG3	1:441:A:GLN:HB2	3	0.21	0.04	0.22
(1,923)	1:441:A:GLN:HB2	1:441:A:GLN:HG2	3	0.21	0.04	0.22
(1,2259)	1:452:A:SER:H	1:451:A:ALA:HA	3	0.2	0.02	0.21
(1,1102)	1:369:A:PRO:HB3	1:387:A:TYR:HD1	3	0.19	0.03	0.19
(1,112)	1:347:A:ASP:H	1:347:A:ASP:HB3	3	0.18	0.03	0.19
(1,505)	1:385:A:MET:HG2	1:373:A:ALA:HB3	3	0.16	0.01	0.15
(1,505)	1:385:A:MET:HG2	1:373:A:ALA:HB2	3	0.16	0.01	0.15
(1,1454)	1:438:A:LEU:HD11	1:376:A:TRP:HH2	3	0.15	0.04	0.16
(1,1454)	1:438:A:LEU:HD13	1:376:A:TRP:HH2	3	0.15	0.04	0.16
(1,2191)	1:403:A:ILE:H	1:397:A:TYR:HB2	3	0.15	0.06	0.11
(1,667)	1:409:A:GLN:HA	1:409:A:GLN:HG2	3	0.14	0.03	0.12
(1,1276)	1:382:A:ARG:HG2	1:382:A:ARG:HB2	3	0.13	0.02	0.15
(1,612)	1:402:A:ILE:HD13	1:400:A:LEU:HB3	3	0.13	0.01	0.12

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,612)	1:402:A:ILE:HD12	1:400:A:LEU:HB3	3	0.13	0.01	0.12
(1,612)	1:402:A:ILE:HD11	1:400:A:LEU:HB3	3	0.13	0.01	0.12
(1,645)	1:406:A:GLU:H	1:405:A:LYS:HG2	3	0.13	0.01	0.12
(1,1877)	1:388:A:GLU:H	1:388:A:GLU:HG2	3	0.13	0.02	0.12
(1,2184)	1:435:A:SER:H	1:432:A:HIS:HA	3	0.13	0.02	0.12
(1,2595)	1:451:A:ALA:H	1:450:A:ILE:HG23	3	0.13	0.01	0.13
(1,2595)	1:451:A:ALA:H	1:450:A:ILE:HG22	3	0.13	0.01	0.13
(1,2719)	1:372:A:LEU:HD11	1:340:A:TYR:HD2	3	0.12	0.02	0.13
(1,2719)	1:372:A:LEU:HD13	1:340:A:TYR:HD2	3	0.12	0.02	0.13
(1,2936)	1:436:A:GLN:H	1:435:A:SER:HB2	3	0.12	0.01	0.12
(1,2967)	1:444:A:GLN:H	1:444:A:GLN:HB3	3	0.12	0.02	0.12
(1,573)	1:399:A:LYS:HB2	1:396:A:HIS:HA	3	0.11	0.01	0.11
(1,451)	1:385:A:MET:HG3	1:389:A:LYS:HB2	2	1.72	0.04	1.72
(1,493)	1:391:A:SER:HB2	1:394:A:LEU:HB2	2	1.16	0.05	1.16
(1,1476)	1:433:A:LEU:HD23	1:433:A:LEU:HA	2	1.1	0.45	1.1
(1,878)	1:436:A:GLN:H	1:436:A:GLN:HG3	2	1.0	0.01	1.0
(1,465)	1:387:A:TYR:HE1	1:390:A:MET:HG2	2	0.9	0.06	0.9
(1,230)	1:356:A:TRP:HE1	1:359:A:LYS:HD2	2	0.8	0.31	0.8
(1,1455)	1:437:A:VAL:H	1:436:A:GLN:HB2	2	0.71	0.02	0.71
(1,1478)	1:433:A:LEU:HD21	1:396:A:HIS:HE1	2	0.71	0.36	0.71
(1,1478)	1:433:A:LEU:HD22	1:396:A:HIS:HE1	2	0.71	0.36	0.71
(1,2514)	1:444:A:GLN:H	1:444:A:GLN:HG3	2	0.7	0.1	0.7
(1,310)	1:450:A:ILE:HD12	1:450:A:ILE:HA	2	0.7	0.01	0.7
(1,310)	1:450:A:ILE:HD13	1:450:A:ILE:HA	2	0.7	0.01	0.7
(1,1471)	1:433:A:LEU:HA	1:436:A:GLN:HG3	2	0.68	0.04	0.68
(1,838)	1:430:A:LEU:HB2	1:430:A:LEU:HD13	2	0.64	0.54	0.64
(1,806)	1:426:A:ARG:HD2	1:426:A:ARG:HA	2	0.64	0.05	0.64
(1,2432)	1:435:A:SER:H	1:436:A:GLN:HB2	2	0.64	0.12	0.64
(1,134)	1:351:A:GLU:HB3	1:351:A:GLU:HG2	2	0.62	0.01	0.62
(1,2857)	1:418:A:THR:HG21	1:342:A:TYR:HE1	2	0.6	0.03	0.6
(1,2857)	1:418:A:THR:HG22	1:342:A:TYR:HE1	2	0.6	0.03	0.6
(1,2767)	1:396:A:HIS:HB3	1:393:A:ALA:HA	2	0.6	0.19	0.6
(1,2767)	1:396:A:HIS:HB3	1:397:A:TYR:HA	2	0.6	0.19	0.6
(1,2106)	1:374:A:ARG:H	1:374:A:ARG:HG3	2	0.49	0.36	0.49
(1,136)	1:351:A:GLU:H	1:351:A:GLU:HG2	2	0.46	0.06	0.46
(1,1980)	1:350:A:TYR:H	1:348:A:SER:HA	2	0.44	0.01	0.44
(1,825)	1:392:A:ARG:HD3	1:392:A:ARG:HB3	2	0.44	0.01	0.44
(1,1660)	1:404:A:ARG:HG3	1:404:A:ARG:HD2	2	0.43	0.01	0.43
(1,1861)	1:436:A:GLN:HG2	1:436:A:GLN:HA	2	0.42	0.01	0.42
(1,1513)	1:424:A:SER:HB2	1:424:A:SER:H	2	0.4	0.04	0.4
(1,482)	1:389:A:LYS:HG2	1:389:A:LYS:HE2	2	0.4	0.01	0.4
(1,2586)	1:446:A:ASP:H	1:445:A:GLU:HG2	2	0.38	0.04	0.38

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2586)	1:431:A:GLU:H	1:431:A:GLU:HG2	2	0.38	0.04	0.38
(1,1005)	1:382:A:ARG:HD2	1:382:A:ARG:HA	2	0.36	0.11	0.36
(1,1554)	1:417:A:LYS:HE3	1:402:A:ILE:HG13	2	0.36	0.06	0.36
(1,187)	1:356:A:TRP:HB2	1:359:A:LYS:HD3	2	0.34	0.08	0.34
(1,1644)	1:404:A:ARG:HD3	1:404:A:ARG:HB3	2	0.34	0.06	0.34
(1,2322)	1:350:A:TYR:H	1:350:A:TYR:HE2	2	0.32	0.06	0.32
(1,1867)	1:380:A:LYS:HE2	1:438:A:LEU:HD13	2	0.31	0.01	0.31
(1,1867)	1:380:A:LYS:HE2	1:438:A:LEU:HD11	2	0.31	0.01	0.31
(1,2818)	1:417:A:LYS:HG2	1:416:A:MET:HB2	2	0.31	0.09	0.31
(1,2405)	1:384:A:ASN:H	1:385:A:MET:HB2	2	0.3	0.12	0.3
(1,353)	1:373:A:ALA:HB3	1:385:A:MET:HG3	2	0.28	0.12	0.28
(1,353)	1:373:A:ALA:HB1	1:385:A:MET:HG3	2	0.28	0.12	0.28
(1,1470)	1:433:A:LEU:HA	1:436:A:GLN:HB2	2	0.27	0.07	0.27
(1,486)	1:391:A:SER:H	1:391:A:SER:HB3	2	0.26	0.01	0.26
(1,1208)	1:360:A:GLU:HA	1:360:A:GLU:HB2	2	0.26	0.0	0.26
(1,1986)	1:351:A:GLU:H	1:351:A:GLU:HG2	2	0.26	0.02	0.26
(1,1986)	1:351:A:GLU:H	1:351:A:GLU:HG3	2	0.26	0.02	0.26
(1,742)	1:349:A:ARG:HB2	1:350:A:TYR:HA	2	0.24	0.08	0.24
(1,1225)	1:357:A:GLU:HG3	1:412:A:LEU:HD21	2	0.24	0.05	0.24
(1,1770)	1:394:A:LEU:HD22	1:337:A:LEU:HD13	2	0.23	0.02	0.23
(1,1770)	1:394:A:LEU:HD21	1:337:A:LEU:HD12	2	0.23	0.02	0.23
(1,2131)	1:380:A:LYS:H	1:380:A:LYS:HG2	2	0.22	0.1	0.22
(1,2800)	1:432:A:HIS:HB3	1:433:A:LEU:HD21	2	0.22	0.03	0.22
(1,2800)	1:432:A:HIS:HB3	1:433:A:LEU:HD12	2	0.22	0.03	0.22
(1,360)	1:374:A:ARG:HA	1:374:A:ARG:HG2	2	0.22	0.08	0.22
(1,650)	1:405:A:LYS:HE2	1:405:A:LYS:HG3	2	0.21	0.0	0.21
(1,647)	1:405:A:LYS:HG2	1:405:A:LYS:HE3	2	0.2	0.0	0.2
(1,2740)	1:362:A:LYS:HG2	1:356:A:TRP:HZ3	2	0.2	0.02	0.2
(1,2792)	1:375:A:LEU:H	1:375:A:LEU:HD22	2	0.19	0.04	0.19
(1,2792)	1:375:A:LEU:H	1:375:A:LEU:HD21	2	0.19	0.04	0.19
(1,60)	1:344:A:LEU:H	1:343:A:GLN:HG3	2	0.18	0.02	0.18
(1,60)	1:344:A:LEU:H	1:343:A:GLN:HG2	2	0.18	0.02	0.18
(1,468)	1:388:A:GLU:HA	1:391:A:SER:HB3	2	0.18	0.06	0.18
(1,2531)	1:383:A:THR:H	1:383:A:THR:HG23	2	0.18	0.01	0.18
(1,2531)	1:383:A:THR:H	1:383:A:THR:HG21	2	0.18	0.01	0.18
(1,1611)	1:410:A:ARG:HG3	1:410:A:ARG:H	2	0.18	0.03	0.18
(1,1263)	1:354:A:ILE:HG22	1:345:A:LEU:H	2	0.17	0.04	0.17
(1,1263)	1:354:A:ILE:HG21	1:345:A:LEU:H	2	0.17	0.04	0.17
(1,1134)	1:367:A:VAL:HG11	1:354:A:ILE:H	2	0.16	0.02	0.16
(1,115)	1:348:A:SER:HA	1:351:A:GLU:H	2	0.16	0.01	0.16
(1,177)	1:345:A:LEU:HD11	1:354:A:ILE:HD11	2	0.16	0.02	0.16
(1,177)	1:345:A:LEU:HD11	1:354:A:ILE:HD12	2	0.16	0.02	0.16

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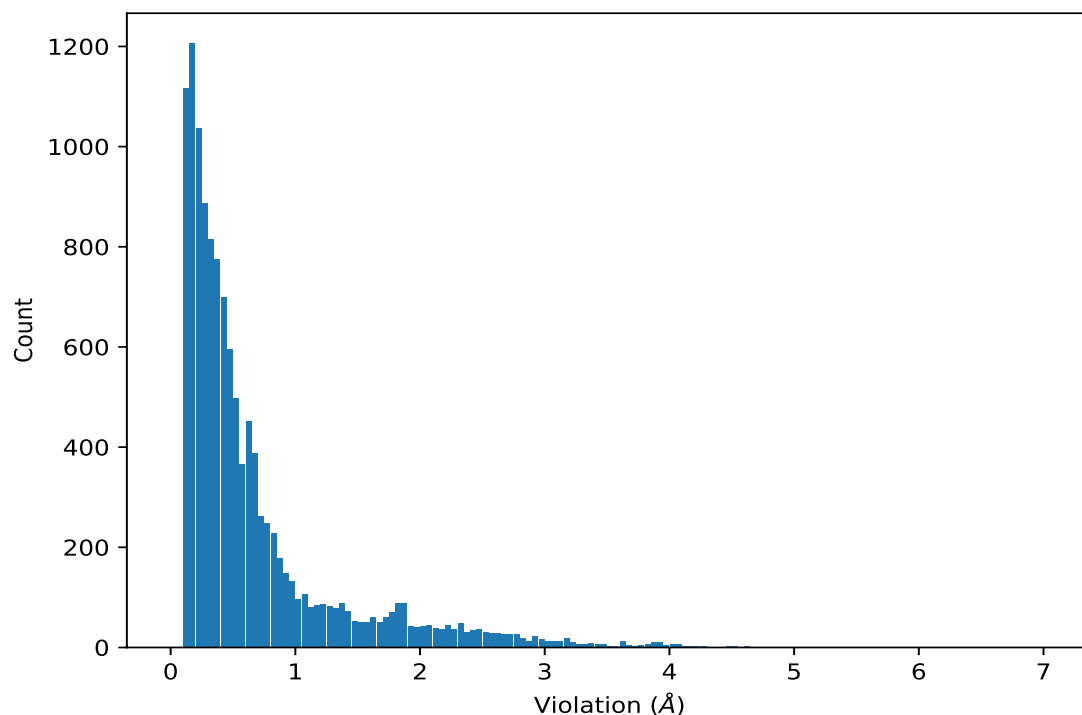
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2139)	1:385:A:MET:H	1:385:A:MET:HB2	2	0.16	0.01	0.16
(1,2890)	1:430:A:LEU:H	1:336:A:LEU:HD11	2	0.16	0.05	0.16
(1,2890)	1:430:A:LEU:H	1:336:A:LEU:HD13	2	0.16	0.05	0.16
(1,930)	1:443:A:TYR:HA	1:443:A:TYR:HB3	2	0.15	0.03	0.15
(1,2838)	1:410:A:ARG:HG2	1:410:A:ARG:HD2	2	0.15	0.03	0.15
(1,2838)	1:392:A:ARG:HG2	1:392:A:ARG:HD3	2	0.15	0.03	0.15
(1,215)	1:359:A:LYS:HA	1:359:A:LYS:HG2	2	0.14	0.04	0.14
(1,794)	1:423:A:MET:H	1:423:A:MET:HG2	2	0.14	0.04	0.14
(1,2989)	1:450:A:ILE:H	1:449:A:THR:HG23	2	0.14	0.0	0.14
(1,2989)	1:450:A:ILE:H	1:449:A:THR:HG21	2	0.14	0.0	0.14
(1,2141)	1:385:A:MET:H	1:384:A:ASN:H	2	0.14	0.04	0.14
(1,318)	1:367:A:VAL:HA	1:367:A:VAL:HG23	2	0.13	0.03	0.13
(1,318)	1:367:A:VAL:HA	1:367:A:VAL:HG21	2	0.13	0.03	0.13
(1,589)	1:400:A:LEU:HA	1:400:A:LEU:HD22	2	0.13	0.01	0.13
(1,589)	1:400:A:LEU:HA	1:400:A:LEU:HD21	2	0.13	0.01	0.13
(1,1320)	1:374:A:ARG:H	1:374:A:ARG:HG2	2	0.12	0.02	0.12
(1,1629)	1:406:A:GLU:HG3	1:412:A:LEU:HD11	2	0.12	0.02	0.12
(1,1629)	1:406:A:GLU:HG3	1:412:A:LEU:HD12	2	0.12	0.02	0.12
(1,342)	1:372:A:LEU:HA	1:372:A:LEU:HD12	2	0.12	0.0	0.12
(1,342)	1:372:A:LEU:HA	1:372:A:LEU:HD13	2	0.12	0.0	0.12
(1,2120)	1:377:A:GLY:H	1:385:A:MET:HB3	2	0.12	0.01	0.12
(1,2266)	1:355:A:ARG:HE	1:367:A:VAL:HB	2	0.12	0.01	0.12
(1,2924)	1:442:A:THR:H	1:441:A:GLN:HA	2	0.12	0.0	0.12
(1,1390)	1:387:A:TYR:HE2	1:390:A:MET:HG2	2	0.11	0.01	0.11
(1,1567)	1:422:A:ILE:HD11	1:415:A:PHE:HD1	2	0.11	0.01	0.11
(1,1567)	1:422:A:ILE:HD12	1:415:A:PHE:HD1	2	0.11	0.01	0.11
(1,1640)	1:405:A:LYS:H	1:404:A:ARG:HB3	2	0.11	0.0	0.11
(1,1729)	1:340:A:TYR:HD2	1:340:A:TYR:HB2	2	0.11	0.0	0.11
(1,2025)	1:381:A:ASN:H	1:381:A:ASN:HB3	2	0.11	0.01	0.11
(1,657)	1:406:A:GLU:HB2	1:412:A:LEU:HB2	2	0.11	0.0	0.11
(1,1236)	1:356:A:TRP:HZ3	1:356:A:TRP:HA	2	0.11	0.0	0.11
(1,2419)	1:443:A:TYR:H	1:442:A:THR:HA	2	0.11	0.0	0.11
(1,1891)	1:394:A:LEU:HD21	1:403:A:ILE:HD13	2	0.1	0.0	0.1
(1,1891)	1:394:A:LEU:HD22	1:403:A:ILE:HD11	2	0.1	0.0	0.1

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

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

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2447)	1:385:A:MET:H	1:444:A:GLN:HE21	17	7.03
(1,888)	1:437:A:VAL:HG22	1:441:A:GLN:HE22	17	6.42
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB3	17	4.61
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	13	4.6
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB2	2	4.57
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB3	3	4.52
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB2	8	4.5
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB2	16	4.48
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	13	4.46
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB2	12	4.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	19	4.32
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB2	1	4.26
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB2	6	4.26
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB3	10	4.25
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB2	15	4.21
(1,52)	1:443:A:TYR:HE2	1:456:A:TRP:HD1	4	4.2
(1,52)	1:443:A:TYR:HE2	1:456:A:TRP:HD1	2	4.19
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB2	5	4.18
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	19	4.18
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB2	7	4.14
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	6	4.14
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	5	4.12
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	9	4.08
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	15	4.08
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	16	4.08
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	4	4.06
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	18	4.06
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB3	18	4.05
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	4	4.05
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	10	4.04
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	7	4.03
(1,52)	1:443:A:TYR:HE2	1:456:A:TRP:HD1	15	4.03
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB3	4	4.02
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB3	13	4.02
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	5	4.0
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	11	4.0
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB2	11	3.98
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	13	3.98
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB3	19	3.96
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	7	3.95
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	6	3.94
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	14	3.94
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	11	3.93
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	18	3.93
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	1	3.93
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	6	3.92
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	8	3.92
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB2	14	3.91
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	9	3.91
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	19	3.91
(1,2761)	1:398:A:TYR:HD2	1:404:A:ARG:HB3	9	3.89
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	1	3.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	2	3.88
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	19	3.88
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	3	3.87
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	16	3.87
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	8	3.86
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	2	3.85
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	13	3.85
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	17	3.85
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	14	3.84
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	13	3.84
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	15	3.83
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	10	3.83
(1,1264)	1:354:A:ILE:HG21	1:364:A:PHE:HD1	15	3.82
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	12	3.82
(1,1069)	1:372:A:LEU:HG	1:387:A:TYR:HD1	12	3.8
(1,1264)	1:354:A:ILE:HG22	1:364:A:PHE:HD1	13	3.79
(1,1898)	1:427:A:THR:HG23	1:430:A:LEU:HD12	18	3.78
(1,1264)	1:354:A:ILE:HG21	1:364:A:PHE:HD1	17	3.77
(1,1264)	1:354:A:ILE:HG22	1:364:A:PHE:HD1	19	3.76
(1,1004)	1:403:A:ILE:HG21	1:398:A:TYR:HE2	19	3.75
(1,1264)	1:354:A:ILE:HG23	1:364:A:PHE:HD1	3	3.72
(1,1004)	1:403:A:ILE:HG23	1:398:A:TYR:HE2	18	3.72
(1,1004)	1:403:A:ILE:HG21	1:398:A:TYR:HE2	14	3.7
(1,1264)	1:354:A:ILE:HG21	1:364:A:PHE:HD1	9	3.68
(1,1264)	1:354:A:ILE:HG21	1:364:A:PHE:HD1	2	3.67
(1,1264)	1:354:A:ILE:HG21	1:364:A:PHE:HD1	18	3.67
(1,1264)	1:354:A:ILE:HG22	1:364:A:PHE:HD1	5	3.65
(1,1264)	1:354:A:ILE:HG23	1:364:A:PHE:HD1	16	3.65
(1,1264)	1:354:A:ILE:HG21	1:364:A:PHE:HD1	7	3.64
(1,1004)	1:403:A:ILE:HG22	1:398:A:TYR:HE2	15	3.64
(1,2629)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	16	3.63
(1,1264)	1:354:A:ILE:HG23	1:364:A:PHE:HD1	14	3.63
(1,1004)	1:403:A:ILE:HG23	1:398:A:TYR:HE2	13	3.63
(1,1658)	1:395:A:ARG:HD3	1:398:A:TYR:HE1	10	3.62
(1,1264)	1:354:A:ILE:HG22	1:364:A:PHE:HD1	4	3.61
(1,1264)	1:354:A:ILE:HG23	1:364:A:PHE:HD1	6	3.61
(1,1264)	1:354:A:ILE:HG22	1:364:A:PHE:HD1	8	3.61
(1,1264)	1:354:A:ILE:HG21	1:364:A:PHE:HD1	10	3.61
(1,1264)	1:354:A:ILE:HG23	1:364:A:PHE:HD1	11	3.61
(1,1264)	1:354:A:ILE:HG22	1:364:A:PHE:HD1	12	3.6
(1,1004)	1:403:A:ILE:HG21	1:398:A:TYR:HE2	11	3.59
(1,2629)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	18	3.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1264)	1:354:A:ILE:HG21	1:364:A:PHE:HD1	1	3.58
(1,2629)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	5	3.52
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	19	3.51
(1,1004)	1:403:A:ILE:HG21	1:398:A:TYR:HE2	8	3.51
(1,1658)	1:395:A:ARG:HD3	1:398:A:TYR:HE1	1	3.48
(1,1658)	1:395:A:ARG:HD3	1:398:A:TYR:HE1	5	3.47
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	4	3.46
(1,1004)	1:403:A:ILE:HG21	1:398:A:TYR:HE2	1	3.46
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	16	3.45
(1,1004)	1:403:A:ILE:HG21	1:398:A:TYR:HE2	4	3.45
(1,52)	1:443:A:TYR:HE2	1:456:A:TRP:HD1	6	3.45
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	9	3.44
(1,1004)	1:403:A:ILE:HG21	1:398:A:TYR:HE2	12	3.44
(1,1004)	1:403:A:ILE:HG22	1:398:A:TYR:HE2	7	3.43
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD23	1	3.42
(1,52)	1:443:A:TYR:HE2	1:456:A:TRP:HD1	3	3.42
(1,388)	1:375:A:LEU:HD23	1:350:A:TYR:HE2	1	3.41
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	15	3.4
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	11	3.39
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	18	3.39
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	19	3.39
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	16	3.38
(1,1658)	1:395:A:ARG:HD3	1:398:A:TYR:HE1	18	3.37
(1,52)	1:443:A:TYR:HE2	1:456:A:TRP:HD1	14	3.37
(1,1658)	1:395:A:ARG:HD3	1:398:A:TYR:HE1	16	3.36
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	4	3.35
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG21	19	3.35
(1,2629)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	1	3.34
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	7	3.34
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	5	3.33
(1,388)	1:375:A:LEU:HD23	1:350:A:TYR:HE2	2	3.33
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	13	3.31
(1,52)	1:443:A:TYR:HE2	1:456:A:TRP:HD1	16	3.31
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG23	18	3.28
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	16	3.27
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	12	3.26
(1,388)	1:375:A:LEU:HD22	1:350:A:TYR:HE2	6	3.26
(1,388)	1:375:A:LEU:HD22	1:350:A:TYR:HE2	12	3.26
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	18	3.25
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	11	3.25
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	5	3.24
(1,2629)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	2	3.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1658)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	3	3.23
(1,1004)	1:403:A:ILE:HG23	1:398:A:TYR:HE2	2	3.23
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD23	2	3.22
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	15	3.22
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	10	3.22
(1,1004)	1:403:A:ILE:HG21	1:398:A:TYR:HE2	6	3.22
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD22	12	3.2
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	13	3.2
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	8	3.19
(1,1004)	1:403:A:ILE:HG21	1:398:A:TYR:HE2	9	3.19
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	10	3.18
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD22	6	3.18
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	10	3.18
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	17	3.17
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG21	11	3.17
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	6	3.17
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	8	3.17
(1,1004)	1:403:A:ILE:HG23	1:398:A:TYR:HE2	16	3.17
(1,1004)	1:403:A:ILE:HG22	1:398:A:TYR:HE2	17	3.17
(1,388)	1:375:A:LEU:HD22	1:350:A:TYR:HE2	4	3.17
(1,1479)	1:433:A:LEU:HD11	1:393:A:ALA:HA	4	3.16
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	9	3.16
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	18	3.16
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	19	3.16
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	1	3.16
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	5	3.15
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG21	14	3.15
(1,2629)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	6	3.14
(1,2629)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	10	3.14
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	4	3.14
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	5	3.14
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	11	3.14
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	14	3.14
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG21	8	3.14
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD22	4	3.12
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD22	8	3.12
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	5	3.12
(1,388)	1:375:A:LEU:HD21	1:350:A:TYR:HE2	5	3.11
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	2	3.1
(1,522)	1:394:A:LEU:HD12	1:413:A:PHE:HE1	5	3.1
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	3	3.09
(1,836)	1:430:A:LEU:HD13	1:427:A:THR:HB	18	3.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	13	3.08
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	10	3.08
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG23	13	3.08
(1,388)	1:375:A:LEU:HD21	1:350:A:TYR:HE2	7	3.08
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD21	7	3.07
(1,388)	1:375:A:LEU:HD22	1:350:A:TYR:HE2	8	3.07
(1,388)	1:375:A:LEU:HD23	1:350:A:TYR:HE2	10	3.07
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	1	3.06
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG22	15	3.06
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	12	3.06
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	8	3.04
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	12	3.04
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	2	3.04
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	5	3.03
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD21	5	3.03
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	14	3.03
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	7	3.02
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	16	3.02
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	11	3.01
(1,1387)	1:388:A:GLU:HA	1:387:A:TYR:HD2	6	3.01
(1,388)	1:375:A:LEU:HD22	1:350:A:TYR:HE2	14	3.01
(1,52)	1:443:A:TYR:HE2	1:456:A:TRP:HD1	7	3.01
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	6	3.0
(1,2629)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	15	2.99
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG21	1	2.99
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG21	12	2.99
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	9	2.98
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	13	2.98
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	19	2.98
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	18	2.97
(1,522)	1:394:A:LEU:HD11	1:413:A:PHE:HE1	7	2.97
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	15	2.96
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	7	2.96
(1,1057)	1:347:A:ASP:HB2	1:350:A:TYR:HE1	10	2.96
(1,2629)	1:395:A:ARG:HD3	1:398:A:TYR:HE1	12	2.95
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	14	2.95
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	4	2.95
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG21	4	2.95
(1,1004)	1:403:A:ILE:HG23	1:398:A:TYR:HE2	3	2.95
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD23	10	2.94
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD21	18	2.94
(1,522)	1:394:A:LEU:HD12	1:413:A:PHE:HE1	4	2.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	1:394:A:LEU:HD13	1:413:A:PHE:HE1	6	2.94
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	1	2.93
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD22	14	2.93
(1,1658)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	2	2.93
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	3	2.93
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	1	2.92
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	3	2.92
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	10	2.92
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	14	2.92
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	17	2.92
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	18	2.92
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	8	2.91
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	2	2.91
(1,388)	1:375:A:LEU:HD22	1:350:A:TYR:HE2	11	2.91
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	2	2.9
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	9	2.9
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD22	11	2.9
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	8	2.9
(1,522)	1:394:A:LEU:HD12	1:413:A:PHE:HE1	14	2.9
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	16	2.89
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	6	2.89
(1,1173)	1:363:A:ILE:HG21	1:364:A:PHE:HD2	12	2.89
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	8	2.88
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	16	2.88
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	4	2.88
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	2	2.87
(1,1173)	1:363:A:ILE:HG23	1:364:A:PHE:HD2	8	2.87
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	3	2.86
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	7	2.86
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	15	2.85
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	19	2.85
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	14	2.85
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	13	2.84
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	19	2.84
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	14	2.84
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD23	9	2.84
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	13	2.84
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG22	7	2.84
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	15	2.84
(1,2629)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	13	2.83
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG21	6	2.83
(1,2629)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	9	2.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	8	2.82
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	18	2.82
(1,2629)	1:395:A:ARG:HD3	1:398:A:TYR:HE1	8	2.81
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	3	2.81
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	10	2.81
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	14	2.81
(1,1173)	1:363:A:ILE:HG21	1:364:A:PHE:HD2	18	2.81
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	19	2.8
(1,1658)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	6	2.8
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	17	2.79
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	17	2.79
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	5	2.79
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD23	15	2.79
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG21	9	2.79
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	17	2.79
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	16	2.78
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD12	16	2.78
(1,1658)	1:395:A:ARG:HD3	1:398:A:TYR:HE1	17	2.78
(1,1173)	1:363:A:ILE:HG21	1:364:A:PHE:HD2	2	2.78
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	19	2.77
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG22	17	2.77
(1,388)	1:375:A:LEU:HD23	1:350:A:TYR:HE2	9	2.77
(1,388)	1:375:A:LEU:HD21	1:350:A:TYR:HE2	18	2.77
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	2	2.76
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	16	2.76
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	4	2.76
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	11	2.76
(1,1173)	1:363:A:ILE:HG21	1:364:A:PHE:HD2	7	2.76
(1,522)	1:394:A:LEU:HD11	1:413:A:PHE:HE1	2	2.76
(1,522)	1:394:A:LEU:HD11	1:413:A:PHE:HE1	13	2.76
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	15	2.75
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	9	2.75
(1,840)	1:430:A:LEU:HD12	1:422:A:ILE:HG23	18	2.75
(1,522)	1:394:A:LEU:HD12	1:413:A:PHE:HE1	16	2.75
(1,388)	1:375:A:LEU:HD23	1:350:A:TYR:HE2	15	2.75
(1,2098)	1:373:A:ALA:H	1:387:A:TYR:HD1	13	2.74
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG23	16	2.74
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	3	2.74
(1,522)	1:394:A:LEU:HD11	1:413:A:PHE:HE1	3	2.74
(1,2629)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	7	2.73
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	15	2.73
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	8	2.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	11	2.73
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	16	2.73
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	4	2.72
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG23	2	2.72
(1,1173)	1:363:A:ILE:HG21	1:364:A:PHE:HD2	11	2.72
(1,522)	1:394:A:LEU:HD12	1:413:A:PHE:HE1	8	2.72
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	1	2.71
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	8	2.71
(1,1173)	1:363:A:ILE:HG21	1:364:A:PHE:HD2	13	2.71
(1,522)	1:394:A:LEU:HD12	1:413:A:PHE:HE1	1	2.71
(1,2629)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	11	2.7
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	7	2.7
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD13	17	2.7
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	1	2.7
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	8	2.7
(1,1173)	1:363:A:ILE:HG21	1:364:A:PHE:HD2	1	2.7
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	11	2.7
(1,1004)	1:403:A:ILE:HG22	1:398:A:TYR:HE2	10	2.7
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	13	2.7
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	18	2.69
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	3	2.69
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	9	2.69
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	16	2.69
(1,1485)	1:432:A:HIS:HD2	1:433:A:LEU:HD21	4	2.69
(1,1173)	1:363:A:ILE:HG22	1:364:A:PHE:HD2	17	2.69
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	9	2.68
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	3	2.68
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	15	2.68
(1,381)	1:375:A:LEU:HD12	1:350:A:TYR:HE2	1	2.68
(1,2629)	1:395:A:ARG:HD3	1:398:A:TYR:HE1	14	2.67
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	5	2.67
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	2	2.67
(1,1173)	1:363:A:ILE:HG21	1:364:A:PHE:HD2	3	2.67
(1,1173)	1:363:A:ILE:HG22	1:364:A:PHE:HD2	19	2.67
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	19	2.67
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	2	2.66
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	14	2.66
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD13	15	2.66
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	12	2.66
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	7	2.66
(1,522)	1:394:A:LEU:HD12	1:413:A:PHE:HE1	10	2.66
(1,381)	1:375:A:LEU:HD12	1:350:A:TYR:HE2	15	2.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	16	2.65
(1,1658)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	15	2.65
(1,1173)	1:363:A:ILE:HG22	1:364:A:PHE:HD2	9	2.65
(1,52)	1:443:A:TYR:HE2	1:456:A:TRP:HD1	12	2.65
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	10	2.64
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	11	2.64
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD13	6	2.64
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	18	2.64
(1,1173)	1:363:A:ILE:HG22	1:364:A:PHE:HD2	4	2.64
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	5	2.64
(1,522)	1:394:A:LEU:HD11	1:413:A:PHE:HE1	9	2.64
(1,52)	1:443:A:TYR:HE2	1:456:A:TRP:HD1	11	2.64
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	4	2.63
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	19	2.63
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	6	2.63
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	7	2.63
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD11	10	2.63
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD11	11	2.63
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	7	2.63
(1,1173)	1:363:A:ILE:HG23	1:364:A:PHE:HD2	6	2.63
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	17	2.63
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	1	2.62
(1,1989)	1:352:A:ASN:H	1:353:A:PHE:HD2	12	2.62
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	10	2.61
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	6	2.61
(1,1658)	1:395:A:ARG:HD3	1:398:A:TYR:HE1	12	2.61
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	16	2.61
(1,302)	1:366:A:ILE:HG21	1:387:A:TYR:HE1	5	2.61
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD13	17	2.6
(1,1173)	1:363:A:ILE:HG23	1:364:A:PHE:HD2	5	2.6
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	1	2.6
(1,307)	1:366:A:ILE:HD12	1:413:A:PHE:HE1	13	2.6
(1,1173)	1:363:A:ILE:HG21	1:364:A:PHE:HD2	16	2.59
(1,52)	1:443:A:TYR:HE2	1:456:A:TRP:HD1	10	2.59
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	1	2.58
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD12	16	2.58
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	3	2.58
(1,1173)	1:363:A:ILE:HG22	1:364:A:PHE:HD2	15	2.58
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	8	2.58
(1,522)	1:394:A:LEU:HD12	1:413:A:PHE:HE1	15	2.58
(1,381)	1:375:A:LEU:HD11	1:350:A:TYR:HE2	12	2.58
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	6	2.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,381)	1:375:A:LEU:HD11	1:350:A:TYR:HE2	4	2.57
(1,307)	1:366:A:ILE:HD11	1:413:A:PHE:HE1	8	2.57
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	7	2.56
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	4	2.56
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	10	2.56
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD13	4	2.56
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	10	2.56
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	7	2.56
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	3	2.55
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	19	2.55
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD11	2	2.55
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD12	5	2.55
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD13	9	2.55
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	6	2.55
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	5	2.55
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	5	2.55
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	9	2.55
(1,382)	1:375:A:LEU:HD12	1:350:A:TYR:HD2	1	2.55
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	10	2.54
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD12	3	2.54
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD12	14	2.54
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD11	19	2.54
(1,1173)	1:363:A:ILE:HG23	1:364:A:PHE:HD2	14	2.54
(1,522)	1:394:A:LEU:HD13	1:413:A:PHE:HE1	11	2.54
(1,2629)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	4	2.53
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	18	2.53
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	17	2.53
(1,1173)	1:363:A:ILE:HG22	1:364:A:PHE:HD2	10	2.53
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	10	2.53
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	10	2.53
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	1	2.53
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	12	2.52
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD22	16	2.52
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	11	2.52
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	14	2.52
(1,388)	1:375:A:LEU:HD22	1:350:A:TYR:HE2	16	2.52
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD11	2	2.51
(1,522)	1:394:A:LEU:HD11	1:413:A:PHE:HE1	12	2.51
(1,52)	1:443:A:TYR:HE2	1:456:A:TRP:HD1	8	2.51
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	6	2.5
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	14	2.5
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	17	2.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD13	6	2.5
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG23	3	2.5
(1,1004)	1:403:A:ILE:HG22	1:398:A:TYR:HE2	5	2.5
(1,381)	1:375:A:LEU:HD12	1:350:A:TYR:HE2	2	2.5
(1,381)	1:375:A:LEU:HD13	1:350:A:TYR:HE2	6	2.5
(1,381)	1:375:A:LEU:HD12	1:350:A:TYR:HE2	11	2.5
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	6	2.49
(1,1658)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	13	2.49
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	2	2.49
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	13	2.49
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	3	2.49
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	7	2.49
(1,302)	1:366:A:ILE:HG21	1:387:A:TYR:HE1	10	2.49
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD11	1	2.48
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD11	14	2.48
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	15	2.48
(1,1658)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	9	2.48
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	2	2.48
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	16	2.48
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	1	2.48
(1,381)	1:375:A:LEU:HD11	1:350:A:TYR:HE2	5	2.48
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	4	2.48
(1,52)	1:443:A:TYR:HE2	1:456:A:TRP:HD1	1	2.48
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	13	2.47
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	12	2.47
(1,1658)	1:395:A:ARG:HD3	1:398:A:TYR:HE1	8	2.47
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD13	7	2.47
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	17	2.47
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	4	2.47
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	18	2.47
(1,522)	1:394:A:LEU:HD13	1:413:A:PHE:HE1	19	2.47
(1,307)	1:366:A:ILE:HD13	1:413:A:PHE:HE1	15	2.47
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	5	2.47
(1,2652)	1:405:A:LYS:HG3	1:398:A:TYR:HD2	17	2.46
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	6	2.46
(1,381)	1:375:A:LEU:HD13	1:350:A:TYR:HE2	7	2.46
(1,2777)	1:387:A:TYR:HE2	1:394:A:LEU:HB2	5	2.45
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	18	2.45
(1,2652)	1:405:A:LYS:HG3	1:398:A:TYR:HD2	3	2.45
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	18	2.45
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD13	1	2.45
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	15	2.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2652)	1:405:A:LYS:HG3	1:398:A:TYR:HD2	15	2.44
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	11	2.44
(1,1495)	1:430:A:LEU:HD23	1:396:A:HIS:HA	18	2.44
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD11	18	2.44
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	15	2.44
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	6	2.44
(1,302)	1:366:A:ILE:HG23	1:387:A:TYR:HE1	4	2.44
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD11	8	2.43
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	12	2.43
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	14	2.43
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	2	2.42
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	13	2.42
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	18	2.42
(1,2209)	1:406:A:GLU:H	1:413:A:PHE:HD2	12	2.42
(1,1541)	1:445:A:GLU:HA	1:443:A:TYR:HD1	16	2.42
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	4	2.42
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	18	2.42
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	2	2.42
(1,522)	1:394:A:LEU:HD11	1:413:A:PHE:HE1	18	2.42
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	6	2.42
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	11	2.42
(1,2789)	1:438:A:LEU:HD13	1:381:A:ASN:HD22	2	2.41
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	8	2.41
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	9	2.41
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	2	2.41
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	15	2.41
(1,382)	1:375:A:LEU:HD12	1:350:A:TYR:HD2	15	2.41
(1,381)	1:375:A:LEU:HD11	1:350:A:TYR:HE2	8	2.41
(1,307)	1:366:A:ILE:HD11	1:413:A:PHE:HE1	18	2.41
(1,2778)	1:366:A:ILE:HD12	1:387:A:TYR:HE1	5	2.4
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	9	2.4
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	8	2.4
(1,1658)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	7	2.4
(1,307)	1:366:A:ILE:HD13	1:413:A:PHE:HE1	6	2.4
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	18	2.4
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	15	2.39
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD11	12	2.39
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	9	2.39
(1,307)	1:366:A:ILE:HD13	1:413:A:PHE:HE1	7	2.39
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	9	2.39
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	1	2.38
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	7	2.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2629)	1:395:A:ARG:HD3	1:398:A:TYR:HE1	19	2.38
(1,1494)	1:430:A:LEU:HD13	1:427:A:THR:H	18	2.38
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	10	2.38
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	9	2.38
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	12	2.38
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	16	2.38
(1,2778)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	10	2.37
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD11	7	2.37
(1,1388)	1:387:A:TYR:HD1	1:366:A:ILE:HD12	13	2.37
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	6	2.37
(1,307)	1:366:A:ILE:HD11	1:413:A:PHE:HE1	19	2.37
(1,302)	1:366:A:ILE:HG23	1:387:A:TYR:HE1	11	2.37
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	4	2.36
(1,1658)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	11	2.36
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	4	2.36
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	18	2.36
(1,307)	1:366:A:ILE:HD11	1:413:A:PHE:HE1	10	2.36
(1,307)	1:366:A:ILE:HD11	1:413:A:PHE:HE1	12	2.36
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	14	2.35
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD12	8	2.35
(1,307)	1:366:A:ILE:HD11	1:413:A:PHE:HE1	2	2.35
(1,307)	1:366:A:ILE:HD12	1:413:A:PHE:HE1	5	2.35
(1,307)	1:366:A:ILE:HD11	1:413:A:PHE:HE1	17	2.35
(1,2789)	1:438:A:LEU:HD12	1:381:A:ASN:HD22	5	2.34
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	3	2.34
(1,2091)	1:372:A:LEU:H	1:353:A:PHE:HD1	13	2.34
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	4	2.34
(1,382)	1:375:A:LEU:HD11	1:350:A:TYR:HD2	12	2.34
(1,2652)	1:405:A:LYS:HG3	1:413:A:PHE:HE2	8	2.33
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	13	2.33
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	18	2.33
(1,1658)	1:395:A:ARG:HD3	1:398:A:TYR:HE1	14	2.33
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	12	2.33
(1,308)	1:366:A:ILE:HD12	1:387:A:TYR:HE1	5	2.33
(1,307)	1:366:A:ILE:HD13	1:413:A:PHE:HE1	9	2.33
(1,302)	1:366:A:ILE:HG22	1:387:A:TYR:HE1	6	2.33
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	16	2.32
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	17	2.32
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	12	2.32
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	17	2.32
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD12	3	2.32
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	3	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	9	2.32
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG22	10	2.32
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	14	2.32
(1,636)	1:405:A:LYS:HA	1:413:A:PHE:HD2	11	2.32
(1,382)	1:375:A:LEU:HD11	1:350:A:TYR:HD2	4	2.32
(1,307)	1:366:A:ILE:HD13	1:413:A:PHE:HE1	1	2.32
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	19	2.31
(1,2634)	1:394:A:LEU:HD21	1:413:A:PHE:HZ	3	2.31
(1,2634)	1:394:A:LEU:HD21	1:413:A:PHE:HZ	17	2.31
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	6	2.31
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD11	4	2.31
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD13	9	2.31
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	15	2.31
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	6	2.31
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	18	2.31
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	5	2.31
(1,381)	1:375:A:LEU:HD11	1:350:A:TYR:HE2	9	2.31
(1,307)	1:366:A:ILE:HD13	1:413:A:PHE:HE1	4	2.31
(1,307)	1:366:A:ILE:HD12	1:413:A:PHE:HE1	14	2.31
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	12	2.3
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	11	2.3
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	15	2.3
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	8	2.3
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	16	2.3
(1,1445)	1:442:A:THR:HG22	1:443:A:TYR:HE2	4	2.3
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	9	2.3
(1,381)	1:375:A:LEU:HD13	1:350:A:TYR:HE2	18	2.3
(1,308)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	10	2.3
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	8	2.3
(1,2652)	1:405:A:LYS:HG3	1:413:A:PHE:HE2	6	2.29
(1,307)	1:366:A:ILE:HD12	1:413:A:PHE:HE1	3	2.29
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	2	2.29
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	12	2.29
(1,2778)	1:366:A:ILE:HD13	1:387:A:TYR:HE1	4	2.28
(1,2634)	1:394:A:LEU:HD21	1:413:A:PHE:HZ	2	2.28
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	5	2.28
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	13	2.28
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	11	2.28
(1,307)	1:366:A:ILE:HD12	1:413:A:PHE:HE1	16	2.28
(1,2634)	1:394:A:LEU:HD21	1:413:A:PHE:HZ	6	2.27
(1,2634)	1:394:A:LEU:HD21	1:413:A:PHE:HZ	18	2.27
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD13	5	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD11	18	2.27
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	11	2.27
(1,1386)	1:373:A:ALA:HB1	1:387:A:TYR:HD1	10	2.27
(1,1345)	1:398:A:TYR:HD1	1:395:A:ARG:HA	19	2.27
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	1	2.27
(1,387)	1:375:A:LEU:HD21	1:353:A:PHE:HE1	19	2.27
(1,381)	1:375:A:LEU:HD11	1:350:A:TYR:HE2	10	2.27
(1,2778)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	11	2.26
(1,2634)	1:394:A:LEU:HD23	1:413:A:PHE:HZ	19	2.26
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	7	2.26
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	8	2.26
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	16	2.26
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	17	2.26
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	5	2.26
(1,381)	1:375:A:LEU:HD11	1:350:A:TYR:HE2	14	2.26
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	10	2.26
(1,2634)	1:394:A:LEU:HD23	1:413:A:PHE:HZ	4	2.25
(1,2634)	1:394:A:LEU:HD22	1:413:A:PHE:HZ	11	2.25
(1,2634)	1:394:A:LEU:HD21	1:413:A:PHE:HZ	14	2.25
(1,2634)	1:394:A:LEU:HD21	1:413:A:PHE:HZ	16	2.25
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	1	2.25
(1,382)	1:375:A:LEU:HD13	1:350:A:TYR:HD2	6	2.25
(1,382)	1:375:A:LEU:HD11	1:350:A:TYR:HD2	8	2.25
(1,382)	1:375:A:LEU:HD12	1:350:A:TYR:HD2	11	2.25
(1,2634)	1:394:A:LEU:HD22	1:413:A:PHE:HZ	1	2.24
(1,2634)	1:394:A:LEU:HD23	1:413:A:PHE:HZ	12	2.24
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	2	2.24
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	19	2.24
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	1	2.24
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	11	2.24
(1,522)	1:394:A:LEU:HD13	1:413:A:PHE:HE1	17	2.24
(1,387)	1:375:A:LEU:HD21	1:353:A:PHE:HE1	13	2.24
(1,381)	1:375:A:LEU:HD13	1:350:A:TYR:HE2	16	2.24
(1,2634)	1:394:A:LEU:HD21	1:413:A:PHE:HZ	7	2.23
(1,2634)	1:394:A:LEU:HD23	1:413:A:PHE:HZ	10	2.23
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	14	2.23
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	9	2.23
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	8	2.23
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	6	2.23
(1,382)	1:375:A:LEU:HD12	1:350:A:TYR:HD2	2	2.23
(1,302)	1:366:A:ILE:HG22	1:387:A:TYR:HE1	14	2.23
(1,302)	1:366:A:ILE:HG21	1:387:A:TYR:HE1	18	2.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	1	2.22
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	16	2.22
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	17	2.22
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD12	15	2.22
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	3	2.22
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	7	2.22
(1,382)	1:375:A:LEU:HD11	1:350:A:TYR:HD2	5	2.22
(1,382)	1:375:A:LEU:HD13	1:350:A:TYR:HD2	7	2.22
(1,113)	1:347:A:ASP:HB3	1:350:A:TYR:HD1	14	2.22
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	1	2.21
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	11	2.21
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	9	2.21
(1,308)	1:366:A:ILE:HD13	1:387:A:TYR:HE1	4	2.21
(1,307)	1:366:A:ILE:HD11	1:413:A:PHE:HE1	11	2.21
(1,302)	1:366:A:ILE:HG23	1:387:A:TYR:HE1	3	2.21
(1,2652)	1:405:A:LYS:HG3	1:398:A:TYR:HD2	4	2.2
(1,2634)	1:394:A:LEU:HD23	1:413:A:PHE:HZ	9	2.2
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD13	19	2.2
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	4	2.2
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	9	2.2
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	14	2.2
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	17	2.2
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	2	2.2
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	6	2.2
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	5	2.2
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	8	2.2
(1,382)	1:375:A:LEU:HD13	1:350:A:TYR:HD2	18	2.2
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD13	13	2.19
(1,1658)	1:395:A:ARG:HD2	1:398:A:TYR:HE1	4	2.19
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	7	2.19
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	4	2.19
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	18	2.19
(1,2806)	1:430:A:LEU:HD13	1:431:A:GLU:HG2	18	2.18
(1,2778)	1:366:A:ILE:HD13	1:387:A:TYR:HE1	15	2.18
(1,2634)	1:394:A:LEU:HD23	1:413:A:PHE:HZ	5	2.18
(1,2634)	1:394:A:LEU:HD23	1:413:A:PHE:HZ	13	2.18
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	5	2.18
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	6	2.18
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	18	2.18
(1,1386)	1:373:A:ALA:HB3	1:387:A:TYR:HD1	11	2.18
(1,1347)	1:398:A:TYR:HD2	1:403:A:ILE:HG22	5	2.18
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	13	2.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	8	2.18
(1,308)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	11	2.18
(1,2778)	1:366:A:ILE:HD13	1:387:A:TYR:HE1	6	2.17
(1,2778)	1:366:A:ILE:HD12	1:387:A:TYR:HE1	14	2.17
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	2	2.17
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD13	2	2.17
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	10	2.17
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	11	2.17
(1,302)	1:366:A:ILE:HG21	1:387:A:TYR:HE1	7	2.17
(1,302)	1:366:A:ILE:HG21	1:387:A:TYR:HE1	16	2.17
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	12	2.16
(1,1349)	1:443:A:TYR:HE1	1:445:A:GLU:HA	16	2.16
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	14	2.16
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	7	2.16
(1,2634)	1:394:A:LEU:HD21	1:413:A:PHE:HZ	15	2.15
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	12	2.15
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	7	2.15
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	4	2.15
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	6	2.15
(1,302)	1:366:A:ILE:HG23	1:387:A:TYR:HE1	9	2.15
(1,302)	1:366:A:ILE:HG23	1:387:A:TYR:HE1	17	2.15
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	1	2.14
(1,1386)	1:373:A:ALA:HB3	1:387:A:TYR:HD1	18	2.14
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	19	2.14
(1,382)	1:375:A:LEU:HD11	1:350:A:TYR:HD2	9	2.14
(1,2778)	1:366:A:ILE:HD13	1:387:A:TYR:HE1	9	2.13
(1,2778)	1:366:A:ILE:HD12	1:387:A:TYR:HE1	16	2.13
(1,2778)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	17	2.13
(1,2652)	1:405:A:LYS:HG3	1:413:A:PHE:HE2	14	2.13
(1,2634)	1:394:A:LEU:HD21	1:413:A:PHE:HZ	8	2.13
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	8	2.13
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	13	2.13
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	5	2.13
(1,302)	1:366:A:ILE:HG22	1:387:A:TYR:HE1	1	2.13
(1,302)	1:366:A:ILE:HG21	1:387:A:TYR:HE1	2	2.13
(1,302)	1:366:A:ILE:HG23	1:387:A:TYR:HE1	15	2.13
(1,2652)	1:405:A:LYS:HG3	1:398:A:TYR:HD2	5	2.12
(1,2294)	1:415:A:PHE:H	1:364:A:PHE:HD2	2	2.12
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	10	2.12
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	8	2.12
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	18	2.12
(1,302)	1:366:A:ILE:HG22	1:387:A:TYR:HE1	8	2.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	13	2.12
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD12	15	2.11
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	7	2.11
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	12	2.11
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	3	2.11
(1,308)	1:366:A:ILE:HD13	1:387:A:TYR:HE1	15	2.11
(1,302)	1:366:A:ILE:HG23	1:387:A:TYR:HE1	12	2.11
(1,2778)	1:366:A:ILE:HD13	1:387:A:TYR:HE1	7	2.1
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	1	2.1
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	7	2.1
(1,1386)	1:373:A:ALA:HB3	1:387:A:TYR:HD1	5	2.1
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	1	2.1
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	6	2.1
(1,1080)	1:372:A:LEU:HD23	1:353:A:PHE:HD1	18	2.1
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	11	2.1
(1,308)	1:366:A:ILE:HD13	1:387:A:TYR:HE1	6	2.1
(1,308)	1:366:A:ILE:HD12	1:387:A:TYR:HE1	14	2.1
(1,2778)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	2	2.09
(1,2778)	1:366:A:ILE:HD12	1:387:A:TYR:HE1	3	2.09
(1,2778)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	19	2.09
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	1	2.09
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	16	2.09
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	18	2.09
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	15	2.09
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	16	2.09
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD12	14	2.09
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	2	2.09
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	3	2.09
(1,387)	1:375:A:LEU:HD22	1:353:A:PHE:HE1	18	2.09
(1,2777)	1:387:A:TYR:HE1	1:369:A:PRO:HG3	13	2.08
(1,2652)	1:405:A:LYS:HG3	1:398:A:TYR:HD2	2	2.08
(1,2652)	1:405:A:LYS:HG3	1:413:A:PHE:HE2	19	2.08
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	9	2.08
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	8	2.08
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	9	2.08
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	7	2.08
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	16	2.08
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	15	2.07
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD13	4	2.07
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	15	2.07
(1,1080)	1:372:A:LEU:HD23	1:353:A:PHE:HD1	11	2.07
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	2	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	8	2.07
(1,172)	1:354:A:ILE:HG23	1:350:A:TYR:HD1	13	2.07
(1,2778)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	18	2.06
(1,2652)	1:405:A:LYS:HG3	1:413:A:PHE:HE2	13	2.06
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	10	2.06
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	3	2.06
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	10	2.06
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	18	2.06
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	8	2.06
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	16	2.06
(1,308)	1:366:A:ILE:HD13	1:387:A:TYR:HE1	9	2.06
(1,308)	1:366:A:ILE:HD12	1:387:A:TYR:HE1	16	2.06
(1,308)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	17	2.06
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	17	2.06
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD11	12	2.05
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	16	2.05
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	10	2.05
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	15	2.05
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	5	2.05
(1,302)	1:366:A:ILE:HG22	1:387:A:TYR:HE1	19	2.05
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	14	2.04
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	15	2.04
(1,1658)	1:395:A:ARG:HD3	1:398:A:TYR:HE1	19	2.04
(1,1386)	1:373:A:ALA:HB1	1:387:A:TYR:HD1	4	2.04
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	15	2.04
(1,2778)	1:366:A:ILE:HD13	1:387:A:TYR:HE1	1	2.03
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	2	2.03
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	11	2.03
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	17	2.03
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	19	2.03
(1,308)	1:366:A:ILE:HD13	1:387:A:TYR:HE1	7	2.03
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	1	2.02
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	6	2.02
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	15	2.02
(1,1080)	1:372:A:LEU:HD23	1:353:A:PHE:HD1	19	2.02
(1,308)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	2	2.02
(1,308)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	19	2.02
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	15	2.02
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	10	2.01
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	1	2.01
(1,1445)	1:442:A:THR:HG21	1:443:A:TYR:HE2	7	2.01
(1,1386)	1:373:A:ALA:HB2	1:387:A:TYR:HD1	9	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	9	2.01
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	2	2.01
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	8	2.01
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	14	2.01
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	12	2.01
(1,1087)	1:371:A:GLY:HA3	1:353:A:PHE:HE1	13	2.01
(1,1080)	1:372:A:LEU:HD23	1:353:A:PHE:HD1	4	2.01
(1,621)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	11	2.01
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	11	2.01
(1,308)	1:366:A:ILE:HD12	1:387:A:TYR:HE1	3	2.01
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD11	10	2.0
(1,1445)	1:442:A:THR:HG22	1:443:A:TYR:HE2	14	2.0
(1,1386)	1:373:A:ALA:HB1	1:387:A:TYR:HD1	14	2.0
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	4	2.0
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	12	2.0
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	9	2.0
(1,1080)	1:372:A:LEU:HD22	1:353:A:PHE:HD1	9	2.0
(1,1080)	1:372:A:LEU:HD23	1:353:A:PHE:HD1	15	2.0
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	19	2.0
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	10	2.0
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	11	2.0
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	19	1.99
(1,1830)	1:387:A:TYR:HE2	1:391:A:SER:HA	7	1.99
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	6	1.99
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	17	1.99
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	2	1.99
(1,1080)	1:372:A:LEU:HD21	1:353:A:PHE:HD1	10	1.99
(1,621)	1:403:A:ILE:HG23	1:413:A:PHE:HD1	3	1.99
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	10	1.99
(1,308)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	18	1.99
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	5	1.98
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	19	1.98
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	17	1.98
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	17	1.98
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	18	1.98
(1,1080)	1:372:A:LEU:HD22	1:353:A:PHE:HD1	3	1.98
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	3	1.98
(1,52)	1:443:A:TYR:HE2	1:456:A:TRP:HD1	18	1.98
(1,2806)	1:430:A:LEU:HD12	1:431:A:GLU:HG2	3	1.97
(1,2652)	1:405:A:LYS:HG3	1:398:A:TYR:HD2	9	1.97
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	11	1.97
(1,1003)	1:409:A:GLN:HG2	1:406:A:GLU:HB2	5	1.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	6	1.96
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	19	1.96
(1,1445)	1:442:A:THR:HG23	1:443:A:TYR:HE2	6	1.96
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	17	1.96
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	10	1.96
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	1	1.96
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	9	1.96
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	14	1.96
(1,621)	1:403:A:ILE:HG23	1:413:A:PHE:HD1	2	1.96
(1,621)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	4	1.96
(1,382)	1:375:A:LEU:HD11	1:350:A:TYR:HD2	10	1.96
(1,382)	1:375:A:LEU:HD11	1:350:A:TYR:HD2	14	1.96
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	2	1.96
(1,2778)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	8	1.95
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD23	19	1.95
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	7	1.95
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	8	1.95
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	13	1.95
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	7	1.95
(1,308)	1:366:A:ILE:HD13	1:387:A:TYR:HE1	1	1.95
(1,1386)	1:373:A:ALA:HB1	1:387:A:TYR:HD1	7	1.94
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	19	1.94
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	16	1.94
(1,621)	1:403:A:ILE:HG22	1:413:A:PHE:HD1	10	1.94
(1,621)	1:403:A:ILE:HG22	1:413:A:PHE:HD1	18	1.94
(1,621)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	19	1.94
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	6	1.94
(1,2778)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	12	1.93
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	7	1.93
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	19	1.93
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	6	1.93
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	8	1.93
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	16	1.93
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	4	1.93
(1,1386)	1:373:A:ALA:HB3	1:387:A:TYR:HD1	8	1.92
(1,1386)	1:373:A:ALA:HB1	1:387:A:TYR:HD1	12	1.92
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	15	1.92
(1,621)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	6	1.92
(1,621)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	12	1.92
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	15	1.92
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	7	1.92
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	12	1.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	19	1.92
(1,2652)	1:405:A:LYS:HG3	1:413:A:PHE:HE2	11	1.91
(1,1828)	1:398:A:TYR:HA	1:399:A:LYS:HD2	1	1.91
(1,1828)	1:398:A:TYR:HA	1:399:A:LYS:HD2	5	1.91
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	7	1.91
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	5	1.91
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	14	1.91
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	13	1.91
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	6	1.91
(1,1080)	1:372:A:LEU:HD23	1:353:A:PHE:HD1	1	1.91
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	14	1.91
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	1	1.91
(1,2821)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	11	1.9
(1,1849)	1:342:A:TYR:HE2	1:345:A:LEU:HD12	11	1.9
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	5	1.9
(1,1172)	1:363:A:ILE:HG23	1:409:A:GLN:HE22	17	1.9
(1,1140)	1:366:A:ILE:HG21	1:387:A:TYR:HD1	5	1.9
(1,621)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	1	1.9
(1,621)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	17	1.9
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	13	1.9
(1,382)	1:375:A:LEU:HD13	1:350:A:TYR:HD2	16	1.9
(1,2806)	1:430:A:LEU:HD12	1:431:A:GLU:HG2	13	1.89
(1,2795)	1:433:A:LEU:HD23	1:440:A:GLU:HG2	18	1.89
(1,2652)	1:405:A:LYS:HG3	1:413:A:PHE:HE2	16	1.89
(1,1828)	1:398:A:TYR:HA	1:399:A:LYS:HD2	7	1.89
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	9	1.89
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	10	1.89
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	7	1.89
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	13	1.89
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	5	1.89
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	3	1.89
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	10	1.89
(1,621)	1:403:A:ILE:HG23	1:413:A:PHE:HD1	16	1.89
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	14	1.89
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	18	1.89
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	4	1.89
(1,2821)	1:403:A:ILE:HG23	1:413:A:PHE:HD1	3	1.88
(1,2806)	1:430:A:LEU:HD12	1:431:A:GLU:HG2	5	1.88
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	19	1.88
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	19	1.88
(1,1809)	1:419:A:PRO:HG2	1:342:A:TYR:HD1	5	1.88
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	3	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1140)	1:366:A:ILE:HG23	1:387:A:TYR:HD1	4	1.88
(1,1080)	1:372:A:LEU:HD21	1:353:A:PHE:HD1	2	1.88
(1,1080)	1:372:A:LEU:HD23	1:353:A:PHE:HD1	14	1.88
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	4	1.88
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	13	1.88
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	18	1.88
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	2	1.88
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	8	1.88
(1,308)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	8	1.88
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	16	1.88
(1,127)	1:349:A:ARG:HD2	1:350:A:TYR:HE1	15	1.88
(1,2778)	1:366:A:ILE:HD12	1:387:A:TYR:HE1	13	1.87
(1,2652)	1:405:A:LYS:HG3	1:398:A:TYR:HD2	1	1.87
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	9	1.87
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	9	1.87
(1,1682)	1:402:A:ILE:HG23	1:415:A:PHE:HB2	10	1.87
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	2	1.87
(1,1386)	1:373:A:ALA:HB3	1:387:A:TYR:HD1	1	1.87
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	19	1.87
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	14	1.87
(1,1140)	1:366:A:ILE:HG23	1:387:A:TYR:HD1	11	1.87
(1,1080)	1:372:A:LEU:HD22	1:353:A:PHE:HD1	16	1.87
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	4	1.87
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	11	1.87
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	16	1.87
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	19	1.87
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	9	1.87
(1,2806)	1:430:A:LEU:HD11	1:431:A:GLU:HG2	16	1.86
(1,2687)	1:400:A:LEU:H	1:430:A:LEU:HD23	18	1.86
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	14	1.86
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	4	1.86
(1,1682)	1:402:A:ILE:HG23	1:415:A:PHE:HB2	3	1.86
(1,1682)	1:402:A:ILE:HG23	1:415:A:PHE:HB2	6	1.86
(1,1682)	1:402:A:ILE:HG22	1:415:A:PHE:HB2	18	1.86
(1,1386)	1:373:A:ALA:HB2	1:387:A:TYR:HD1	6	1.86
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	4	1.86
(1,1091)	1:369:A:PRO:HA	1:387:A:TYR:HE1	13	1.86
(1,1080)	1:372:A:LEU:HD22	1:353:A:PHE:HD1	5	1.86
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	16	1.86
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	2	1.86
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	3	1.86
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	19	1.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	3	1.86
(1,308)	1:366:A:ILE:HD11	1:387:A:TYR:HE1	12	1.86
(1,302)	1:366:A:ILE:HG23	1:387:A:TYR:HE1	13	1.86
(1,2821)	1:403:A:ILE:HG23	1:413:A:PHE:HD1	2	1.85
(1,2821)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	4	1.85
(1,2806)	1:430:A:LEU:HD13	1:431:A:GLU:HG2	1	1.85
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	11	1.85
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	18	1.85
(1,1682)	1:402:A:ILE:HG22	1:415:A:PHE:HB2	4	1.85
(1,1682)	1:402:A:ILE:HG22	1:415:A:PHE:HB2	14	1.85
(1,1682)	1:402:A:ILE:HG22	1:415:A:PHE:HB2	17	1.85
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	8	1.85
(1,1446)	1:442:A:THR:HG22	1:443:A:TYR:HD2	4	1.85
(1,1386)	1:373:A:ALA:HB3	1:387:A:TYR:HD1	16	1.85
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	2	1.85
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	6	1.85
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	10	1.85
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	18	1.85
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	12	1.85
(1,1140)	1:366:A:ILE:HG21	1:387:A:TYR:HD1	10	1.85
(1,1080)	1:372:A:LEU:HD22	1:353:A:PHE:HD1	8	1.85
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	6	1.85
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	15	1.85
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	3	1.85
(1,383)	1:375:A:LEU:HD12	1:353:A:PHE:HE1	19	1.85
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	18	1.84
(1,1682)	1:402:A:ILE:HG21	1:415:A:PHE:HB2	5	1.84
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	5	1.84
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	17	1.84
(1,1386)	1:373:A:ALA:HB3	1:387:A:TYR:HD1	3	1.84
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	4	1.84
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	9	1.84
(1,1256)	1:410:A:ARG:HD2	1:412:A:LEU:HB3	5	1.84
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	4	1.84
(1,900)	1:438:A:LEU:HD11	1:434:A:GLU:HB2	17	1.84
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	9	1.84
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	13	1.84
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	1	1.84
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	11	1.84
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	15	1.84
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	17	1.84
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	1	1.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2821)	1:403:A:ILE:HG22	1:413:A:PHE:HD1	10	1.83
(1,2821)	1:403:A:ILE:HG22	1:413:A:PHE:HD1	18	1.83
(1,2821)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	19	1.83
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	4	1.83
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	18	1.83
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	4	1.83
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	13	1.83
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	19	1.83
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	15	1.83
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	2	1.83
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	12	1.83
(1,1682)	1:402:A:ILE:HG23	1:415:A:PHE:HB2	15	1.83
(1,1682)	1:402:A:ILE:HG23	1:415:A:PHE:HB2	16	1.83
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	1	1.83
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	6	1.83
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	16	1.83
(1,1386)	1:373:A:ALA:HB1	1:387:A:TYR:HD1	2	1.83
(1,1386)	1:373:A:ALA:HB2	1:387:A:TYR:HD1	19	1.83
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	12	1.83
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	8	1.83
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	1	1.83
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	5	1.83
(1,621)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	9	1.83
(1,621)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	14	1.83
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	6	1.83
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	7	1.83
(1,127)	1:349:A:ARG:HD2	1:350:A:TYR:HE1	12	1.83
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	7	1.83
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	14	1.82
(1,2254)	1:443:A:TYR:H	1:443:A:TYR:HD2	14	1.82
(1,1682)	1:402:A:ILE:HG23	1:415:A:PHE:HB2	1	1.82
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	4	1.82
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	9	1.82
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	18	1.82
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	5	1.82
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	16	1.82
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	12	1.82
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	14	1.82
(1,2821)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	6	1.81
(1,2821)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	12	1.81
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD12	15	1.81
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	13	1.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1682)	1:402:A:ILE:HG21	1:415:A:PHE:HB2	2	1.81
(1,1682)	1:402:A:ILE:HG22	1:415:A:PHE:HB2	12	1.81
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	3	1.81
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	15	1.81
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	9	1.81
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	7	1.81
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	11	1.81
(1,1080)	1:372:A:LEU:HD21	1:353:A:PHE:HD1	7	1.81
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	7	1.81
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	17	1.81
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	9	1.81
(1,2795)	1:433:A:LEU:HD23	1:440:A:GLU:HG2	2	1.8
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD11	1	1.8
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	17	1.8
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	3	1.8
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	15	1.8
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	15	1.8
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	2	1.8
(1,1682)	1:402:A:ILE:HG22	1:415:A:PHE:HB2	7	1.8
(1,1682)	1:402:A:ILE:HG21	1:415:A:PHE:HB2	9	1.8
(1,1682)	1:402:A:ILE:HG22	1:415:A:PHE:HB2	13	1.8
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	10	1.8
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	11	1.8
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	14	1.8
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	19	1.8
(1,1446)	1:442:A:THR:HG21	1:443:A:TYR:HD2	7	1.8
(1,1080)	1:372:A:LEU:HD21	1:353:A:PHE:HD1	13	1.8
(1,621)	1:403:A:ILE:HG22	1:413:A:PHE:HD1	7	1.8
(1,308)	1:366:A:ILE:HD12	1:387:A:TYR:HE1	13	1.8
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	18	1.8
(1,2821)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	1	1.79
(1,2821)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	17	1.79
(1,2795)	1:433:A:LEU:HD21	1:440:A:GLU:HG2	7	1.79
(1,2795)	1:433:A:LEU:HD21	1:440:A:GLU:HG2	13	1.79
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	13	1.79
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	1	1.79
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	1	1.79
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	4	1.79
(1,1684)	1:402:A:ILE:HG21	1:397:A:TYR:HB2	19	1.79
(1,1682)	1:402:A:ILE:HG21	1:415:A:PHE:HB2	19	1.79
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	19	1.79
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	4	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	12	1.79
(1,1080)	1:372:A:LEU:HD23	1:353:A:PHE:HD1	6	1.79
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	12	1.79
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	8	1.79
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	12	1.79
(1,127)	1:349:A:ARG:HD2	1:350:A:TYR:HE1	13	1.79
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	5	1.79
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	16	1.79
(1,2821)	1:403:A:ILE:HG23	1:413:A:PHE:HD1	16	1.78
(1,2806)	1:430:A:LEU:HD11	1:431:A:GLU:HG2	6	1.78
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	6	1.78
(1,2652)	1:405:A:LYS:HG3	1:398:A:TYR:HD2	10	1.78
(1,2447)	1:385:A:MET:H	1:444:A:GLN:HE21	15	1.78
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	7	1.78
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	11	1.78
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	11	1.78
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	14	1.78
(1,1684)	1:402:A:ILE:HG22	1:397:A:TYR:HB2	17	1.78
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	6	1.78
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	8	1.78
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	19	1.78
(1,621)	1:403:A:ILE:HG23	1:413:A:PHE:HD1	13	1.78
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	13	1.77
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	6	1.77
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	11	1.77
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	17	1.77
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	6	1.77
(1,1682)	1:402:A:ILE:HG22	1:415:A:PHE:HB2	11	1.77
(1,1579)	1:413:A:PHE:HD1	1:364:A:PHE:HZ	12	1.77
(1,1442)	1:443:A:TYR:HE2	1:445:A:GLU:HG2	9	1.77
(1,1386)	1:373:A:ALA:HB3	1:387:A:TYR:HD1	15	1.77
(1,1262)	1:354:A:ILE:HG12	1:364:A:PHE:HD1	1	1.77
(1,1140)	1:366:A:ILE:HG22	1:387:A:TYR:HD1	6	1.77
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	15	1.77
(1,621)	1:403:A:ILE:HG22	1:413:A:PHE:HD1	5	1.77
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	17	1.77
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	14	1.77
(1,2652)	1:405:A:LYS:HG3	1:413:A:PHE:HE2	18	1.76
(1,1386)	1:373:A:ALA:HB3	1:387:A:TYR:HD1	17	1.76
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	1	1.76
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	14	1.76
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	16	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	2	1.76
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	10	1.76
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	5	1.75
(1,1684)	1:402:A:ILE:HG22	1:397:A:TYR:HB2	11	1.75
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	3	1.75
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	10	1.75
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	12	1.75
(1,1140)	1:366:A:ILE:HG23	1:387:A:TYR:HD1	3	1.75
(1,1140)	1:366:A:ILE:HG23	1:387:A:TYR:HD1	15	1.75
(1,1140)	1:366:A:ILE:HG21	1:387:A:TYR:HD1	16	1.75
(1,1140)	1:366:A:ILE:HG23	1:387:A:TYR:HD1	17	1.75
(1,1090)	1:369:A:PRO:HA	1:387:A:TYR:HD1	13	1.75
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	19	1.75
(1,451)	1:385:A:MET:HG3	1:389:A:LYS:HB2	15	1.75
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	4	1.75
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	15	1.75
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD23	19	1.74
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	8	1.74
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	12	1.74
(1,1682)	1:402:A:ILE:HG21	1:415:A:PHE:HB2	8	1.74
(1,1541)	1:445:A:GLU:HA	1:443:A:TYR:HD1	10	1.74
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	2	1.74
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	3	1.74
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	16	1.74
(1,2790)	1:438:A:LEU:HD21	1:437:A:VAL:HB	4	1.73
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	12	1.73
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	16	1.73
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	7	1.73
(1,1256)	1:410:A:ARG:HD3	1:412:A:LEU:HB3	9	1.73
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	3	1.73
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	12	1.73
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	18	1.73
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	9	1.73
(1,387)	1:375:A:LEU:HD23	1:353:A:PHE:HE1	4	1.73
(1,292)	1:366:A:ILE:HG13	1:413:A:PHE:HD1	5	1.73
(1,2821)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	9	1.72
(1,2821)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	14	1.72
(1,2795)	1:433:A:LEU:HD23	1:440:A:GLU:HG2	15	1.72
(1,2790)	1:438:A:LEU:HD22	1:437:A:VAL:HB	6	1.72
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD13	16	1.72
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	4	1.72
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	10	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	5	1.72
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	4	1.72
(1,1684)	1:402:A:ILE:HG22	1:397:A:TYR:HB2	18	1.72
(1,1445)	1:442:A:THR:HG22	1:443:A:TYR:HE2	3	1.72
(1,1403)	1:383:A:THR:HG22	1:382:A:ARG:HD2	18	1.72
(1,1256)	1:410:A:ARG:HD2	1:412:A:LEU:HB3	18	1.72
(1,1140)	1:366:A:ILE:HG21	1:387:A:TYR:HD1	18	1.72
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	10	1.72
(1,621)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	8	1.72
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	1	1.72
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD13	14	1.71
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	9	1.71
(1,2254)	1:443:A:TYR:H	1:443:A:TYR:HD2	17	1.71
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	2	1.71
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	17	1.71
(1,1392)	1:386:A:THR:HG22	1:389:A:LYS:HG2	3	1.71
(1,1366)	1:391:A:SER:HB2	1:387:A:TYR:HE2	7	1.71
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	13	1.71
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD11	1	1.71
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD11	9	1.71
(1,1088)	1:371:A:GLY:HA3	1:353:A:PHE:HD1	13	1.71
(1,734)	1:416:A:MET:HG2	1:403:A:ILE:HA	8	1.71
(1,85)	1:344:A:LEU:HD21	1:350:A:TYR:HD1	13	1.71
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD12	12	1.7
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD11	13	1.7
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	16	1.7
(1,2652)	1:405:A:LYS:HG3	1:398:A:TYR:HD2	12	1.7
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	7	1.7
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	15	1.7
(1,1386)	1:373:A:ALA:HB1	1:387:A:TYR:HD1	13	1.7
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	14	1.7
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD11	7	1.7
(1,1172)	1:363:A:ILE:HG22	1:409:A:GLN:HE22	3	1.7
(1,1140)	1:366:A:ILE:HG22	1:387:A:TYR:HD1	14	1.7
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	14	1.7
(1,2790)	1:438:A:LEU:HD23	1:437:A:VAL:HB	11	1.69
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	10	1.69
(1,1694)	1:353:A:PHE:HD2	1:350:A:TYR:HA	16	1.69
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	14	1.69
(1,1256)	1:410:A:ARG:HD2	1:412:A:LEU:HB3	15	1.69
(1,1140)	1:366:A:ILE:HG21	1:387:A:TYR:HD1	2	1.69
(1,1140)	1:366:A:ILE:HG23	1:387:A:TYR:HD1	9	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1140)	1:366:A:ILE:HG23	1:387:A:TYR:HD1	12	1.69
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	19	1.69
(1,621)	1:403:A:ILE:HG22	1:413:A:PHE:HD1	15	1.69
(1,2821)	1:403:A:ILE:HG22	1:413:A:PHE:HD1	7	1.68
(1,2790)	1:438:A:LEU:HD23	1:437:A:VAL:HB	9	1.68
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	14	1.68
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	3	1.68
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	19	1.68
(1,1442)	1:443:A:TYR:HE2	1:445:A:GLU:HG2	7	1.68
(1,1392)	1:386:A:THR:HG21	1:389:A:LYS:HG2	11	1.68
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	15	1.68
(1,1158)	1:403:A:ILE:HG23	1:364:A:PHE:HE2	17	1.68
(1,1140)	1:366:A:ILE:HG22	1:387:A:TYR:HD1	8	1.68
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	5	1.68
(1,451)	1:385:A:MET:HG3	1:389:A:LYS:HB2	19	1.68
(1,2790)	1:438:A:LEU:HD23	1:437:A:VAL:HB	13	1.67
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD12	6	1.67
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	18	1.67
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	9	1.67
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	16	1.67
(1,1445)	1:442:A:THR:HG23	1:443:A:TYR:HE2	1	1.67
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	2	1.67
(1,1158)	1:403:A:ILE:HG21	1:364:A:PHE:HE2	3	1.67
(1,1140)	1:366:A:ILE:HG22	1:387:A:TYR:HD1	1	1.67
(1,1080)	1:372:A:LEU:HD21	1:353:A:PHE:HD1	12	1.67
(1,900)	1:438:A:LEU:HD13	1:434:A:GLU:HB2	9	1.67
(1,2821)	1:403:A:ILE:HG22	1:413:A:PHE:HD1	5	1.66
(1,2821)	1:403:A:ILE:HG23	1:413:A:PHE:HD1	13	1.66
(1,2790)	1:438:A:LEU:HD22	1:437:A:VAL:HB	18	1.66
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	8	1.66
(1,1684)	1:402:A:ILE:HG21	1:397:A:TYR:HB2	16	1.66
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	2	1.66
(1,172)	1:354:A:ILE:HG21	1:350:A:TYR:HD1	19	1.66
(1,2795)	1:433:A:LEU:HD22	1:440:A:GLU:HG2	11	1.65
(1,2790)	1:438:A:LEU:HD22	1:437:A:VAL:HB	17	1.65
(1,2735)	1:403:A:ILE:HG23	1:364:A:PHE:HE2	17	1.65
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	3	1.65
(1,1392)	1:386:A:THR:HG23	1:389:A:LYS:HG2	12	1.65
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD11	3	1.65
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	19	1.65
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	8	1.65
(1,383)	1:375:A:LEU:HD11	1:353:A:PHE:HE1	13	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	10	1.65
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	11	1.65
(1,2790)	1:438:A:LEU:HD23	1:437:A:VAL:HB	12	1.64
(1,2652)	1:405:A:LYS:HG3	1:398:A:TYR:HD2	7	1.64
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	1	1.64
(1,2463)	1:415:A:PHE:H	1:364:A:PHE:HE2	2	1.64
(1,1864)	1:350:A:TYR:HD2	1:375:A:LEU:HD23	13	1.64
(1,1525)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	17	1.64
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	11	1.64
(1,734)	1:416:A:MET:HG2	1:403:A:ILE:HA	13	1.64
(1,695)	1:412:A:LEU:HA	1:413:A:PHE:HD2	13	1.64
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	17	1.64
(1,561)	1:398:A:TYR:HA	1:398:A:TYR:HD2	5	1.64
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	17	1.64
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD22	4	1.63
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG23	4	1.63
(1,2735)	1:403:A:ILE:HG21	1:364:A:PHE:HE2	3	1.63
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	3	1.63
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	11	1.63
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	8	1.63
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	3	1.63
(1,1140)	1:366:A:ILE:HG21	1:387:A:TYR:HD1	7	1.63
(1,900)	1:438:A:LEU:HD12	1:434:A:GLU:HB2	3	1.63
(1,387)	1:375:A:LEU:HD23	1:353:A:PHE:HE1	14	1.63
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	8	1.63
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	6	1.63
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	8	1.63
(1,2790)	1:438:A:LEU:HD22	1:437:A:VAL:HB	7	1.62
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG21	6	1.62
(1,1684)	1:402:A:ILE:HG23	1:397:A:TYR:HB2	3	1.62
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	16	1.62
(1,1525)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	6	1.62
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	15	1.62
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	18	1.62
(1,1140)	1:366:A:ILE:HG22	1:387:A:TYR:HD1	19	1.62
(1,1003)	1:409:A:GLN:HG2	1:406:A:GLU:HB2	19	1.62
(1,946)	1:447:A:GLU:HG2	1:446:A:ASP:H	11	1.62
(1,547)	1:395:A:ARG:HD2	1:395:A:ARG:H	14	1.62
(1,387)	1:375:A:LEU:HD21	1:353:A:PHE:HE1	2	1.62
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	12	1.62
(1,2821)	1:403:A:ILE:HG21	1:413:A:PHE:HD1	8	1.61
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD11	7	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD11	8	1.61
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	12	1.61
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	15	1.61
(1,2447)	1:385:A:MET:H	1:444:A:GLN:HE21	10	1.61
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	4	1.61
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	5	1.61
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	19	1.61
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	16	1.61
(1,2790)	1:438:A:LEU:HD23	1:437:A:VAL:HB	14	1.6
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	1	1.6
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	8	1.6
(1,1704)	1:350:A:TYR:HD1	1:344:A:LEU:HA	12	1.6
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	5	1.6
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	18	1.6
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	14	1.6
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	14	1.6
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	10	1.6
(1,547)	1:395:A:ARG:HD2	1:395:A:ARG:H	18	1.6
(1,387)	1:375:A:LEU:HD21	1:353:A:PHE:HE1	10	1.6
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	13	1.6
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	15	1.6
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD13	5	1.59
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	4	1.59
(1,1256)	1:410:A:ARG:HD3	1:412:A:LEU:HB3	12	1.59
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	16	1.59
(1,547)	1:395:A:ARG:HD2	1:395:A:ARG:H	16	1.59
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	2	1.59
(1,2821)	1:403:A:ILE:HG22	1:413:A:PHE:HD1	15	1.58
(1,2790)	1:438:A:LEU:HD21	1:437:A:VAL:HB	1	1.58
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	13	1.58
(1,1684)	1:402:A:ILE:HG21	1:397:A:TYR:HB2	9	1.58
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	19	1.58
(1,1523)	1:422:A:ILE:HG21	1:426:A:ARG:HG2	5	1.58
(1,1446)	1:442:A:THR:HG23	1:443:A:TYR:HD2	6	1.58
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	14	1.58
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	14	1.57
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	4	1.57
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	5	1.57
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	9	1.57
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	11	1.57
(1,2941)	1:411:A:LEU:H	1:412:A:LEU:HD11	18	1.56
(1,2797)	1:430:A:LEU:HA	1:433:A:LEU:HD11	4	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2795)	1:433:A:LEU:HD23	1:440:A:GLU:HG2	1	1.56
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD12	2	1.56
(1,1847)	1:398:A:TYR:HE2	1:398:A:TYR:HA	5	1.56
(1,1684)	1:402:A:ILE:HG22	1:397:A:TYR:HB2	14	1.56
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	10	1.56
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	19	1.56
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	2	1.56
(1,1445)	1:442:A:THR:HG21	1:443:A:TYR:HE2	18	1.56
(1,1183)	1:363:A:ILE:HD12	1:362:A:LYS:HG3	6	1.56
(1,900)	1:438:A:LEU:HD11	1:434:A:GLU:HB2	8	1.56
(1,900)	1:438:A:LEU:HD13	1:434:A:GLU:HB2	11	1.56
(1,900)	1:438:A:LEU:HD11	1:434:A:GLU:HB2	16	1.56
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	11	1.56
(1,547)	1:395:A:ARG:HD2	1:395:A:ARG:H	8	1.56
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	6	1.56
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	19	1.56
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD11	11	1.55
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD12	18	1.55
(1,1777)	1:337:A:LEU:HD13	1:340:A:TYR:HB2	1	1.55
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	3	1.55
(1,1476)	1:433:A:LEU:HD23	1:433:A:LEU:HA	4	1.55
(1,1392)	1:386:A:THR:HG22	1:389:A:LYS:HG2	15	1.55
(1,1158)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	19	1.55
(1,900)	1:438:A:LEU:HD12	1:434:A:GLU:HB2	10	1.55
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	7	1.55
(1,547)	1:395:A:ARG:HD2	1:395:A:ARG:H	1	1.55
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	1	1.55
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	3	1.55
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	7	1.55
(1,2790)	1:438:A:LEU:HD23	1:437:A:VAL:HB	2	1.54
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG22	2	1.54
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG21	14	1.54
(1,1158)	1:403:A:ILE:HG21	1:364:A:PHE:HE2	16	1.54
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	6	1.54
(1,293)	1:366:A:ILE:HG13	1:364:A:PHE:HE1	18	1.54
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD12	9	1.53
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	16	1.53
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	6	1.53
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	17	1.53
(1,1348)	1:395:A:ARG:HA	1:398:A:TYR:HE1	19	1.53
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	7	1.53
(1,946)	1:447:A:GLU:HG2	1:446:A:ASP:H	10	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	7	1.53
(1,1777)	1:337:A:LEU:HD12	1:340:A:TYR:HB2	5	1.52
(1,1777)	1:337:A:LEU:HD11	1:340:A:TYR:HB2	18	1.52
(1,1684)	1:402:A:ILE:HG22	1:397:A:TYR:HB2	4	1.52
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	8	1.52
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	13	1.52
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	16	1.52
(1,1446)	1:442:A:THR:HG21	1:443:A:TYR:HD2	18	1.52
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	5	1.52
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	19	1.52
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	1	1.52
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	5	1.52
(1,2795)	1:433:A:LEU:HD22	1:440:A:GLU:HG2	16	1.51
(1,2794)	1:375:A:LEU:HD23	1:353:A:PHE:HB2	4	1.51
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD12	3	1.51
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG23	15	1.51
(1,2735)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	19	1.51
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	7	1.51
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB1	8	1.51
(1,1777)	1:337:A:LEU:HD12	1:340:A:TYR:HB2	13	1.51
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	6	1.51
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	1	1.51
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	7	1.51
(1,387)	1:375:A:LEU:HD23	1:353:A:PHE:HE1	3	1.51
(1,2878)	1:403:A:ILE:HG22	1:414:A:ARG:HB3	2	1.5
(1,2789)	1:438:A:LEU:HD11	1:381:A:ASN:HD22	18	1.5
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB3	6	1.5
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG23	12	1.5
(1,2735)	1:403:A:ILE:HG21	1:364:A:PHE:HE2	16	1.5
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	11	1.5
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	12	1.5
(1,1445)	1:442:A:THR:HG21	1:443:A:TYR:HE2	17	1.5
(1,1183)	1:363:A:ILE:HD13	1:362:A:LYS:HG3	4	1.5
(1,900)	1:438:A:LEU:HD13	1:434:A:GLU:HB2	5	1.5
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	18	1.5
(1,387)	1:375:A:LEU:HD23	1:353:A:PHE:HE1	11	1.5
(1,383)	1:375:A:LEU:HD12	1:353:A:PHE:HE1	18	1.5
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	15	1.49
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	5	1.49
(1,1003)	1:409:A:GLN:HG2	1:406:A:GLU:HB2	18	1.49
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	2	1.49
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	13	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	17	1.49
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	1	1.49
(1,234)	1:356:A:TRP:HE1	1:359:A:LYS:HE2	16	1.49
(1,2553)	1:454:A:VAL:H	1:454:A:VAL:HG22	2	1.48
(1,1777)	1:337:A:LEU:HD13	1:340:A:TYR:HB2	12	1.48
(1,1684)	1:402:A:ILE:HG23	1:397:A:TYR:HB2	7	1.48
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	17	1.48
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	4	1.48
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	14	1.48
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	17	1.48
(1,1183)	1:363:A:ILE:HD11	1:362:A:LYS:HG3	8	1.48
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	12	1.48
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	12	1.48
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	14	1.48
(1,2790)	1:438:A:LEU:HD22	1:437:A:VAL:HB	10	1.47
(1,2553)	1:454:A:VAL:H	1:454:A:VAL:HG23	8	1.47
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	12	1.47
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	3	1.47
(1,1623)	1:407:A:PRO:HD3	1:406:A:GLU:HG3	10	1.47
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	6	1.47
(1,1183)	1:363:A:ILE:HD12	1:362:A:LYS:HG3	19	1.47
(1,1158)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	8	1.47
(1,1003)	1:409:A:GLN:HG2	1:406:A:GLU:HB2	6	1.47
(1,837)	1:430:A:LEU:HD13	1:427:A:THR:HA	18	1.47
(1,2795)	1:433:A:LEU:HD23	1:440:A:GLU:HG2	9	1.46
(1,2790)	1:438:A:LEU:HD23	1:437:A:VAL:HB	3	1.46
(1,2671)	1:415:A:PHE:HD2	1:364:A:PHE:HE2	2	1.46
(1,2547)	1:442:A:THR:H	1:442:A:THR:HG21	9	1.46
(1,1777)	1:337:A:LEU:HD11	1:340:A:TYR:HB2	16	1.46
(1,1684)	1:402:A:ILE:HG22	1:397:A:TYR:HB2	2	1.46
(1,1684)	1:402:A:ILE:HG21	1:397:A:TYR:HB2	5	1.46
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	2	1.46
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	15	1.46
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	3	1.46
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	18	1.46
(1,1541)	1:445:A:GLU:HA	1:443:A:TYR:HD1	3	1.46
(1,387)	1:375:A:LEU:HD21	1:353:A:PHE:HE1	9	1.46
(1,2553)	1:454:A:VAL:H	1:454:A:VAL:HG23	10	1.45
(1,1541)	1:445:A:GLU:HA	1:443:A:TYR:HD1	14	1.45
(1,1407)	1:456:A:TRP:HB3	1:456:A:TRP:HZ3	11	1.45
(1,1392)	1:386:A:THR:HG22	1:389:A:LYS:HG2	9	1.45
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	17	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1256)	1:410:A:ARG:HD2	1:412:A:LEU:HB3	14	1.45
(1,1256)	1:410:A:ARG:HD2	1:412:A:LEU:HB3	19	1.45
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	9	1.45
(1,1183)	1:363:A:ILE:HD12	1:362:A:LYS:HG3	12	1.45
(1,1158)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	9	1.45
(1,387)	1:375:A:LEU:HD23	1:353:A:PHE:HE1	8	1.45
(1,2735)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	8	1.44
(1,2553)	1:454:A:VAL:H	1:454:A:VAL:HG21	4	1.44
(1,1684)	1:402:A:ILE:HG21	1:397:A:TYR:HB2	1	1.44
(1,1684)	1:402:A:ILE:HG23	1:397:A:TYR:HB2	12	1.44
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	11	1.44
(1,1525)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	8	1.44
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	5	1.44
(1,1140)	1:366:A:ILE:HG23	1:387:A:TYR:HD1	13	1.44
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	1	1.44
(1,1003)	1:409:A:GLN:HG2	1:406:A:GLU:HB2	9	1.44
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	4	1.44
(1,547)	1:395:A:ARG:HD2	1:395:A:ARG:H	19	1.44
(1,236)	1:361:A:SER:HB3	1:358:A:ASP:HB2	1	1.44
(1,172)	1:354:A:ILE:HG23	1:350:A:TYR:HD1	10	1.44
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	2	1.44
(1,2816)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	17	1.43
(1,1777)	1:337:A:LEU:HD11	1:340:A:TYR:HB2	2	1.43
(1,1777)	1:337:A:LEU:HD13	1:340:A:TYR:HB2	6	1.43
(1,1777)	1:337:A:LEU:HD13	1:340:A:TYR:HB2	11	1.43
(1,1777)	1:337:A:LEU:HD12	1:340:A:TYR:HB2	17	1.43
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	4	1.43
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	9	1.43
(1,1525)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	2	1.43
(1,1234)	1:356:A:TRP:HH2	1:342:A:TYR:HE2	11	1.43
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	16	1.43
(1,1183)	1:363:A:ILE:HD13	1:362:A:LYS:HG3	13	1.43
(1,1183)	1:363:A:ILE:HD13	1:362:A:LYS:HG3	17	1.43
(1,1158)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	4	1.43
(1,900)	1:438:A:LEU:HD12	1:434:A:GLU:HB2	18	1.43
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	2	1.43
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	9	1.43
(1,2790)	1:438:A:LEU:HD21	1:437:A:VAL:HB	15	1.42
(1,2726)	1:367:A:VAL:HG13	1:355:A:ARG:HD2	6	1.42
(1,2254)	1:443:A:TYR:H	1:443:A:TYR:HD2	11	1.42
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD23	4	1.42
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	11	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1407)	1:456:A:TRP:HB3	1:456:A:TRP:HZ3	9	1.42
(1,1407)	1:456:A:TRP:HB3	1:456:A:TRP:HZ3	14	1.42
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	13	1.42
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	19	1.42
(1,1172)	1:363:A:ILE:HG21	1:409:A:GLN:HE22	8	1.42
(1,900)	1:438:A:LEU:HD12	1:434:A:GLU:HB2	2	1.42
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	14	1.42
(1,85)	1:344:A:LEU:HD23	1:350:A:TYR:HD1	19	1.42
(1,2816)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	6	1.41
(1,2735)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	9	1.41
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	18	1.41
(1,1684)	1:402:A:ILE:HG23	1:397:A:TYR:HB2	15	1.41
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	6	1.41
(1,1407)	1:456:A:TRP:HB3	1:456:A:TRP:HZ3	10	1.41
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	7	1.41
(1,1158)	1:403:A:ILE:HG23	1:364:A:PHE:HE2	10	1.41
(1,1158)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	11	1.41
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	2	1.41
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	10	1.41
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	14	1.41
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	16	1.41
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	12	1.41
(1,734)	1:416:A:MET:HG2	1:403:A:ILE:HA	15	1.41
(1,388)	1:375:A:LEU:HD23	1:350:A:TYR:HE2	19	1.41
(1,387)	1:375:A:LEU:HD22	1:353:A:PHE:HE1	7	1.41
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD11	10	1.4
(1,2735)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	4	1.4
(1,1684)	1:402:A:ILE:HG23	1:397:A:TYR:HB2	6	1.4
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	7	1.4
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	17	1.4
(1,1446)	1:442:A:THR:HG22	1:443:A:TYR:HD2	14	1.4
(1,1407)	1:456:A:TRP:HB3	1:456:A:TRP:HZ3	19	1.4
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	3	1.4
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	8	1.4
(1,1172)	1:363:A:ILE:HG22	1:409:A:GLN:HE22	1	1.4
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	11	1.4
(1,900)	1:438:A:LEU:HD11	1:434:A:GLU:HB2	19	1.4
(1,1777)	1:337:A:LEU:HD13	1:340:A:TYR:HB2	14	1.39
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	9	1.39
(1,1183)	1:363:A:ILE:HD13	1:362:A:LYS:HG3	18	1.39
(1,547)	1:395:A:ARG:HD2	1:395:A:ARG:H	5	1.39
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB1	10	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:375:A:LEU:HD23	1:353:A:PHE:HE1	16	1.39
(1,2790)	1:438:A:LEU:HD22	1:437:A:VAL:HB	16	1.38
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	4	1.38
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	17	1.38
(1,1684)	1:402:A:ILE:HG23	1:397:A:TYR:HB2	13	1.38
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	9	1.38
(1,1525)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	10	1.38
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	1	1.38
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	2	1.38
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	7	1.38
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	9	1.38
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	11	1.38
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	12	1.38
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	11	1.38
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	15	1.38
(1,1183)	1:363:A:ILE:HD12	1:362:A:LYS:HG3	1	1.38
(1,1172)	1:363:A:ILE:HG22	1:409:A:GLN:HE22	13	1.38
(1,1172)	1:363:A:ILE:HG22	1:409:A:GLN:HE22	16	1.38
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	5	1.38
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	7	1.38
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	19	1.38
(1,382)	1:375:A:LEU:HD13	1:350:A:TYR:HD2	19	1.38
(1,2735)	1:403:A:ILE:HG23	1:364:A:PHE:HE2	10	1.37
(1,2735)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	11	1.37
(1,2447)	1:385:A:MET:H	1:444:A:GLN:HE21	9	1.37
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	6	1.37
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	5	1.37
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	1	1.37
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	7	1.37
(1,1525)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	1	1.37
(1,1445)	1:442:A:THR:HG22	1:443:A:TYR:HE2	11	1.37
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	3	1.37
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	6	1.37
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	8	1.37
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	13	1.37
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	14	1.37
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	18	1.37
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	19	1.37
(1,1183)	1:363:A:ILE:HD11	1:362:A:LYS:HG3	16	1.37
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	4	1.37
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	13	1.37
(1,946)	1:447:A:GLU:HG2	1:446:A:ASP:H	19	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	3	1.37
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	8	1.37
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	9	1.37
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	9	1.37
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	4	1.37
(1,234)	1:356:A:TRP:HE1	1:359:A:LYS:HE2	8	1.37
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB1	17	1.36
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	11	1.36
(1,1777)	1:337:A:LEU:HD11	1:340:A:TYR:HB2	9	1.36
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	18	1.36
(1,1684)	1:402:A:ILE:HG23	1:397:A:TYR:HB2	10	1.36
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	8	1.36
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	13	1.36
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	4	1.36
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	4	1.36
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	5	1.36
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	10	1.36
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	15	1.36
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	16	1.36
(1,1420)	1:407:A:PRO:HB2	1:407:A:PRO:HD2	17	1.36
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	9	1.36
(1,1183)	1:363:A:ILE:HD13	1:362:A:LYS:HG3	10	1.36
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	1	1.36
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	8	1.36
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	18	1.36
(1,383)	1:375:A:LEU:HD11	1:353:A:PHE:HE1	3	1.36
(1,111)	1:347:A:ASP:HB3	1:350:A:TYR:HE1	10	1.36
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	16	1.35
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	13	1.35
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	19	1.35
(1,1777)	1:337:A:LEU:HD12	1:340:A:TYR:HB2	3	1.35
(1,1777)	1:337:A:LEU:HD11	1:340:A:TYR:HB2	7	1.35
(1,1525)	1:422:A:ILE:HG22	1:417:A:LYS:HD3	11	1.35
(1,1446)	1:442:A:THR:HG22	1:443:A:TYR:HD2	3	1.35
(1,1392)	1:386:A:THR:HG21	1:389:A:LYS:HG2	13	1.35
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	1	1.35
(1,1183)	1:363:A:ILE:HD12	1:362:A:LYS:HG3	3	1.35
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	6	1.35
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	15	1.35
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	15	1.35
(1,236)	1:361:A:SER:HB3	1:358:A:ASP:HB2	3	1.35
(1,2795)	1:433:A:LEU:HD23	1:440:A:GLU:HG2	19	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2774)	1:443:A:TYR:HD1	1:444:A:GLN:HB3	9	1.34
(1,2687)	1:430:A:LEU:HD21	1:396:A:HIS:H	4	1.34
(1,2687)	1:430:A:LEU:HD22	1:396:A:HIS:H	10	1.34
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	4	1.34
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	10	1.34
(1,1158)	1:403:A:ILE:HG21	1:364:A:PHE:HE2	13	1.34
(1,1158)	1:403:A:ILE:HG23	1:364:A:PHE:HE2	15	1.34
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	9	1.34
(1,900)	1:438:A:LEU:HD13	1:434:A:GLU:HB2	14	1.34
(1,743)	1:417:A:LYS:HD3	1:402:A:ILE:HG13	10	1.34
(1,734)	1:416:A:MET:HG2	1:403:A:ILE:HA	1	1.34
(1,236)	1:361:A:SER:HB3	1:358:A:ASP:HB2	7	1.34
(1,172)	1:354:A:ILE:HG22	1:350:A:TYR:HD1	6	1.34
(1,172)	1:354:A:ILE:HG22	1:350:A:TYR:HD1	14	1.34
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	16	1.34
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	15	1.33
(1,1777)	1:337:A:LEU:HD11	1:340:A:TYR:HB2	4	1.33
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	16	1.33
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	17	1.33
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	12	1.33
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	9	1.33
(1,1407)	1:456:A:TRP:HB3	1:456:A:TRP:HZ3	8	1.33
(1,1392)	1:386:A:THR:HG22	1:389:A:LYS:HG2	2	1.33
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	9	1.33
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	10	1.33
(1,387)	1:375:A:LEU:HD21	1:353:A:PHE:HE1	1	1.33
(1,2795)	1:433:A:LEU:HD21	1:440:A:GLU:HG2	12	1.32
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB2	13	1.32
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	8	1.32
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	16	1.32
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	11	1.32
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	1	1.32
(1,1525)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	18	1.32
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	19	1.32
(1,1206)	1:360:A:GLU:HA	1:362:A:LYS:HG3	8	1.32
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	5	1.32
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	18	1.32
(1,734)	1:416:A:MET:HG2	1:403:A:ILE:HA	14	1.32
(1,381)	1:375:A:LEU:HD13	1:350:A:TYR:HE2	19	1.32
(1,2878)	1:403:A:ILE:HG22	1:414:A:ARG:HB3	18	1.31
(1,2735)	1:403:A:ILE:HG21	1:364:A:PHE:HE2	13	1.31
(1,2694)	1:438:A:LEU:HD13	1:435:A:SER:HB2	17	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2447)	1:385:A:MET:H	1:444:A:GLN:HE21	13	1.31
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	1	1.31
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	11	1.31
(1,1777)	1:337:A:LEU:HD11	1:340:A:TYR:HB2	10	1.31
(1,1777)	1:337:A:LEU:HD13	1:340:A:TYR:HB2	19	1.31
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	8	1.31
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	10	1.31
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	2	1.31
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	10	1.31
(1,1392)	1:386:A:THR:HG23	1:389:A:LYS:HG2	19	1.31
(1,1158)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	1	1.31
(1,1158)	1:403:A:ILE:HG23	1:364:A:PHE:HE2	5	1.31
(1,1158)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	6	1.31
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	3	1.31
(1,2851)	1:344:A:LEU:HD12	1:372:A:LEU:HB3	3	1.3
(1,2735)	1:403:A:ILE:HG23	1:364:A:PHE:HE2	15	1.3
(1,2687)	1:400:A:LEU:H	1:430:A:LEU:HD21	5	1.3
(1,2687)	1:400:A:LEU:H	1:430:A:LEU:HD22	12	1.3
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	15	1.3
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	2	1.3
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	5	1.3
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	19	1.3
(1,1777)	1:337:A:LEU:HD11	1:340:A:TYR:HB2	15	1.3
(1,1720)	1:356:A:TRP:HZ2	1:342:A:TYR:HE2	10	1.3
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	14	1.3
(1,1392)	1:386:A:THR:HG21	1:389:A:LYS:HG2	6	1.3
(1,1256)	1:410:A:ARG:HD3	1:412:A:LEU:HB3	6	1.3
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	13	1.3
(1,1183)	1:363:A:ILE:HD12	1:362:A:LYS:HG3	5	1.3
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	9	1.3
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	18	1.3
(1,734)	1:416:A:MET:HG2	1:403:A:ILE:HA	2	1.3
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB3	5	1.3
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB3	11	1.3
(1,266)	1:363:A:ILE:HG21	1:406:A:GLU:HG2	12	1.3
(1,236)	1:361:A:SER:HB3	1:358:A:ASP:HB2	9	1.3
(1,2851)	1:344:A:LEU:HD11	1:372:A:LEU:HB3	15	1.29
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB2	7	1.29
(1,2687)	1:430:A:LEU:HD23	1:396:A:HIS:H	14	1.29
(1,2687)	1:400:A:LEU:H	1:430:A:LEU:HD23	19	1.29
(1,2685)	1:430:A:LEU:HD11	1:336:A:LEU:HD13	18	1.29
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	10	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	18	1.29
(1,1684)	1:402:A:ILE:HG22	1:397:A:TYR:HB2	8	1.29
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	15	1.29
(1,1445)	1:442:A:THR:HG22	1:443:A:TYR:HE2	15	1.29
(1,1256)	1:410:A:ARG:HD3	1:412:A:LEU:HB3	16	1.29
(1,1183)	1:363:A:ILE:HD12	1:362:A:LYS:HG3	9	1.29
(1,1183)	1:363:A:ILE:HD12	1:362:A:LYS:HG3	14	1.29
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	12	1.29
(1,387)	1:375:A:LEU:HD21	1:353:A:PHE:HE1	15	1.29
(1,383)	1:375:A:LEU:HD11	1:353:A:PHE:HE1	15	1.29
(1,236)	1:361:A:SER:HB3	1:358:A:ASP:HB2	4	1.29
(1,2873)	1:430:A:LEU:H	1:427:A:THR:HG23	7	1.28
(1,2851)	1:344:A:LEU:HD12	1:372:A:LEU:HB3	1	1.28
(1,2789)	1:438:A:LEU:HD12	1:381:A:ASN:HD22	16	1.28
(1,2735)	1:403:A:ILE:HG23	1:364:A:PHE:HE2	5	1.28
(1,2735)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	6	1.28
(1,2687)	1:430:A:LEU:HD23	1:396:A:HIS:H	13	1.28
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	5	1.28
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	7	1.28
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	5	1.28
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	12	1.28
(1,1392)	1:386:A:THR:HG22	1:389:A:LYS:HG2	8	1.28
(1,1172)	1:363:A:ILE:HG23	1:409:A:GLN:HE22	15	1.28
(1,1003)	1:409:A:GLN:HG2	1:406:A:GLU:HB2	4	1.28
(1,172)	1:354:A:ILE:HG23	1:350:A:TYR:HD1	18	1.28
(1,2873)	1:418:A:THR:HG22	1:417:A:LYS:H	11	1.27
(1,2735)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	1	1.27
(1,2547)	1:442:A:THR:H	1:442:A:THR:HG22	14	1.27
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	1	1.27
(1,2254)	1:443:A:TYR:H	1:443:A:TYR:HD2	6	1.27
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	4	1.27
(1,1777)	1:337:A:LEU:HD11	1:340:A:TYR:HB2	8	1.27
(1,1525)	1:422:A:ILE:HG22	1:417:A:LYS:HD3	7	1.27
(1,1525)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	12	1.27
(1,1525)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	15	1.27
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	11	1.27
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	17	1.27
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	12	1.27
(1,236)	1:361:A:SER:HB3	1:358:A:ASP:HB2	2	1.27
(1,2790)	1:438:A:LEU:HD21	1:390:A:MET:HB2	19	1.26
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB1	1	1.26
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB2	2	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	18	1.26
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	9	1.26
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	16	1.26
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	13	1.26
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	1	1.26
(1,1485)	1:432:A:HIS:HD2	1:433:A:LEU:HD23	17	1.26
(1,1407)	1:456:A:TRP:HB3	1:456:A:TRP:HZ3	12	1.26
(1,1392)	1:386:A:THR:HG22	1:389:A:LYS:HG2	17	1.26
(1,1256)	1:410:A:ARG:HD3	1:412:A:LEU:HB3	3	1.26
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	11	1.26
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	16	1.26
(1,1158)	1:403:A:ILE:HG21	1:364:A:PHE:HE2	18	1.26
(1,734)	1:416:A:MET:HG2	1:403:A:ILE:HA	3	1.26
(1,734)	1:416:A:MET:HG2	1:403:A:ILE:HA	17	1.26
(1,388)	1:375:A:LEU:HD23	1:350:A:TYR:HE2	13	1.26
(1,383)	1:375:A:LEU:HD13	1:353:A:PHE:HE1	9	1.26
(1,266)	1:363:A:ILE:HG23	1:406:A:GLU:HG2	18	1.26
(1,2851)	1:344:A:LEU:HD13	1:372:A:LEU:HB3	16	1.25
(1,2795)	1:433:A:LEU:HD21	1:440:A:GLU:HG2	14	1.25
(1,2687)	1:430:A:LEU:HD21	1:396:A:HIS:H	9	1.25
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	3	1.25
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	12	1.25
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	14	1.25
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	3	1.25
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	4	1.25
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	9	1.25
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	15	1.25
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	6	1.25
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	18	1.25
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG11	8	1.25
(1,1158)	1:403:A:ILE:HG21	1:364:A:PHE:HE2	2	1.25
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	7	1.25
(1,900)	1:438:A:LEU:HD12	1:434:A:GLU:HB2	4	1.25
(1,266)	1:363:A:ILE:HG23	1:406:A:GLU:HG2	11	1.25
(1,172)	1:354:A:ILE:HG23	1:350:A:TYR:HD1	2	1.25
(1,2794)	1:433:A:LEU:HD21	1:429:A:ARG:HD3	11	1.24
(1,2790)	1:438:A:LEU:HD21	1:437:A:VAL:HB	5	1.24
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB1	3	1.24
(1,2687)	1:430:A:LEU:HD21	1:396:A:HIS:H	6	1.24
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	9	1.24
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	13	1.24
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	7	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	15	1.24
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	7	1.24
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	12	1.24
(1,1397)	1:385:A:MET:HB2	1:374:A:ARG:HA	19	1.24
(1,1392)	1:386:A:THR:HG21	1:389:A:LYS:HG2	4	1.24
(1,1183)	1:363:A:ILE:HD12	1:362:A:LYS:HG3	7	1.24
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB1	4	1.24
(1,387)	1:375:A:LEU:HD23	1:353:A:PHE:HE1	6	1.24
(1,172)	1:354:A:ILE:HG21	1:350:A:TYR:HD1	8	1.24
(1,2816)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	8	1.23
(1,2745)	1:360:A:GLU:HA	1:359:A:LYS:HG2	17	1.23
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	4	1.23
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	7	1.23
(1,1525)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	19	1.23
(1,1446)	1:442:A:THR:HG23	1:443:A:TYR:HD2	1	1.23
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	13	1.23
(1,1183)	1:363:A:ILE:HD11	1:362:A:LYS:HG3	11	1.23
(1,1158)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	14	1.23
(1,900)	1:438:A:LEU:HD11	1:434:A:GLU:HB2	15	1.23
(1,266)	1:363:A:ILE:HG21	1:406:A:GLU:HG2	9	1.23
(1,2878)	1:403:A:ILE:HG21	1:414:A:ARG:HB3	7	1.22
(1,2878)	1:403:A:ILE:HG22	1:414:A:ARG:HB3	16	1.22
(1,2851)	1:344:A:LEU:HD11	1:372:A:LEU:HB3	5	1.22
(1,2851)	1:344:A:LEU:HD13	1:372:A:LEU:HB3	6	1.22
(1,2851)	1:344:A:LEU:HD11	1:372:A:LEU:HB3	13	1.22
(1,2816)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	2	1.22
(1,2735)	1:403:A:ILE:HG21	1:364:A:PHE:HE2	18	1.22
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	1	1.22
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	14	1.22
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	8	1.22
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	1	1.22
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	2	1.22
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	5	1.22
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	8	1.22
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	10	1.22
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	14	1.22
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	1	1.22
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	18	1.22
(1,1477)	1:433:A:LEU:HD23	1:436:A:GLN:HB3	4	1.22
(1,1430)	1:447:A:GLU:HB2	1:448:A:PRO:HD3	18	1.22
(1,1407)	1:456:A:TRP:HB3	1:456:A:TRP:HZ3	17	1.22
(1,1397)	1:385:A:MET:HB2	1:374:A:ARG:HA	15	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,900)	1:438:A:LEU:HD11	1:434:A:GLU:HB2	6	1.22
(1,2878)	1:403:A:ILE:HG22	1:414:A:ARG:HB3	3	1.21
(1,2851)	1:344:A:LEU:HD11	1:372:A:LEU:HB3	8	1.21
(1,2851)	1:344:A:LEU:HD12	1:372:A:LEU:HB3	9	1.21
(1,2851)	1:344:A:LEU:HD13	1:372:A:LEU:HB3	11	1.21
(1,2735)	1:403:A:ILE:HG21	1:364:A:PHE:HE2	2	1.21
(1,2553)	1:454:A:VAL:H	1:454:A:VAL:HG21	7	1.21
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	3	1.21
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	7	1.21
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	7	1.21
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	8	1.21
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	13	1.21
(1,1541)	1:445:A:GLU:HA	1:443:A:TYR:HD1	8	1.21
(1,1256)	1:410:A:ARG:HD3	1:412:A:LEU:HB3	10	1.21
(1,1172)	1:363:A:ILE:HG23	1:409:A:GLN:HE22	10	1.21
(1,493)	1:391:A:SER:HB2	1:394:A:LEU:HB2	8	1.21
(1,387)	1:375:A:LEU:HD23	1:353:A:PHE:HE1	12	1.21
(1,383)	1:375:A:LEU:HD13	1:353:A:PHE:HE1	14	1.21
(1,172)	1:354:A:ILE:HG22	1:350:A:TYR:HD1	16	1.21
(1,2873)	1:418:A:THR:HG21	1:417:A:LYS:H	4	1.2
(1,2735)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	14	1.2
(1,2687)	1:430:A:LEU:HD22	1:396:A:HIS:H	2	1.2
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	18	1.2
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	9	1.2
(1,2254)	1:443:A:TYR:H	1:443:A:TYR:HD2	2	1.2
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	10	1.2
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	11	1.2
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	9	1.2
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	14	1.2
(1,1393)	1:386:A:THR:HG22	1:388:A:GLU:HB3	3	1.2
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	12	1.2
(1,1047)	1:350:A:TYR:HD2	1:350:A:TYR:HA	15	1.2
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	19	1.2
(1,900)	1:438:A:LEU:HD11	1:434:A:GLU:HB2	13	1.2
(1,400)	1:377:A:GLY:HA3	1:382:A:ARG:HB3	10	1.2
(1,381)	1:375:A:LEU:HD12	1:350:A:TYR:HE2	13	1.2
(1,266)	1:363:A:ILE:HG23	1:406:A:GLU:HG2	1	1.2
(1,2878)	1:403:A:ILE:HG23	1:414:A:ARG:HB3	6	1.19
(1,2790)	1:438:A:LEU:HD21	1:437:A:VAL:HB	8	1.19
(1,2687)	1:430:A:LEU:HD21	1:396:A:HIS:H	7	1.19
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	4	1.19
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	19	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	15	1.19
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	18	1.19
(1,1445)	1:442:A:THR:HG23	1:443:A:TYR:HE2	2	1.19
(1,1430)	1:447:A:GLU:HB2	1:448:A:PRO:HD3	10	1.19
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	1	1.19
(1,1158)	1:403:A:ILE:HG23	1:364:A:PHE:HE2	7	1.19
(1,900)	1:438:A:LEU:HD12	1:434:A:GLU:HB2	1	1.19
(1,234)	1:356:A:TRP:HE1	1:359:A:LYS:HE2	9	1.19
(1,234)	1:356:A:TRP:HE1	1:359:A:LYS:HE2	15	1.19
(1,2851)	1:344:A:LEU:HD11	1:372:A:LEU:HB3	4	1.18
(1,2851)	1:344:A:LEU:HD11	1:372:A:LEU:HB3	17	1.18
(1,2687)	1:430:A:LEU:HD21	1:396:A:HIS:H	16	1.18
(1,2075)	1:367:A:VAL:H	1:369:A:PRO:HD2	18	1.18
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	6	1.18
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	17	1.18
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	8	1.18
(1,1525)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	14	1.18
(1,1172)	1:363:A:ILE:HG22	1:409:A:GLN:HE22	7	1.18
(1,838)	1:430:A:LEU:HB2	1:430:A:LEU:HD13	18	1.18
(1,550)	1:396:A:HIS:HB2	1:430:A:LEU:HD23	18	1.18
(1,383)	1:375:A:LEU:HD13	1:353:A:PHE:HE1	4	1.18
(1,383)	1:375:A:LEU:HD11	1:353:A:PHE:HE1	11	1.18
(1,234)	1:356:A:TRP:HE1	1:359:A:LYS:HE2	12	1.18
(1,2878)	1:403:A:ILE:HG23	1:414:A:ARG:HB3	11	1.17
(1,2878)	1:403:A:ILE:HG23	1:414:A:ARG:HB3	14	1.17
(1,2873)	1:418:A:THR:HG22	1:417:A:LYS:H	8	1.17
(1,2793)	1:433:A:LEU:HD21	1:393:A:ALA:HA	19	1.17
(1,2787)	1:440:A:GLU:HA	1:433:A:LEU:HD23	17	1.17
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB1	8	1.17
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	2	1.17
(1,1834)	1:361:A:SER:HB2	1:358:A:ASP:HB2	2	1.17
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	2	1.17
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	15	1.17
(1,1430)	1:447:A:GLU:HB2	1:448:A:PRO:HD3	11	1.17
(1,1403)	1:383:A:THR:HG22	1:382:A:ARG:HD2	11	1.17
(1,1304)	1:376:A:TRP:HZ2	1:380:A:LYS:HE3	10	1.17
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	3	1.17
(1,1158)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	12	1.17
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	12	1.17
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	13	1.17
(1,900)	1:438:A:LEU:HD11	1:434:A:GLU:HB2	12	1.17
(1,820)	1:429:A:ARG:HA	1:432:A:HIS:HB2	4	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB3	18	1.17
(1,383)	1:375:A:LEU:HD12	1:353:A:PHE:HE1	16	1.17
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	6	1.17
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	17	1.17
(1,2816)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	1	1.16
(1,2816)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	10	1.16
(1,2795)	1:433:A:LEU:HD23	1:440:A:GLU:HG2	8	1.16
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	8	1.16
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	12	1.16
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	3	1.16
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	11	1.16
(1,1659)	1:404:A:ARG:HB2	1:404:A:ARG:HD3	10	1.16
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	5	1.16
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	19	1.16
(1,1446)	1:442:A:THR:HG22	1:443:A:TYR:HD2	8	1.16
(1,1403)	1:383:A:THR:HG21	1:382:A:ARG:HD2	13	1.16
(1,1392)	1:386:A:THR:HG23	1:389:A:LYS:HG2	18	1.16
(1,1256)	1:410:A:ARG:HD3	1:412:A:LEU:HB3	1	1.16
(1,1183)	1:363:A:ILE:HD13	1:362:A:LYS:HG3	2	1.16
(1,1003)	1:409:A:GLN:HG2	1:406:A:GLU:HB2	12	1.16
(1,884)	1:437:A:VAL:HG21	1:392:A:ARG:HG3	10	1.16
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB1	14	1.16
(1,266)	1:363:A:ILE:HG23	1:406:A:GLU:HG2	7	1.16
(1,2984)	1:410:A:ARG:HE	1:366:A:ILE:HG22	11	1.15
(1,2879)	1:344:A:LEU:HD13	1:350:A:TYR:HE1	16	1.15
(1,2851)	1:344:A:LEU:HD12	1:372:A:LEU:HB3	12	1.15
(1,2831)	1:411:A:LEU:HD13	1:413:A:PHE:HZ	3	1.15
(1,2735)	1:403:A:ILE:HG23	1:364:A:PHE:HE2	7	1.15
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	17	1.15
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	13	1.15
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	6	1.15
(1,1541)	1:445:A:GLU:HA	1:443:A:TYR:HD1	1	1.15
(1,1445)	1:442:A:THR:HG22	1:443:A:TYR:HE2	8	1.15
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	16	1.15
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB2	9	1.15
(1,172)	1:354:A:ILE:HG21	1:350:A:TYR:HD1	4	1.15
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	2	1.15
(1,2878)	1:403:A:ILE:HG21	1:414:A:ARG:HB3	5	1.14
(1,2851)	1:344:A:LEU:HD13	1:372:A:LEU:HB3	7	1.14
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	3	1.14
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	8	1.14
(1,1991)	1:353:A:PHE:H	1:353:A:PHE:HD2	6	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	14	1.14
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	19	1.14
(1,2878)	1:403:A:ILE:HG23	1:414:A:ARG:HB3	1	1.13
(1,2878)	1:403:A:ILE:HG21	1:414:A:ARG:HB3	17	1.13
(1,2851)	1:344:A:LEU:HD13	1:372:A:LEU:HB3	2	1.13
(1,2851)	1:344:A:LEU:HD12	1:372:A:LEU:HB3	18	1.13
(1,2816)	1:422:A:ILE:HG22	1:417:A:LYS:HD3	11	1.13
(1,2813)	1:418:A:THR:HG22	1:362:A:LYS:HD3	2	1.13
(1,2794)	1:433:A:LEU:HD23	1:429:A:ARG:HD2	7	1.13
(1,2735)	1:403:A:ILE:HG22	1:364:A:PHE:HE2	12	1.13
(1,2687)	1:430:A:LEU:HD22	1:396:A:HIS:H	1	1.13
(1,2687)	1:430:A:LEU:HD22	1:396:A:HIS:H	15	1.13
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	5	1.13
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	19	1.13
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	4	1.13
(1,1430)	1:447:A:GLU:HB2	1:448:A:PRO:HD3	16	1.13
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	3	1.13
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	9	1.13
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	10	1.13
(1,900)	1:438:A:LEU:HD12	1:434:A:GLU:HB2	7	1.13
(1,266)	1:363:A:ILE:HG21	1:406:A:GLU:HG2	17	1.13
(1,172)	1:354:A:ILE:HG23	1:350:A:TYR:HD1	7	1.13
(1,172)	1:354:A:ILE:HG23	1:350:A:TYR:HD1	12	1.13
(1,2879)	1:344:A:LEU:HD13	1:350:A:TYR:HE1	10	1.12
(1,2878)	1:403:A:ILE:HG23	1:414:A:ARG:HB3	12	1.12
(1,2878)	1:403:A:ILE:HG22	1:414:A:ARG:HB3	13	1.12
(1,2687)	1:430:A:LEU:HD21	1:396:A:HIS:H	3	1.12
(1,2684)	1:429:A:ARG:HG3	1:430:A:LEU:HD23	4	1.12
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	1	1.12
(1,1874)	1:382:A:ARG:HD3	1:382:A:ARG:HA	10	1.12
(1,2873)	1:418:A:THR:HG22	1:417:A:LYS:H	2	1.11
(1,2873)	1:418:A:THR:HG21	1:417:A:LYS:H	13	1.11
(1,2851)	1:344:A:LEU:HD12	1:372:A:LEU:HB3	14	1.11
(1,2851)	1:344:A:LEU:HD12	1:372:A:LEU:HB3	19	1.11
(1,2816)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	18	1.11
(1,2794)	1:433:A:LEU:HD23	1:429:A:ARG:HD2	13	1.11
(1,2726)	1:367:A:VAL:HG11	1:355:A:ARG:HD3	17	1.11
(1,2687)	1:400:A:LEU:H	1:430:A:LEU:HD21	17	1.11
(1,2447)	1:385:A:MET:H	1:444:A:GLN:HE21	19	1.11
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	11	1.11
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	12	1.11
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	16	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	16	1.11
(1,2254)	1:443:A:TYR:H	1:443:A:TYR:HD2	15	1.11
(1,1659)	1:404:A:ARG:HB2	1:404:A:ARG:HD3	4	1.11
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	6	1.11
(1,1403)	1:383:A:THR:HG22	1:382:A:ARG:HD2	14	1.11
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	14	1.11
(1,715)	1:414:A:ARG:HD2	1:414:A:ARG:HH12	12	1.11
(1,646)	1:405:A:LYS:HG2	1:413:A:PHE:HE2	11	1.11
(1,493)	1:391:A:SER:HB2	1:394:A:LEU:HB2	13	1.11
(1,419)	1:380:A:LYS:HB3	1:377:A:GLY:HA3	9	1.11
(1,230)	1:356:A:TRP:HE1	1:359:A:LYS:HD2	14	1.11
(1,172)	1:354:A:ILE:HG21	1:350:A:TYR:HD1	5	1.11
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	7	1.11
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	14	1.11
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	15	1.11
(1,2879)	1:344:A:LEU:HD11	1:350:A:TYR:HE1	14	1.1
(1,2879)	1:344:A:LEU:HD11	1:350:A:TYR:HE1	18	1.1
(1,2873)	1:418:A:THR:HG23	1:417:A:LYS:H	18	1.1
(1,2851)	1:344:A:LEU:HD11	1:372:A:LEU:HB3	10	1.1
(1,2831)	1:411:A:LEU:HD12	1:413:A:PHE:HZ	10	1.1
(1,2694)	1:438:A:LEU:HD13	1:434:A:GLU:HA	11	1.1
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	6	1.1
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	7	1.1
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	10	1.1
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	16	1.1
(1,1525)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	3	1.1
(1,1442)	1:443:A:TYR:HE2	1:445:A:GLU:HG2	2	1.1
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	5	1.1
(1,1183)	1:363:A:ILE:HD12	1:362:A:LYS:HG3	15	1.1
(1,734)	1:416:A:MET:HG2	1:403:A:ILE:HA	12	1.1
(1,383)	1:375:A:LEU:HD11	1:353:A:PHE:HE1	2	1.1
(1,383)	1:375:A:LEU:HD13	1:353:A:PHE:HE1	10	1.1
(1,354)	1:393:A:ALA:HB1	1:438:A:LEU:HD23	12	1.1
(1,57)	1:343:A:GLN:HG3	1:344:A:LEU:HD21	11	1.1
(1,2984)	1:410:A:ARG:HE	1:366:A:ILE:HG21	8	1.09
(1,2878)	1:403:A:ILE:HG21	1:414:A:ARG:HB3	10	1.09
(1,2873)	1:418:A:THR:HG22	1:417:A:LYS:H	17	1.09
(1,2831)	1:411:A:LEU:HD13	1:413:A:PHE:HZ	1	1.09
(1,2831)	1:411:A:LEU:HD12	1:413:A:PHE:HZ	8	1.09
(1,2831)	1:411:A:LEU:HD13	1:413:A:PHE:HZ	11	1.09
(1,2831)	1:411:A:LEU:HD13	1:368:A:ASP:H	18	1.09
(1,2694)	1:438:A:LEU:HD13	1:434:A:GLU:HA	9	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	11	1.09
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	8	1.09
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	14	1.09
(1,1541)	1:445:A:GLU:HA	1:443:A:TYR:HD1	6	1.09
(1,1525)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	5	1.09
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG11	2	1.09
(1,1430)	1:447:A:GLU:HB2	1:448:A:PRO:HD3	14	1.09
(1,1424)	1:450:A:ILE:HG22	1:452:A:SER:HB2	6	1.09
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	17	1.09
(1,1403)	1:383:A:THR:HG23	1:382:A:ARG:HD2	16	1.09
(1,2879)	1:344:A:LEU:HD13	1:350:A:TYR:HE1	8	1.08
(1,2879)	1:344:A:LEU:HD11	1:350:A:TYR:HE1	9	1.08
(1,2831)	1:411:A:LEU:HD11	1:413:A:PHE:HZ	9	1.08
(1,2831)	1:411:A:LEU:HD13	1:413:A:PHE:HZ	19	1.08
(1,2794)	1:433:A:LEU:HD21	1:429:A:ARG:HD2	10	1.08
(1,2774)	1:443:A:TYR:HD2	1:445:A:GLU:HB2	14	1.08
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	13	1.08
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	14	1.08
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	17	1.08
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	7	1.08
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	6	1.08
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	3	1.08
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	14	1.08
(1,1424)	1:450:A:ILE:HG22	1:452:A:SER:HB2	10	1.08
(1,1424)	1:450:A:ILE:HG21	1:452:A:SER:HB2	12	1.08
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	16	1.08
(1,1349)	1:443:A:TYR:HE1	1:445:A:GLU:HA	10	1.08
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	4	1.08
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	5	1.08
(1,884)	1:437:A:VAL:HG23	1:392:A:ARG:HG3	16	1.08
(1,383)	1:375:A:LEU:HD12	1:353:A:PHE:HE1	7	1.08
(1,383)	1:375:A:LEU:HD13	1:353:A:PHE:HE1	8	1.08
(1,266)	1:363:A:ILE:HG23	1:406:A:GLU:HG2	2	1.08
(1,2878)	1:403:A:ILE:HG23	1:414:A:ARG:HB3	4	1.07
(1,2873)	1:418:A:THR:HG23	1:417:A:LYS:H	15	1.07
(1,2831)	1:411:A:LEU:HD13	1:413:A:PHE:HZ	7	1.07
(1,2760)	1:400:A:LEU:HD23	1:401:A:ASN:H	15	1.07
(1,2694)	1:438:A:LEU:HD12	1:434:A:GLU:HA	3	1.07
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	14	1.07
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	9	1.07
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	11	1.07
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	12	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1834)	1:361:A:SER:HB2	1:358:A:ASP:HB2	4	1.07
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	5	1.07
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	7	1.07
(1,1677)	1:402:A:ILE:HG12	1:400:A:LEU:HA	16	1.07
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	13	1.07
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	14	1.07
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	13	1.07
(1,1478)	1:433:A:LEU:HD22	1:396:A:HIS:HE1	2	1.07
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG13	16	1.07
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	11	1.07
(1,864)	1:433:A:LEU:HA	1:433:A:LEU:HD12	17	1.07
(1,820)	1:429:A:ARG:HA	1:432:A:HIS:HB2	8	1.07
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB3	3	1.07
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB3	8	1.07
(1,440)	1:383:A:THR:HA	1:383:A:THR:HG22	3	1.07
(1,2984)	1:410:A:ARG:HE	1:367:A:VAL:HG22	2	1.06
(1,2831)	1:411:A:LEU:HD11	1:413:A:PHE:HZ	6	1.06
(1,2816)	1:422:A:ILE:HG22	1:417:A:LYS:HD3	7	1.06
(1,2795)	1:433:A:LEU:HD22	1:440:A:GLU:HG2	3	1.06
(1,2793)	1:433:A:LEU:HD23	1:429:A:ARG:HA	12	1.06
(1,2694)	1:438:A:LEU:HD12	1:434:A:GLU:HA	4	1.06
(1,2687)	1:430:A:LEU:HD23	1:396:A:HIS:H	8	1.06
(1,2633)	1:394:A:LEU:HD13	1:366:A:ILE:HD12	13	1.06
(1,2447)	1:385:A:MET:H	1:444:A:GLN:HE21	6	1.06
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	18	1.06
(1,2254)	1:443:A:TYR:H	1:443:A:TYR:HD2	4	1.06
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	1	1.06
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	11	1.06
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	8	1.06
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	10	1.06
(1,1624)	1:407:A:PRO:HD3	1:406:A:GLU:HB2	15	1.06
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG11	14	1.06
(1,1424)	1:450:A:ILE:HG23	1:452:A:SER:HB2	18	1.06
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	8	1.06
(1,865)	1:438:A:LEU:HD11	1:380:A:LYS:HE3	19	1.06
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB1	7	1.06
(1,172)	1:354:A:ILE:HG23	1:350:A:TYR:HD1	9	1.06
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	5	1.06
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	8	1.06
(1,2873)	1:418:A:THR:HG23	1:417:A:LYS:H	3	1.05
(1,2873)	1:430:A:LEU:H	1:427:A:THR:HG23	10	1.05
(1,2831)	1:411:A:LEU:HD12	1:413:A:PHE:HZ	17	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2816)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	12	1.05
(1,2816)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	15	1.05
(1,2799)	1:412:A:LEU:HD21	1:365:A:ARG:HD3	7	1.05
(1,2791)	1:438:A:LEU:HD21	1:385:A:MET:HG2	3	1.05
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	8	1.05
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	16	1.05
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	5	1.05
(1,1665)	1:403:A:ILE:HG12	1:364:A:PHE:HE2	2	1.05
(1,1446)	1:442:A:THR:HG22	1:443:A:TYR:HD2	15	1.05
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	4	1.05
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	6	1.05
(1,383)	1:375:A:LEU:HD11	1:353:A:PHE:HE1	1	1.05
(1,236)	1:361:A:SER:HB3	1:358:A:ASP:HB2	14	1.05
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	1	1.05
(1,2972)	1:435:A:SER:H	1:434:A:GLU:HG2	19	1.04
(1,2879)	1:344:A:LEU:HD12	1:350:A:TYR:HE2	19	1.04
(1,2760)	1:400:A:LEU:HD22	1:401:A:ASN:H	9	1.04
(1,2694)	1:438:A:LEU:HD12	1:434:A:GLU:HA	10	1.04
(1,2684)	1:429:A:ARG:HG2	1:430:A:LEU:HD22	17	1.04
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	10	1.04
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	15	1.04
(1,1495)	1:430:A:LEU:HD21	1:396:A:HIS:HA	17	1.04
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG13	6	1.04
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	3	1.04
(1,926)	1:442:A:THR:H	1:441:A:GLN:HG2	13	1.04
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB1	12	1.04
(1,57)	1:343:A:GLN:HG3	1:344:A:LEU:HD23	4	1.04
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	4	1.04
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	19	1.04
(1,2831)	1:411:A:LEU:HD13	1:413:A:PHE:HZ	2	1.03
(1,2831)	1:411:A:LEU:HD11	1:413:A:PHE:HZ	16	1.03
(1,2760)	1:400:A:LEU:HD22	1:401:A:ASN:H	2	1.03
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	15	1.03
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	15	1.03
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	14	1.03
(1,1479)	1:433:A:LEU:HD11	1:393:A:ALA:HA	17	1.03
(1,1442)	1:443:A:TYR:HE2	1:445:A:GLU:HG2	17	1.03
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	12	1.03
(1,1392)	1:386:A:THR:HG23	1:389:A:LYS:HG2	14	1.03
(1,1164)	1:363:A:ILE:HG13	1:358:A:ASP:HB2	9	1.03
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	3	1.03
(1,2984)	1:410:A:ARG:HE	1:366:A:ILE:HG23	10	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2873)	1:418:A:THR:HG21	1:417:A:LYS:H	9	1.02
(1,2831)	1:411:A:LEU:HD11	1:413:A:PHE:HZ	14	1.02
(1,2816)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	19	1.02
(1,2760)	1:400:A:LEU:HD22	1:401:A:ASN:H	10	1.02
(1,2760)	1:400:A:LEU:HD23	1:401:A:ASN:H	13	1.02
(1,2694)	1:438:A:LEU:HD12	1:434:A:GLU:HA	18	1.02
(1,2687)	1:430:A:LEU:HD22	1:396:A:HIS:H	11	1.02
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	2	1.02
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	10	1.02
(1,1900)	1:430:A:LEU:HD12	1:402:A:ILE:HD12	18	1.02
(1,1899)	1:430:A:LEU:HD12	1:400:A:LEU:HD22	18	1.02
(1,1776)	1:337:A:LEU:HD12	1:390:A:MET:HG2	18	1.02
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	4	1.02
(1,1525)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	4	1.02
(1,1525)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	13	1.02
(1,1424)	1:450:A:ILE:HG22	1:452:A:SER:HB2	14	1.02
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	17	1.02
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	4	1.02
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	11	1.02
(1,354)	1:393:A:ALA:HB1	1:438:A:LEU:HD22	13	1.02
(1,172)	1:354:A:ILE:HG22	1:350:A:TYR:HD1	11	1.02
(1,2879)	1:344:A:LEU:HD12	1:350:A:TYR:HE1	6	1.01
(1,2878)	1:403:A:ILE:HG23	1:414:A:ARG:HB3	9	1.01
(1,2873)	1:418:A:THR:HG21	1:417:A:LYS:H	19	1.01
(1,2840)	1:403:A:ILE:HG23	1:416:A:MET:H	14	1.01
(1,2831)	1:411:A:LEU:HD13	1:413:A:PHE:HZ	4	1.01
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB1	16	1.01
(1,2726)	1:367:A:VAL:HG12	1:365:A:ARG:HD2	5	1.01
(1,2633)	1:394:A:LEU:HD11	1:366:A:ILE:HD12	8	1.01
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	5	1.01
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	8	1.01
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	14	1.01
(1,1834)	1:361:A:SER:HB2	1:358:A:ASP:HB2	14	1.01
(1,1827)	1:430:A:LEU:HB3	1:430:A:LEU:HD21	18	1.01
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	10	1.01
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG13	5	1.01
(1,1442)	1:443:A:TYR:HE2	1:445:A:GLU:HG2	10	1.01
(1,1442)	1:443:A:TYR:HE2	1:445:A:GLU:HG2	11	1.01
(1,1442)	1:443:A:TYR:HE2	1:445:A:GLU:HG2	15	1.01
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	1	1.01
(1,1393)	1:386:A:THR:HG21	1:388:A:GLU:HB3	13	1.01
(1,1256)	1:410:A:ARG:HD3	1:412:A:LEU:HB3	17	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	15	1.01
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	3	1.01
(1,298)	1:366:A:ILE:HG22	1:369:A:PRO:HD2	17	1.01
(1,2879)	1:344:A:LEU:HD12	1:350:A:TYR:HE1	2	1.0
(1,2879)	1:344:A:LEU:HD12	1:350:A:TYR:HE1	7	1.0
(1,2840)	1:403:A:ILE:HG22	1:416:A:MET:H	13	1.0
(1,2831)	1:411:A:LEU:HD13	1:413:A:PHE:HZ	15	1.0
(1,2799)	1:412:A:LEU:HD23	1:365:A:ARG:HD3	6	1.0
(1,2799)	1:412:A:LEU:HD22	1:365:A:ARG:HD3	16	1.0
(1,2794)	1:433:A:LEU:HD22	1:429:A:ARG:HD3	1	1.0
(1,2726)	1:367:A:VAL:HG11	1:355:A:ARG:HD3	16	1.0
(1,2696)	1:438:A:LEU:HD23	1:382:A:ARG:HD2	17	1.0
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	1	1.0
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	5	1.0
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	4	1.0
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	6	1.0
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	9	1.0
(1,1917)	1:394:A:LEU:HD13	1:366:A:ILE:HD12	13	1.0
(1,1525)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	16	1.0
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	18	1.0
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	3	1.0
(1,878)	1:436:A:GLN:H	1:436:A:GLN:HG3	4	1.0
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	16	1.0
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB1	2	1.0
(1,298)	1:366:A:ILE:HG22	1:369:A:PRO:HD2	11	1.0
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	3	1.0
(1,2878)	1:403:A:ILE:HG21	1:414:A:ARG:HB3	15	0.99
(1,2873)	1:418:A:THR:HG21	1:417:A:LYS:H	14	0.99
(1,2693)	1:437:A:VAL:HG21	1:441:A:GLN:HE22	2	0.99
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	6	0.99
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	7	0.99
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	1	0.99
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	16	0.99
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	3	0.99
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	9	0.99
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	19	0.99
(1,1442)	1:443:A:TYR:HE2	1:445:A:GLU:HG2	8	0.99
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	8	0.99
(1,1407)	1:456:A:TRP:HB3	1:456:A:TRP:HZ3	2	0.99
(1,1331)	1:400:A:LEU:HD22	1:397:A:TYR:HA	17	0.99
(1,878)	1:436:A:GLN:H	1:436:A:GLN:HG3	19	0.99
(1,734)	1:416:A:MET:HG2	1:403:A:ILE:HA	5	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB3	1	0.99
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB2	6	0.99
(1,382)	1:375:A:LEU:HD12	1:350:A:TYR:HD2	13	0.99
(1,2831)	1:411:A:LEU:HD11	1:413:A:PHE:HZ	5	0.98
(1,2813)	1:418:A:THR:HG23	1:362:A:LYS:HD3	15	0.98
(1,2760)	1:400:A:LEU:HD21	1:401:A:ASN:H	3	0.98
(1,2760)	1:400:A:LEU:HD21	1:401:A:ASN:H	7	0.98
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	16	0.98
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	3	0.98
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	19	0.98
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	2	0.98
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	13	0.98
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	15	0.98
(1,1496)	1:430:A:LEU:HD21	1:427:A:THR:HA	5	0.98
(1,1491)	1:430:A:LEU:HA	1:430:A:LEU:HD22	18	0.98
(1,1456)	1:436:A:GLN:HB2	1:433:A:LEU:HD11	19	0.98
(1,1445)	1:442:A:THR:HG23	1:443:A:TYR:HE2	12	0.98
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	4	0.98
(1,1349)	1:443:A:TYR:HE1	1:445:A:GLU:HA	3	0.98
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	14	0.98
(1,1256)	1:410:A:ARG:HD2	1:412:A:LEU:HB3	4	0.98
(1,1164)	1:363:A:ILE:HG13	1:358:A:ASP:HB2	1	0.98
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	18	0.98
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	6	0.98
(1,1024)	1:336:A:LEU:HD22	1:338:A:TRP:HZ2	11	0.98
(1,354)	1:393:A:ALA:HB2	1:438:A:LEU:HD23	4	0.98
(1,172)	1:354:A:ILE:HG23	1:350:A:TYR:HD1	1	0.98
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	12	0.98
(1,2873)	1:418:A:THR:HG22	1:417:A:LYS:H	12	0.97
(1,2840)	1:403:A:ILE:HG23	1:416:A:MET:H	8	0.97
(1,2840)	1:403:A:ILE:HG21	1:416:A:MET:H	15	0.97
(1,2696)	1:438:A:LEU:HD22	1:382:A:ARG:HD2	8	0.97
(1,2696)	1:438:A:LEU:HD23	1:382:A:ARG:HD2	10	0.97
(1,2167)	1:392:A:ARG:H	1:392:A:ARG:HG2	18	0.97
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	7	0.97
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	17	0.97
(1,1834)	1:361:A:SER:HB2	1:358:A:ASP:HB2	15	0.97
(1,1776)	1:337:A:LEU:HD11	1:390:A:MET:HG2	12	0.97
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG13	12	0.97
(1,1442)	1:443:A:TYR:HE2	1:445:A:GLU:HG2	3	0.97
(1,1430)	1:447:A:GLU:HB2	1:448:A:PRO:HD3	12	0.97
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	13	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1403)	1:383:A:THR:HG21	1:382:A:ARG:HD2	12	0.97
(1,1392)	1:386:A:THR:HG22	1:389:A:LYS:HG2	10	0.97
(1,1256)	1:410:A:ARG:HD3	1:412:A:LEU:HB3	2	0.97
(1,1231)	1:356:A:TRP:HZ2	1:342:A:TYR:HD2	10	0.97
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	5	0.97
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	4	0.97
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	8	0.97
(1,1024)	1:336:A:LEU:HD23	1:338:A:TRP:HZ2	19	0.97
(1,455)	1:386:A:THR:HG22	1:389:A:LYS:HE2	13	0.97
(1,384)	1:344:A:LEU:HD13	1:375:A:LEU:HD23	10	0.97
(1,298)	1:366:A:ILE:HG22	1:369:A:PRO:HD2	9	0.97
(1,298)	1:366:A:ILE:HG21	1:369:A:PRO:HD2	19	0.97
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	9	0.97
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	11	0.97
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	17	0.96
(1,2879)	1:344:A:LEU:HD11	1:350:A:TYR:HE1	5	0.96
(1,2878)	1:403:A:ILE:HG23	1:414:A:ARG:HB3	8	0.96
(1,2862)	1:379:A:HIS:HB3	1:340:A:TYR:HE1	10	0.96
(1,2831)	1:411:A:LEU:HD11	1:413:A:PHE:HZ	13	0.96
(1,2816)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	14	0.96
(1,2795)	1:433:A:LEU:HD23	1:440:A:GLU:HG2	5	0.96
(1,2795)	1:433:A:LEU:HD22	1:440:A:GLU:HG2	10	0.96
(1,2774)	1:443:A:TYR:HD1	1:445:A:GLU:HB2	19	0.96
(1,2760)	1:400:A:LEU:HD23	1:401:A:ASN:H	1	0.96
(1,2760)	1:400:A:LEU:HD22	1:401:A:ASN:H	5	0.96
(1,2760)	1:400:A:LEU:HD21	1:401:A:ASN:H	6	0.96
(1,2760)	1:400:A:LEU:HD22	1:401:A:ASN:H	8	0.96
(1,2447)	1:385:A:MET:H	1:444:A:GLN:HE21	5	0.96
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	11	0.96
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	18	0.96
(1,1609)	1:411:A:LEU:HD23	1:387:A:TYR:HB2	19	0.96
(1,1583)	1:413:A:PHE:HE2	1:411:A:LEU:HA	8	0.96
(1,1446)	1:442:A:THR:HG23	1:443:A:TYR:HD2	2	0.96
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	12	0.96
(1,1403)	1:383:A:THR:HG21	1:382:A:ARG:HD2	6	0.96
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	15	0.96
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	15	0.96
(1,927)	1:441:A:GLN:H	1:441:A:GLN:HG2	2	0.96
(1,687)	1:411:A:LEU:HD23	1:369:A:PRO:HD2	9	0.96
(1,687)	1:411:A:LEU:HD22	1:369:A:PRO:HD2	16	0.96
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB3	16	0.96
(1,478)	1:389:A:LYS:HG3	1:389:A:LYS:HE2	11	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,465)	1:387:A:TYR:HE1	1:390:A:MET:HG2	12	0.96
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	18	0.96
(1,2879)	1:344:A:LEU:HD11	1:350:A:TYR:HE1	12	0.95
(1,2879)	1:344:A:LEU:HD11	1:350:A:TYR:HE2	13	0.95
(1,2873)	1:418:A:THR:HG22	1:417:A:LYS:H	6	0.95
(1,2795)	1:433:A:LEU:HD23	1:440:A:GLU:HG2	6	0.95
(1,2760)	1:400:A:LEU:HD22	1:401:A:ASN:H	4	0.95
(1,2760)	1:400:A:LEU:HD22	1:401:A:ASN:H	11	0.95
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	16	0.95
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	19	0.95
(1,1917)	1:394:A:LEU:HD11	1:366:A:ILE:HD12	8	0.95
(1,1804)	1:422:A:ILE:HD13	1:336:A:LEU:HD11	14	0.95
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	12	0.95
(1,1525)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	9	0.95
(1,1495)	1:430:A:LEU:HD23	1:396:A:HIS:HA	2	0.95
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG13	7	0.95
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG12	15	0.95
(1,1446)	1:442:A:THR:HG23	1:443:A:TYR:HD2	12	0.95
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	1	0.95
(1,1331)	1:400:A:LEU:HD23	1:397:A:TYR:HA	10	0.95
(1,820)	1:429:A:ARG:HA	1:432:A:HIS:HB2	18	0.95
(1,687)	1:411:A:LEU:HD22	1:369:A:PRO:HD2	18	0.95
(1,624)	1:403:A:ILE:HG22	1:397:A:TYR:HB3	6	0.95
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB3	17	0.95
(1,478)	1:389:A:LYS:HG3	1:389:A:LYS:HE2	13	0.95
(1,384)	1:344:A:LEU:HD11	1:375:A:LEU:HD23	1	0.95
(1,298)	1:366:A:ILE:HG23	1:369:A:PRO:HD2	2	0.95
(1,298)	1:366:A:ILE:HG22	1:369:A:PRO:HD2	3	0.95
(1,298)	1:366:A:ILE:HG23	1:369:A:PRO:HD2	5	0.95
(1,298)	1:366:A:ILE:HG21	1:369:A:PRO:HD2	6	0.95
(1,298)	1:366:A:ILE:HG22	1:369:A:PRO:HD2	15	0.95
(1,298)	1:366:A:ILE:HG23	1:369:A:PRO:HD2	16	0.95
(1,298)	1:366:A:ILE:HG23	1:369:A:PRO:HD2	18	0.95
(1,2984)	1:410:A:ARG:HE	1:367:A:VAL:HG22	15	0.94
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD22	8	0.94
(1,2932)	1:420:A:ASP:H	1:418:A:THR:HG23	19	0.94
(1,2840)	1:403:A:ILE:HG22	1:416:A:MET:H	2	0.94
(1,2840)	1:403:A:ILE:HG21	1:416:A:MET:H	10	0.94
(1,2793)	1:433:A:LEU:HD23	1:429:A:ARG:HA	13	0.94
(1,2762)	1:394:A:LEU:HD21	1:398:A:TYR:HE1	8	0.94
(1,2762)	1:394:A:LEU:HD23	1:398:A:TYR:HE1	9	0.94
(1,2760)	1:400:A:LEU:HD22	1:401:A:ASN:H	14	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2760)	1:400:A:LEU:HD21	1:401:A:ASN:H	16	0.94
(1,2760)	1:400:A:LEU:HD23	1:401:A:ASN:H	18	0.94
(1,2555)	1:340:A:TYR:HA	1:339:A:ASP:HB2	18	0.94
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	3	0.94
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	6	0.94
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	3	0.94
(1,2063)	1:365:A:ARG:H	1:364:A:PHE:HD1	12	0.94
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG12	1	0.94
(1,1424)	1:450:A:ILE:HG21	1:452:A:SER:HB2	16	0.94
(1,1331)	1:400:A:LEU:HD22	1:397:A:TYR:HA	7	0.94
(1,1164)	1:363:A:ILE:HG13	1:358:A:ASP:HB2	7	0.94
(1,958)	1:449:A:THR:H	1:449:A:THR:HG23	2	0.94
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	13	0.94
(1,687)	1:411:A:LEU:HD21	1:369:A:PRO:HD2	11	0.94
(1,624)	1:403:A:ILE:HG22	1:397:A:TYR:HB3	8	0.94
(1,384)	1:344:A:LEU:HD12	1:375:A:LEU:HD22	6	0.94
(1,298)	1:366:A:ILE:HG23	1:369:A:PRO:HD2	10	0.94
(1,298)	1:366:A:ILE:HG22	1:369:A:PRO:HD2	12	0.94
(1,2972)	1:435:A:SER:H	1:434:A:GLU:HG2	4	0.93
(1,2862)	1:379:A:HIS:HB3	1:340:A:TYR:HE1	7	0.93
(1,2760)	1:400:A:LEU:HD23	1:401:A:ASN:H	17	0.93
(1,2681)	1:418:A:THR:HG21	1:342:A:TYR:HD1	16	0.93
(1,2644)	1:402:A:ILE:HD12	1:397:A:TYR:HE1	2	0.93
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	12	0.93
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	13	0.93
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	15	0.93
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	18	0.93
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	19	0.93
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	19	0.93
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	11	0.93
(1,1804)	1:422:A:ILE:HD12	1:336:A:LEU:HD11	12	0.93
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	4	0.93
(1,1609)	1:411:A:LEU:HD22	1:387:A:TYR:HB2	13	0.93
(1,1522)	1:422:A:ILE:HG22	1:430:A:LEU:HG	1	0.93
(1,1496)	1:430:A:LEU:HD21	1:427:A:THR:HA	3	0.93
(1,1437)	1:444:A:GLN:HG2	1:444:A:GLN:HA	17	0.93
(1,1331)	1:400:A:LEU:HD23	1:397:A:TYR:HA	4	0.93
(1,1331)	1:400:A:LEU:HD22	1:397:A:TYR:HA	15	0.93
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	5	0.93
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	17	0.93
(1,1024)	1:336:A:LEU:HD22	1:338:A:TRP:HZ2	9	0.93
(1,687)	1:411:A:LEU:HD23	1:369:A:PRO:HD2	2	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,687)	1:411:A:LEU:HD23	1:369:A:PRO:HD2	3	0.93
(1,687)	1:411:A:LEU:HD23	1:369:A:PRO:HD2	10	0.93
(1,687)	1:411:A:LEU:HD23	1:369:A:PRO:HD2	14	0.93
(1,354)	1:393:A:ALA:HB1	1:438:A:LEU:HD23	1	0.93
(1,298)	1:366:A:ILE:HG21	1:369:A:PRO:HD2	8	0.93
(1,2879)	1:344:A:LEU:HD11	1:350:A:TYR:HE2	17	0.92
(1,2873)	1:418:A:THR:HG21	1:417:A:LYS:H	1	0.92
(1,2873)	1:418:A:THR:HG23	1:417:A:LYS:H	16	0.92
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG21	8	0.92
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	2	0.92
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	7	0.92
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	5	0.92
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	6	0.92
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	11	0.92
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD23	17	0.92
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	18	0.92
(1,1541)	1:445:A:GLU:HA	1:443:A:TYR:HD1	11	0.92
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG12	13	0.92
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG13	17	0.92
(1,1331)	1:400:A:LEU:HD23	1:397:A:TYR:HA	5	0.92
(1,1331)	1:400:A:LEU:HD21	1:397:A:TYR:HA	8	0.92
(1,1331)	1:400:A:LEU:HD23	1:397:A:TYR:HA	11	0.92
(1,1164)	1:363:A:ILE:HG13	1:358:A:ASP:HB2	3	0.92
(1,1164)	1:363:A:ILE:HG13	1:358:A:ASP:HB2	15	0.92
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	8	0.92
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	4	0.92
(1,1024)	1:336:A:LEU:HD22	1:338:A:TRP:HZ2	12	0.92
(1,687)	1:411:A:LEU:HD21	1:369:A:PRO:HD2	4	0.92
(1,687)	1:411:A:LEU:HD21	1:369:A:PRO:HD2	6	0.92
(1,687)	1:411:A:LEU:HD23	1:369:A:PRO:HD2	15	0.92
(1,624)	1:403:A:ILE:HG21	1:397:A:TYR:HB3	2	0.92
(1,384)	1:344:A:LEU:HD13	1:375:A:LEU:HD22	16	0.92
(1,354)	1:393:A:ALA:HB2	1:438:A:LEU:HD22	11	0.92
(1,298)	1:366:A:ILE:HG21	1:369:A:PRO:HD2	14	0.92
(1,2984)	1:410:A:ARG:HE	1:366:A:ILE:HG22	13	0.91
(1,2840)	1:403:A:ILE:HG22	1:416:A:MET:H	18	0.91
(1,2831)	1:411:A:LEU:HD11	1:413:A:PHE:HZ	12	0.91
(1,2799)	1:412:A:LEU:HD22	1:365:A:ARG:HD3	12	0.91
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG22	3	0.91
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	4	0.91
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	11	0.91
(1,2254)	1:443:A:TYR:H	1:443:A:TYR:HD2	18	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	14	0.91
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	4	0.91
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	11	0.91
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	14	0.91
(1,1804)	1:422:A:ILE:HD12	1:336:A:LEU:HD13	11	0.91
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	10	0.91
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	11	0.91
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG13	10	0.91
(1,1424)	1:450:A:ILE:HG22	1:452:A:SER:HB2	5	0.91
(1,1357)	1:394:A:LEU:HD22	1:390:A:MET:HG3	18	0.91
(1,1331)	1:400:A:LEU:HD23	1:397:A:TYR:HA	9	0.91
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	1	0.91
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	16	0.91
(1,1256)	1:410:A:ARG:HD3	1:412:A:LEU:HB3	11	0.91
(1,1176)	1:363:A:ILE:HD11	1:414:A:ARG:HH11	12	0.91
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	9	0.91
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	18	0.91
(1,1024)	1:336:A:LEU:HD22	1:338:A:TRP:HZ2	6	0.91
(1,1024)	1:336:A:LEU:HD21	1:338:A:TRP:HZ2	14	0.91
(1,888)	1:437:A:VAL:HG21	1:441:A:GLN:HE22	2	0.91
(1,687)	1:411:A:LEU:HD23	1:369:A:PRO:HD2	1	0.91
(1,687)	1:411:A:LEU:HD22	1:369:A:PRO:HD2	12	0.91
(1,687)	1:411:A:LEU:HD21	1:369:A:PRO:HD2	13	0.91
(1,687)	1:411:A:LEU:HD23	1:369:A:PRO:HD2	17	0.91
(1,687)	1:411:A:LEU:HD22	1:369:A:PRO:HD2	19	0.91
(1,624)	1:403:A:ILE:HG21	1:397:A:TYR:HB3	13	0.91
(1,384)	1:344:A:LEU:HD11	1:375:A:LEU:HD22	14	0.91
(1,354)	1:393:A:ALA:HB2	1:438:A:LEU:HD21	7	0.91
(1,298)	1:366:A:ILE:HG21	1:369:A:PRO:HD2	1	0.91
(1,298)	1:366:A:ILE:HG22	1:369:A:PRO:HD2	13	0.91
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HG23	5	0.9
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	15	0.9
(1,2760)	1:400:A:LEU:HD22	1:401:A:ASN:H	12	0.9
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG21	5	0.9
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	2	0.9
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	6	0.9
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	17	0.9
(1,2694)	1:438:A:LEU:HD12	1:434:A:GLU:HA	2	0.9
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	12	0.9
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	4	0.9
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	16	0.9
(1,1715)	1:342:A:TYR:HA	1:342:A:TYR:HE2	13	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	2	0.9
(1,1653)	1:404:A:ARG:HG2	1:414:A:ARG:HD3	10	0.9
(1,1496)	1:430:A:LEU:HD22	1:427:A:THR:HA	11	0.9
(1,1446)	1:442:A:THR:HG21	1:443:A:TYR:HD2	17	0.9
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	15	0.9
(1,1331)	1:400:A:LEU:HD21	1:397:A:TYR:HA	1	0.9
(1,1331)	1:400:A:LEU:HD22	1:397:A:TYR:HA	3	0.9
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	11	0.9
(1,1182)	1:363:A:ILE:HD11	1:406:A:GLU:HG2	11	0.9
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	2	0.9
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	10	0.9
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	17	0.9
(1,298)	1:366:A:ILE:HG22	1:369:A:PRO:HD2	4	0.9
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	10	0.9
(1,2932)	1:420:A:ASP:H	1:422:A:ILE:HB	12	0.89
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HG23	18	0.89
(1,2862)	1:379:A:HIS:HB3	1:340:A:TYR:HE1	8	0.89
(1,2840)	1:403:A:ILE:HG21	1:416:A:MET:H	17	0.89
(1,2840)	1:403:A:ILE:HG23	1:416:A:MET:H	19	0.89
(1,2794)	1:375:A:LEU:HD21	1:353:A:PHE:HB2	17	0.89
(1,2762)	1:394:A:LEU:HD21	1:398:A:TYR:HE1	16	0.89
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG22	1	0.89
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG22	13	0.89
(1,2472)	1:409:A:GLN:HE22	1:412:A:LEU:HD11	15	0.89
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	13	0.89
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	10	0.89
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	14	0.89
(1,1871)	1:426:A:ARG:HD2	1:426:A:ARG:HB3	3	0.89
(1,1609)	1:411:A:LEU:HD21	1:387:A:TYR:HB2	17	0.89
(1,1496)	1:430:A:LEU:HD22	1:427:A:THR:HA	1	0.89
(1,1496)	1:430:A:LEU:HD21	1:427:A:THR:HA	6	0.89
(1,1456)	1:436:A:GLN:HB2	1:433:A:LEU:HD12	4	0.89
(1,1445)	1:442:A:THR:HG21	1:443:A:TYR:HE2	10	0.89
(1,1430)	1:447:A:GLU:HB2	1:448:A:PRO:HD3	15	0.89
(1,1402)	1:383:A:THR:HG23	1:384:A:ASN:HD21	4	0.89
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	10	0.89
(1,1357)	1:394:A:LEU:HD21	1:390:A:MET:HG3	12	0.89
(1,1331)	1:400:A:LEU:HD21	1:397:A:TYR:HA	12	0.89
(1,1256)	1:410:A:ARG:HD3	1:412:A:LEU:HB3	7	0.89
(1,1182)	1:363:A:ILE:HD12	1:406:A:GLU:HG2	7	0.89
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	2	0.89
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	10	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	12	0.89
(1,1003)	1:409:A:GLN:HG2	1:406:A:GLU:HB2	2	0.89
(1,964)	1:451:A:ALA:H	1:450:A:ILE:HA	15	0.89
(1,687)	1:411:A:LEU:HD21	1:369:A:PRO:HD2	7	0.89
(1,687)	1:411:A:LEU:HD21	1:369:A:PRO:HD2	8	0.89
(1,387)	1:375:A:LEU:HD22	1:353:A:PHE:HE1	5	0.89
(1,354)	1:393:A:ALA:HB2	1:438:A:LEU:HD22	14	0.89
(1,298)	1:366:A:ILE:HG23	1:369:A:PRO:HD2	7	0.89
(1,2932)	1:420:A:ASP:H	1:418:A:THR:HG23	4	0.88
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	8	0.88
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	13	0.88
(1,2878)	1:403:A:ILE:HG23	1:414:A:ARG:HB3	19	0.88
(1,2876)	1:372:A:LEU:HD11	1:374:A:ARG:H	16	0.88
(1,2862)	1:379:A:HIS:HB3	1:340:A:TYR:HE1	5	0.88
(1,2862)	1:376:A:TRP:HB3	1:340:A:TYR:HE2	19	0.88
(1,2816)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	3	0.88
(1,2791)	1:438:A:LEU:HD21	1:385:A:MET:HG2	2	0.88
(1,2472)	1:409:A:GLN:HE22	1:412:A:LEU:HD12	8	0.88
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	1	0.88
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	8	0.88
(1,2254)	1:443:A:TYR:H	1:443:A:TYR:HD2	12	0.88
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	10	0.88
(1,1804)	1:422:A:ILE:HD11	1:336:A:LEU:HD12	19	0.88
(1,1723)	1:341:A:VAL:HG12	1:338:A:TRP:HE3	16	0.88
(1,1522)	1:422:A:ILE:HG21	1:430:A:LEU:HG	8	0.88
(1,1495)	1:430:A:LEU:HD21	1:396:A:HIS:HA	9	0.88
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG13	3	0.88
(1,1331)	1:400:A:LEU:HD22	1:397:A:TYR:HA	13	0.88
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	6	0.88
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	6	0.88
(1,1024)	1:336:A:LEU:HD21	1:338:A:TRP:HZ2	5	0.88
(1,1024)	1:336:A:LEU:HD21	1:338:A:TRP:HZ2	17	0.88
(1,964)	1:451:A:ALA:H	1:450:A:ILE:HA	7	0.88
(1,964)	1:451:A:ALA:H	1:450:A:ILE:HA	11	0.88
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	2	0.88
(1,383)	1:375:A:LEU:HD12	1:353:A:PHE:HE1	6	0.88
(1,354)	1:393:A:ALA:HB2	1:438:A:LEU:HD21	6	0.88
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD13	18	0.88
(1,45)	1:342:A:TYR:HA	1:342:A:TYR:HD2	13	0.88
(1,2862)	1:379:A:HIS:HB3	1:340:A:TYR:HE1	11	0.87
(1,2862)	1:379:A:HIS:HB3	1:340:A:TYR:HE1	12	0.87
(1,2840)	1:403:A:ILE:HG23	1:416:A:MET:H	9	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2816)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	5	0.87
(1,2760)	1:400:A:LEU:HD22	1:401:A:ASN:H	19	0.87
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG22	7	0.87
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG23	9	0.87
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG23	19	0.87
(1,2681)	1:418:A:THR:HG22	1:342:A:TYR:HD1	19	0.87
(1,2633)	1:394:A:LEU:HD13	1:366:A:ILE:HD12	12	0.87
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	9	0.87
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	12	0.87
(1,1871)	1:426:A:ARG:HD2	1:426:A:ARG:HB3	5	0.87
(1,1609)	1:411:A:LEU:HD21	1:387:A:TYR:HB2	15	0.87
(1,1496)	1:430:A:LEU:HD22	1:427:A:THR:HA	16	0.87
(1,1446)	1:442:A:THR:HG21	1:443:A:TYR:HD2	16	0.87
(1,1430)	1:447:A:GLU:HB2	1:448:A:PRO:HD3	8	0.87
(1,1393)	1:386:A:THR:HG22	1:388:A:GLU:HB3	2	0.87
(1,1331)	1:400:A:LEU:HD23	1:397:A:TYR:HA	14	0.87
(1,1331)	1:400:A:LEU:HD22	1:397:A:TYR:HA	16	0.87
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	1	0.87
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	14	0.87
(1,1024)	1:336:A:LEU:HD22	1:338:A:TRP:HZ2	7	0.87
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	1	0.87
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	16	0.87
(1,687)	1:411:A:LEU:HD21	1:369:A:PRO:HD2	5	0.87
(1,624)	1:403:A:ILE:HG22	1:397:A:TYR:HB3	14	0.87
(1,624)	1:403:A:ILE:HG23	1:397:A:TYR:HB3	15	0.87
(1,384)	1:344:A:LEU:HD11	1:375:A:LEU:HD21	5	0.87
(1,384)	1:344:A:LEU:HD12	1:375:A:LEU:HD22	8	0.87
(1,384)	1:344:A:LEU:HD11	1:375:A:LEU:HD23	9	0.87
(1,384)	1:344:A:LEU:HD11	1:375:A:LEU:HD23	17	0.87
(1,384)	1:344:A:LEU:HD11	1:375:A:LEU:HD21	18	0.87
(1,354)	1:393:A:ALA:HB2	1:438:A:LEU:HD21	17	0.87
(1,354)	1:393:A:ALA:HB3	1:438:A:LEU:HD21	18	0.87
(1,234)	1:356:A:TRP:HE1	1:359:A:LYS:HE2	5	0.87
(1,2932)	1:420:A:ASP:H	1:418:A:THR:HG23	14	0.86
(1,2841)	1:403:A:ILE:HD13	1:397:A:TYR:HA	11	0.86
(1,2841)	1:403:A:ILE:HD12	1:397:A:TYR:HA	18	0.86
(1,2841)	1:403:A:ILE:HD11	1:397:A:TYR:HA	19	0.86
(1,2826)	1:413:A:PHE:H	1:412:A:LEU:HD23	4	0.86
(1,2826)	1:366:A:ILE:H	1:412:A:LEU:HD21	8	0.86
(1,2797)	1:433:A:LEU:HD12	1:434:A:GLU:HA	8	0.86
(1,2793)	1:433:A:LEU:HD23	1:429:A:ARG:HA	14	0.86
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG23	10	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2696)	1:438:A:LEU:HD22	1:382:A:ARG:HD2	4	0.86
(1,2681)	1:418:A:THR:HG23	1:342:A:TYR:HD1	11	0.86
(1,2633)	1:394:A:LEU:HD13	1:366:A:ILE:HD11	18	0.86
(1,2472)	1:409:A:GLN:HE22	1:412:A:LEU:HD11	13	0.86
(1,2472)	1:409:A:GLN:HE22	1:412:A:LEU:HD13	17	0.86
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	6	0.86
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	17	0.86
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	18	0.86
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	19	0.86
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	4	0.86
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	7	0.86
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	18	0.86
(1,1782)	1:337:A:LEU:HD13	1:397:A:TYR:HE2	1	0.86
(1,1723)	1:341:A:VAL:HG13	1:338:A:TRP:HE3	3	0.86
(1,1430)	1:447:A:GLU:HB2	1:448:A:PRO:HD3	19	0.86
(1,1331)	1:400:A:LEU:HD22	1:397:A:TYR:HA	6	0.86
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	12	0.86
(1,1212)	1:359:A:LYS:HG3	1:356:A:TRP:HZ2	17	0.86
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	13	0.86
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	19	0.86
(1,1024)	1:336:A:LEU:HD22	1:338:A:TRP:HZ2	1	0.86
(1,964)	1:451:A:ALA:H	1:450:A:ILE:HA	9	0.86
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	5	0.86
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	6	0.86
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	8	0.86
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	11	0.86
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	12	0.86
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	18	0.86
(1,624)	1:403:A:ILE:HG22	1:397:A:TYR:HB3	1	0.86
(1,384)	1:344:A:LEU:HD11	1:375:A:LEU:HD22	12	0.86
(1,354)	1:393:A:ALA:HB3	1:438:A:LEU:HD22	2	0.86
(1,2984)	1:410:A:ARG:HE	1:366:A:ILE:HG22	12	0.85
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HG21	1	0.85
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HG22	9	0.85
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HG22	12	0.85
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	1	0.85
(1,2879)	1:344:A:LEU:HD12	1:350:A:TYR:HE1	1	0.85
(1,2862)	1:376:A:TRP:HB3	1:340:A:TYR:HE2	3	0.85
(1,2862)	1:376:A:TRP:HB3	1:340:A:TYR:HE2	17	0.85
(1,2841)	1:403:A:ILE:HD13	1:397:A:TYR:HA	9	0.85
(1,2826)	1:413:A:PHE:H	1:412:A:LEU:HD23	14	0.85
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	7	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	12	0.85
(1,2694)	1:438:A:LEU:HD12	1:434:A:GLU:HA	19	0.85
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	2	0.85
(1,2472)	1:409:A:GLN:HE22	1:412:A:LEU:HD13	7	0.85
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	10	0.85
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	15	0.85
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	16	0.85
(1,2106)	1:374:A:ARG:H	1:374:A:ARG:HG3	3	0.85
(1,1782)	1:337:A:LEU:HD13	1:397:A:TYR:HE2	6	0.85
(1,1782)	1:337:A:LEU:HD11	1:397:A:TYR:HE2	16	0.85
(1,1723)	1:341:A:VAL:HG11	1:338:A:TRP:HE3	9	0.85
(1,1723)	1:341:A:VAL:HG11	1:338:A:TRP:HE3	19	0.85
(1,1522)	1:422:A:ILE:HG21	1:430:A:LEU:HG	11	0.85
(1,1442)	1:443:A:TYR:HE2	1:445:A:GLU:HG2	5	0.85
(1,1331)	1:400:A:LEU:HD21	1:397:A:TYR:HA	2	0.85
(1,1256)	1:410:A:ARG:HD3	1:412:A:LEU:HB3	8	0.85
(1,964)	1:451:A:ALA:H	1:450:A:ILE:HA	16	0.85
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	3	0.85
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	4	0.85
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	10	0.85
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	13	0.85
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB2	19	0.85
(1,384)	1:344:A:LEU:HD12	1:375:A:LEU:HD23	2	0.85
(1,383)	1:375:A:LEU:HD13	1:353:A:PHE:HE1	5	0.85
(1,354)	1:393:A:ALA:HB1	1:438:A:LEU:HD21	16	0.85
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD23	12	0.84
(1,2932)	1:420:A:ASP:H	1:418:A:THR:HG21	5	0.84
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HG22	4	0.84
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HG23	7	0.84
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	5	0.84
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	6	0.84
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	7	0.84
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	12	0.84
(1,2862)	1:376:A:TRP:HB3	1:340:A:TYR:HE2	1	0.84
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	10	0.84
(1,2826)	1:413:A:PHE:H	1:412:A:LEU:HD22	3	0.84
(1,2826)	1:413:A:PHE:H	1:412:A:LEU:HD23	5	0.84
(1,2794)	1:433:A:LEU:HD22	1:429:A:ARG:HD2	9	0.84
(1,2793)	1:433:A:LEU:HD22	1:429:A:ARG:HA	15	0.84
(1,2791)	1:380:A:LYS:HE3	1:438:A:LEU:HD22	14	0.84
(1,2762)	1:394:A:LEU:HD21	1:398:A:TYR:HE1	17	0.84
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG22	16	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2254)	1:443:A:TYR:H	1:443:A:TYR:HD2	7	0.84
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	1	0.84
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	9	0.84
(1,1782)	1:337:A:LEU:HD12	1:397:A:TYR:HE2	9	0.84
(1,1723)	1:341:A:VAL:HG11	1:338:A:TRP:HE3	17	0.84
(1,1723)	1:341:A:VAL:HG12	1:338:A:TRP:HE3	18	0.84
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	12	0.84
(1,1609)	1:411:A:LEU:HD21	1:387:A:TYR:HB2	2	0.84
(1,1609)	1:411:A:LEU:HD21	1:387:A:TYR:HB2	9	0.84
(1,1599)	1:412:A:LEU:HD22	1:364:A:PHE:H	15	0.84
(1,1541)	1:445:A:GLU:HA	1:443:A:TYR:HD1	7	0.84
(1,1522)	1:422:A:ILE:HG21	1:430:A:LEU:HG	4	0.84
(1,1496)	1:430:A:LEU:HD21	1:427:A:THR:HA	14	0.84
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG11	19	0.84
(1,1450)	1:442:A:THR:HG21	1:445:A:GLU:HB3	17	0.84
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	13	0.84
(1,1331)	1:400:A:LEU:HD21	1:397:A:TYR:HA	18	0.84
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	5	0.84
(1,1024)	1:336:A:LEU:HD21	1:338:A:TRP:HZ2	15	0.84
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	9	0.84
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	14	0.84
(1,715)	1:414:A:ARG:HD2	1:414:A:ARG:HH12	14	0.84
(1,624)	1:403:A:ILE:HG23	1:397:A:TYR:HB3	10	0.84
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB1	13	0.84
(1,504)	1:387:A:TYR:HB3	1:373:A:ALA:HB3	15	0.84
(1,384)	1:344:A:LEU:HD12	1:375:A:LEU:HD21	7	0.84
(1,384)	1:344:A:LEU:HD13	1:375:A:LEU:HD23	15	0.84
(1,2984)	1:410:A:ARG:HE	1:367:A:VAL:HG22	3	0.83
(1,2932)	1:420:A:ASP:H	1:418:A:THR:HG23	13	0.83
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HD13	6	0.83
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HD11	10	0.83
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HG22	13	0.83
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HG21	14	0.83
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HD12	16	0.83
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	9	0.83
(1,2876)	1:372:A:LEU:HD11	1:374:A:ARG:H	8	0.83
(1,2873)	1:418:A:THR:HG22	1:417:A:LYS:H	5	0.83
(1,2840)	1:403:A:ILE:HG23	1:416:A:MET:H	11	0.83
(1,2840)	1:403:A:ILE:HG23	1:416:A:MET:H	12	0.83
(1,2826)	1:413:A:PHE:H	1:412:A:LEU:HD23	1	0.83
(1,2826)	1:413:A:PHE:H	1:412:A:LEU:HD21	7	0.83
(1,2826)	1:413:A:PHE:H	1:412:A:LEU:HD22	15	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2826)	1:366:A:ILE:H	1:412:A:LEU:HD21	17	0.83
(1,2789)	1:438:A:LEU:HD13	1:381:A:ASN:HD22	1	0.83
(1,2762)	1:394:A:LEU:HD21	1:398:A:TYR:HE1	3	0.83
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	9	0.83
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	14	0.83
(1,2640)	1:400:A:LEU:HD22	1:402:A:ILE:HD12	16	0.83
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	11	0.83
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	18	0.83
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	8	0.83
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	8	0.83
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB3	7	0.83
(1,1804)	1:422:A:ILE:HD12	1:336:A:LEU:HD11	7	0.83
(1,1782)	1:337:A:LEU:HD12	1:397:A:TYR:HE2	7	0.83
(1,1782)	1:337:A:LEU:HD13	1:397:A:TYR:HE2	11	0.83
(1,1782)	1:337:A:LEU:HD11	1:397:A:TYR:HE2	19	0.83
(1,1723)	1:341:A:VAL:HG11	1:338:A:TRP:HE3	2	0.83
(1,1723)	1:341:A:VAL:HG11	1:338:A:TRP:HE3	7	0.83
(1,1723)	1:341:A:VAL:HG13	1:338:A:TRP:HE3	12	0.83
(1,1723)	1:341:A:VAL:HG13	1:338:A:TRP:HE3	14	0.83
(1,1609)	1:411:A:LEU:HD23	1:387:A:TYR:HB2	16	0.83
(1,1522)	1:422:A:ILE:HG22	1:430:A:LEU:HG	16	0.83
(1,1496)	1:430:A:LEU:HD21	1:427:A:THR:HA	9	0.83
(1,1495)	1:430:A:LEU:HD23	1:396:A:HIS:HA	19	0.83
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	3	0.83
(1,1402)	1:383:A:THR:HG23	1:384:A:ASN:HD21	9	0.83
(1,1331)	1:400:A:LEU:HD21	1:397:A:TYR:HA	19	0.83
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	8	0.83
(1,1133)	1:367:A:VAL:HG13	1:352:A:ASN:HB3	8	0.83
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	7	0.83
(1,624)	1:403:A:ILE:HG22	1:397:A:TYR:HB3	12	0.83
(1,624)	1:403:A:ILE:HG22	1:397:A:TYR:HB3	19	0.83
(1,465)	1:387:A:TYR:HE1	1:390:A:MET:HG2	18	0.83
(1,384)	1:344:A:LEU:HD12	1:375:A:LEU:HD22	3	0.83
(1,383)	1:375:A:LEU:HD13	1:353:A:PHE:HE1	12	0.83
(1,354)	1:393:A:ALA:HB1	1:438:A:LEU:HD22	9	0.83
(1,234)	1:356:A:TRP:HE1	1:359:A:LYS:HE2	13	0.83
(1,2932)	1:420:A:ASP:H	1:422:A:ILE:HB	10	0.82
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HD11	2	0.82
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HD12	3	0.82
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HD11	8	0.82
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HD11	17	0.82
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HG21	19	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	16	0.82
(1,2841)	1:403:A:ILE:HD11	1:397:A:TYR:HA	8	0.82
(1,2841)	1:403:A:ILE:HD12	1:397:A:TYR:HA	15	0.82
(1,2840)	1:403:A:ILE:HG23	1:416:A:MET:H	4	0.82
(1,2840)	1:403:A:ILE:HG21	1:416:A:MET:H	7	0.82
(1,2826)	1:413:A:PHE:H	1:412:A:LEU:HD21	9	0.82
(1,2826)	1:413:A:PHE:H	1:412:A:LEU:HD21	19	0.82
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	16	0.82
(1,2725)	1:367:A:VAL:HG22	1:365:A:ARG:HB3	12	0.82
(1,2579)	1:358:A:ASP:HB2	1:363:A:ILE:HG23	15	0.82
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG21	13	0.82
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD21	6	0.82
(1,2319)	1:349:A:ARG:H	1:350:A:TYR:HD1	12	0.82
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	9	0.82
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	17	0.82
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	9	0.82
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	5	0.82
(1,1917)	1:394:A:LEU:HD13	1:366:A:ILE:HD12	12	0.82
(1,1782)	1:337:A:LEU:HD11	1:397:A:TYR:HE2	8	0.82
(1,1723)	1:341:A:VAL:HG12	1:338:A:TRP:HE3	11	0.82
(1,1599)	1:412:A:LEU:HD21	1:364:A:PHE:H	17	0.82
(1,1541)	1:445:A:GLU:HA	1:443:A:TYR:HD1	4	0.82
(1,1496)	1:430:A:LEU:HD21	1:427:A:THR:HA	13	0.82
(1,1496)	1:430:A:LEU:HD23	1:427:A:THR:HA	19	0.82
(1,1495)	1:430:A:LEU:HD21	1:396:A:HIS:HA	13	0.82
(1,1448)	1:442:A:THR:HG21	1:456:A:TRP:HB3	7	0.82
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	13	0.82
(1,1142)	1:450:A:ILE:HD11	1:454:A:VAL:HA	2	0.82
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	12	0.82
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	19	0.82
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	1	0.82
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	19	0.82
(1,1024)	1:336:A:LEU:HD22	1:338:A:TRP:HZ2	13	0.82
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	15	0.82
(1,458)	1:386:A:THR:HG23	1:389:A:LYS:HD2	1	0.82
(1,455)	1:386:A:THR:HG23	1:389:A:LYS:HE2	15	0.82
(1,234)	1:356:A:TRP:HE1	1:359:A:LYS:HE2	3	0.82
(1,172)	1:354:A:ILE:HG23	1:350:A:TYR:HD1	15	0.82
(1,2932)	1:420:A:ASP:H	1:418:A:THR:HG21	11	0.81
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HG22	11	0.81
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	14	0.81
(1,2862)	1:376:A:TRP:HB3	1:340:A:TYR:HE2	16	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2862)	1:376:A:TRP:HB3	1:340:A:TYR:HE2	18	0.81
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	5	0.81
(1,2826)	1:413:A:PHE:H	1:412:A:LEU:HD22	16	0.81
(1,2816)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	4	0.81
(1,2816)	1:422:A:ILE:HG23	1:417:A:LYS:HD3	13	0.81
(1,2813)	1:418:A:THR:HG23	1:362:A:LYS:HD2	6	0.81
(1,2793)	1:433:A:LEU:HD21	1:429:A:ARG:HA	11	0.81
(1,2791)	1:438:A:LEU:HD23	1:385:A:MET:HG2	19	0.81
(1,2789)	1:438:A:LEU:HD12	1:381:A:ASN:HD22	12	0.81
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD11	9	0.81
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	10	0.81
(1,2708)	1:349:A:ARG:HD2	1:350:A:TYR:HE2	15	0.81
(1,2696)	1:438:A:LEU:HD21	1:382:A:ARG:HD2	2	0.81
(1,2694)	1:438:A:LEU:HD13	1:434:A:GLU:HA	5	0.81
(1,2644)	1:402:A:ILE:HD13	1:397:A:TYR:HE1	6	0.81
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	12	0.81
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	15	0.81
(1,2258)	1:450:A:ILE:H	1:450:A:ILE:HG13	11	0.81
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	2	0.81
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	14	0.81
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	2	0.81
(1,1917)	1:394:A:LEU:HD13	1:366:A:ILE:HD11	18	0.81
(1,1774)	1:337:A:LEU:HD12	1:393:A:ALA:HB3	12	0.81
(1,1723)	1:341:A:VAL:HG11	1:338:A:TRP:HE3	1	0.81
(1,1723)	1:341:A:VAL:HG12	1:338:A:TRP:HE3	15	0.81
(1,1522)	1:422:A:ILE:HG21	1:430:A:LEU:HG	19	0.81
(1,1495)	1:430:A:LEU:HD21	1:396:A:HIS:HA	5	0.81
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG11	4	0.81
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG12	9	0.81
(1,1446)	1:442:A:THR:HG22	1:443:A:TYR:HD2	11	0.81
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	2	0.81
(1,1403)	1:383:A:THR:HG21	1:382:A:ARG:HD2	19	0.81
(1,1360)	1:392:A:ARG:HD2	1:392:A:ARG:HB3	16	0.81
(1,1256)	1:410:A:ARG:HD3	1:412:A:LEU:HB3	13	0.81
(1,1182)	1:363:A:ILE:HD12	1:406:A:GLU:HG2	1	0.81
(1,1024)	1:336:A:LEU:HD21	1:338:A:TRP:HZ2	3	0.81
(1,833)	1:430:A:LEU:HD12	1:338:A:TRP:HD1	18	0.81
(1,458)	1:386:A:THR:HG22	1:389:A:LYS:HD2	17	0.81
(1,354)	1:393:A:ALA:HB1	1:438:A:LEU:HD22	3	0.81
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD13	3	0.81
(1,236)	1:361:A:SER:HB3	1:358:A:ASP:HB2	15	0.81
(1,2984)	1:410:A:ARG:HE	1:366:A:ILE:HG23	7	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD22	9	0.8
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD23	16	0.8
(1,2910)	1:366:A:ILE:H	1:366:A:ILE:HG22	15	0.8
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	2	0.8
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	18	0.8
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	17	0.8
(1,2841)	1:403:A:ILE:HD12	1:397:A:TYR:HA	1	0.8
(1,2841)	1:403:A:ILE:HD11	1:397:A:TYR:HA	12	0.8
(1,2826)	1:413:A:PHE:H	1:412:A:LEU:HD23	6	0.8
(1,2813)	1:418:A:THR:HG22	1:362:A:LYS:HD3	11	0.8
(1,2793)	1:433:A:LEU:HD22	1:429:A:ARG:HA	1	0.8
(1,2768)	1:394:A:LEU:HD12	1:387:A:TYR:HD1	7	0.8
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	13	0.8
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG23	17	0.8
(1,2726)	1:367:A:VAL:HG13	1:365:A:ARG:HD2	11	0.8
(1,2645)	1:402:A:ILE:HD12	1:338:A:TRP:HB3	9	0.8
(1,2644)	1:402:A:ILE:HD13	1:397:A:TYR:HE1	7	0.8
(1,2633)	1:394:A:LEU:HD12	1:366:A:ILE:HD11	6	0.8
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	8	0.8
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG23	13	0.8
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	5	0.8
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD23	1	0.8
(1,2258)	1:450:A:ILE:H	1:450:A:ILE:HG13	18	0.8
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	3	0.8
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	5	0.8
(1,1782)	1:337:A:LEU:HD13	1:397:A:TYR:HE2	5	0.8
(1,1723)	1:341:A:VAL:HG12	1:338:A:TRP:HE3	8	0.8
(1,1599)	1:412:A:LEU:HD23	1:364:A:PHE:H	6	0.8
(1,1599)	1:412:A:LEU:HD21	1:364:A:PHE:H	7	0.8
(1,1599)	1:412:A:LEU:HD23	1:364:A:PHE:H	13	0.8
(1,1599)	1:412:A:LEU:HD22	1:364:A:PHE:H	16	0.8
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	10	0.8
(1,1496)	1:430:A:LEU:HD22	1:427:A:THR:HA	4	0.8
(1,1496)	1:430:A:LEU:HD21	1:427:A:THR:HA	8	0.8
(1,1496)	1:430:A:LEU:HD23	1:427:A:THR:HA	15	0.8
(1,1430)	1:447:A:GLU:HB2	1:448:A:PRO:HD3	4	0.8
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	16	0.8
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	14	0.8
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	16	0.8
(1,624)	1:403:A:ILE:HG21	1:397:A:TYR:HB3	16	0.8
(1,530)	1:394:A:LEU:HD23	1:397:A:TYR:HB3	8	0.8
(1,384)	1:344:A:LEU:HD11	1:375:A:LEU:HD23	19	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:393:A:ALA:HB3	1:438:A:LEU:HD23	8	0.8
(1,2984)	1:410:A:ARG:HE	1:367:A:VAL:HG21	9	0.79
(1,2932)	1:420:A:ASP:H	1:418:A:THR:HG22	3	0.79
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	10	0.79
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	17	0.79
(1,2876)	1:372:A:LEU:HD11	1:374:A:ARG:H	18	0.79
(1,2862)	1:379:A:HIS:HB3	1:340:A:TYR:HE1	6	0.79
(1,2862)	1:379:A:HIS:HB3	1:340:A:TYR:HE1	14	0.79
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	4	0.79
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	18	0.79
(1,2840)	1:403:A:ILE:HG22	1:416:A:MET:H	3	0.79
(1,2826)	1:366:A:ILE:H	1:412:A:LEU:HD23	10	0.79
(1,2826)	1:413:A:PHE:H	1:412:A:LEU:HD23	11	0.79
(1,2816)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	16	0.79
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	19	0.79
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD12	5	0.79
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG22	11	0.79
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	3	0.79
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	19	0.79
(1,2694)	1:438:A:LEU:HD11	1:434:A:GLU:HA	16	0.79
(1,2633)	1:394:A:LEU:HD11	1:366:A:ILE:HD13	5	0.79
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	7	0.79
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG21	19	0.79
(1,2514)	1:444:A:GLN:H	1:444:A:GLN:HG3	17	0.79
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD23	18	0.79
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	14	0.79
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	6	0.79
(1,1804)	1:422:A:ILE:HD12	1:336:A:LEU:HD13	6	0.79
(1,1782)	1:337:A:LEU:HD11	1:397:A:TYR:HE2	4	0.79
(1,1782)	1:337:A:LEU:HD13	1:397:A:TYR:HE2	14	0.79
(1,1723)	1:341:A:VAL:HG13	1:338:A:TRP:HE3	6	0.79
(1,1599)	1:412:A:LEU:HD21	1:364:A:PHE:H	9	0.79
(1,1599)	1:412:A:LEU:HD23	1:364:A:PHE:H	10	0.79
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	18	0.79
(1,1522)	1:422:A:ILE:HG22	1:430:A:LEU:HG	6	0.79
(1,1522)	1:422:A:ILE:HG23	1:430:A:LEU:HG	7	0.79
(1,1496)	1:430:A:LEU:HD23	1:427:A:THR:HA	10	0.79
(1,1495)	1:430:A:LEU:HD22	1:396:A:HIS:HA	4	0.79
(1,1495)	1:430:A:LEU:HD22	1:396:A:HIS:HA	12	0.79
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG12	11	0.79
(1,1466)	1:434:A:GLU:HB2	1:437:A:VAL:HG12	18	0.79
(1,1445)	1:442:A:THR:HG21	1:443:A:TYR:HE2	16	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1424)	1:450:A:ILE:HG23	1:452:A:SER:HB2	11	0.79
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	2	0.79
(1,1182)	1:363:A:ILE:HD13	1:406:A:GLU:HG2	9	0.79
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	9	0.79
(1,1024)	1:336:A:LEU:HD23	1:338:A:TRP:HZ2	10	0.79
(1,1024)	1:336:A:LEU:HD22	1:338:A:TRP:HZ2	18	0.79
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	19	0.79
(1,715)	1:414:A:ARG:HD2	1:414:A:ARG:HH12	1	0.79
(1,715)	1:414:A:ARG:HD2	1:414:A:ARG:HH12	5	0.79
(1,624)	1:403:A:ILE:HG22	1:397:A:TYR:HB3	9	0.79
(1,549)	1:396:A:HIS:HB3	1:430:A:LEU:HD23	18	0.79
(1,354)	1:393:A:ALA:HB3	1:438:A:LEU:HD21	10	0.79
(1,354)	1:393:A:ALA:HB3	1:438:A:LEU:HD21	19	0.79
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD23	7	0.78
(1,2876)	1:372:A:LEU:HD13	1:374:A:ARG:H	1	0.78
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	12	0.78
(1,2841)	1:403:A:ILE:HD12	1:397:A:TYR:HA	7	0.78
(1,2841)	1:403:A:ILE:HD12	1:397:A:TYR:HA	17	0.78
(1,2826)	1:413:A:PHE:H	1:412:A:LEU:HD22	12	0.78
(1,2767)	1:396:A:HIS:HB3	1:397:A:TYR:HA	2	0.78
(1,2694)	1:438:A:LEU:HD12	1:434:A:GLU:HA	1	0.78
(1,2694)	1:438:A:LEU:HD11	1:434:A:GLU:HA	12	0.78
(1,2633)	1:394:A:LEU:HD11	1:366:A:ILE:HD13	14	0.78
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG23	2	0.78
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	10	0.78
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD21	3	0.78
(1,2343)	1:361:A:SER:H	1:362:A:LYS:HG3	2	0.78
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	2	0.78
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	11	0.78
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	10	0.78
(1,1804)	1:422:A:ILE:HD11	1:336:A:LEU:HD13	5	0.78
(1,1782)	1:337:A:LEU:HD11	1:397:A:TYR:HE2	15	0.78
(1,1782)	1:337:A:LEU:HD12	1:397:A:TYR:HE2	17	0.78
(1,1774)	1:337:A:LEU:HD13	1:393:A:ALA:HB2	18	0.78
(1,1723)	1:341:A:VAL:HG11	1:338:A:TRP:HE3	10	0.78
(1,1599)	1:412:A:LEU:HD23	1:364:A:PHE:H	1	0.78
(1,1599)	1:412:A:LEU:HD23	1:364:A:PHE:H	5	0.78
(1,1599)	1:412:A:LEU:HD21	1:364:A:PHE:H	8	0.78
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	2	0.78
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	3	0.78
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	4	0.78
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	13	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	16	0.78
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	17	0.78
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	19	0.78
(1,1446)	1:442:A:THR:HG21	1:443:A:TYR:HD2	10	0.78
(1,1360)	1:392:A:ARG:HD2	1:392:A:ARG:HB3	10	0.78
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	17	0.78
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	13	0.78
(1,624)	1:403:A:ILE:HG23	1:397:A:TYR:HB3	7	0.78
(1,458)	1:386:A:THR:HG22	1:389:A:LYS:HD2	3	0.78
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD12	10	0.78
(1,127)	1:349:A:ARG:HD2	1:350:A:TYR:HE1	3	0.78
(1,2984)	1:410:A:ARG:HE	1:367:A:VAL:HG23	18	0.77
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD22	5	0.77
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD22	13	0.77
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	3	0.77
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	4	0.77
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	6	0.77
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	11	0.77
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	14	0.77
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	19	0.77
(1,2841)	1:403:A:ILE:HD12	1:397:A:TYR:HA	2	0.77
(1,2841)	1:403:A:ILE:HD11	1:397:A:TYR:HA	13	0.77
(1,2841)	1:403:A:ILE:HD11	1:397:A:TYR:HA	14	0.77
(1,2840)	1:403:A:ILE:HG23	1:416:A:MET:H	6	0.77
(1,2813)	1:418:A:THR:HG21	1:362:A:LYS:HD3	7	0.77
(1,2806)	1:430:A:LEU:HD12	1:431:A:GLU:HG2	4	0.77
(1,2806)	1:430:A:LEU:HD11	1:431:A:GLU:HG2	9	0.77
(1,2793)	1:433:A:LEU:HD23	1:429:A:ARG:HA	3	0.77
(1,2791)	1:380:A:LYS:HE3	1:438:A:LEU:HD23	8	0.77
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD12	15	0.77
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	1	0.77
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	11	0.77
(1,2644)	1:402:A:ILE:HD13	1:397:A:TYR:HE1	13	0.77
(1,2633)	1:394:A:LEU:HD11	1:366:A:ILE:HD11	4	0.77
(1,2607)	1:367:A:VAL:HA	1:365:A:ARG:HD2	12	0.77
(1,2473)	1:409:A:GLN:HE21	1:412:A:LEU:HD11	11	0.77
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD22	11	0.77
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	15	0.77
(1,2254)	1:443:A:TYR:H	1:443:A:TYR:HD2	3	0.77
(1,2254)	1:443:A:TYR:H	1:443:A:TYR:HD2	10	0.77
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	6	0.77
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	9	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1804)	1:422:A:ILE:HD11	1:336:A:LEU:HD13	10	0.77
(1,1782)	1:337:A:LEU:HD12	1:397:A:TYR:HE2	3	0.77
(1,1723)	1:341:A:VAL:HG12	1:338:A:TRP:HE3	5	0.77
(1,1690)	1:402:A:ILE:HD11	1:400:A:LEU:HA	10	0.77
(1,1609)	1:411:A:LEU:HD23	1:387:A:TYR:HB2	12	0.77
(1,1599)	1:412:A:LEU:HD22	1:364:A:PHE:H	3	0.77
(1,1599)	1:412:A:LEU:HD23	1:364:A:PHE:H	4	0.77
(1,1599)	1:412:A:LEU:HD21	1:364:A:PHE:H	19	0.77
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	6	0.77
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	7	0.77
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	8	0.77
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	9	0.77
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	11	0.77
(1,1522)	1:422:A:ILE:HG21	1:430:A:LEU:HG	17	0.77
(1,1495)	1:430:A:LEU:HD22	1:396:A:HIS:HA	7	0.77
(1,1482)	1:433:A:LEU:HB3	1:433:A:LEU:HD11	4	0.77
(1,1393)	1:386:A:THR:HG23	1:388:A:GLU:HB3	18	0.77
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG23	4	0.77
(1,1024)	1:336:A:LEU:HD22	1:338:A:TRP:HZ2	16	0.77
(1,1006)	1:380:A:LYS:HA	1:380:A:LYS:HD3	18	0.77
(1,2984)	1:410:A:ARG:HE	1:366:A:ILE:HG21	1	0.76
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD22	14	0.76
(1,2932)	1:420:A:ASP:H	1:422:A:ILE:HB	6	0.76
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	19	0.76
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	8	0.76
(1,2841)	1:403:A:ILE:HD11	1:397:A:TYR:HA	4	0.76
(1,2841)	1:403:A:ILE:HD11	1:397:A:TYR:HA	6	0.76
(1,2841)	1:403:A:ILE:HD12	1:397:A:TYR:HA	10	0.76
(1,2841)	1:403:A:ILE:HD11	1:397:A:TYR:HA	16	0.76
(1,2806)	1:430:A:LEU:HD13	1:431:A:GLU:HG2	8	0.76
(1,2793)	1:433:A:LEU:HD23	1:429:A:ARG:HA	7	0.76
(1,2768)	1:394:A:LEU:HD13	1:387:A:TYR:HD1	1	0.76
(1,2762)	1:394:A:LEU:HD22	1:398:A:TYR:HE1	11	0.76
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD12	1	0.76
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD12	4	0.76
(1,2726)	1:367:A:VAL:HG12	1:355:A:ARG:HD3	4	0.76
(1,2694)	1:438:A:LEU:HD11	1:434:A:GLU:HA	13	0.76
(1,2644)	1:402:A:ILE:HD11	1:397:A:TYR:HE1	16	0.76
(1,2633)	1:394:A:LEU:HD11	1:366:A:ILE:HD11	1	0.76
(1,2633)	1:394:A:LEU:HD13	1:366:A:ILE:HD13	3	0.76
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG21	6	0.76
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	12	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2472)	1:409:A:GLN:HE22	1:412:A:LEU:HD13	3	0.76
(1,2432)	1:435:A:SER:H	1:436:A:GLN:HB2	4	0.76
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	19	0.76
(1,2352)	1:354:A:ILE:H	1:353:A:PHE:HD2	5	0.76
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	13	0.76
(1,2254)	1:443:A:TYR:H	1:443:A:TYR:HD2	8	0.76
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	1	0.76
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	16	0.76
(1,2207)	1:406:A:GLU:H	1:412:A:LEU:HB2	2	0.76
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	6	0.76
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	13	0.76
(1,1923)	1:344:A:LEU:HD22	1:375:A:LEU:HD22	6	0.76
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB3	4	0.76
(1,1782)	1:337:A:LEU:HD12	1:397:A:TYR:HE2	13	0.76
(1,1703)	1:344:A:LEU:HA	1:350:A:TYR:HE1	1	0.76
(1,1609)	1:411:A:LEU:HD22	1:387:A:TYR:HB2	4	0.76
(1,1609)	1:411:A:LEU:HD21	1:387:A:TYR:HB2	14	0.76
(1,1599)	1:412:A:LEU:HD22	1:364:A:PHE:H	2	0.76
(1,1599)	1:412:A:LEU:HD23	1:364:A:PHE:H	14	0.76
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	1	0.76
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	5	0.76
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	12	0.76
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	14	0.76
(1,1578)	1:413:A:PHE:HD2	1:413:A:PHE:HA	15	0.76
(1,1495)	1:430:A:LEU:HD23	1:396:A:HIS:HA	10	0.76
(1,1495)	1:430:A:LEU:HD21	1:396:A:HIS:HA	14	0.76
(1,1393)	1:386:A:THR:HG22	1:388:A:GLU:HB3	9	0.76
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG21	6	0.76
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	15	0.76
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	19	0.76
(1,458)	1:386:A:THR:HG23	1:389:A:LYS:HD2	12	0.76
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD13	19	0.76
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD22	13	0.76
(1,2984)	1:410:A:ARG:HE	1:366:A:ILE:HG22	17	0.75
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD23	1	0.75
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD21	2	0.75
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	16	0.75
(1,2826)	1:413:A:PHE:H	1:412:A:LEU:HD22	2	0.75
(1,2806)	1:430:A:LEU:HD11	1:431:A:GLU:HG2	14	0.75
(1,2793)	1:433:A:LEU:HD22	1:429:A:ARG:HA	9	0.75
(1,2793)	1:433:A:LEU:HD23	1:429:A:ARG:HA	16	0.75
(1,2768)	1:394:A:LEU:HD11	1:387:A:TYR:HD1	19	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2726)	1:367:A:VAL:HG12	1:355:A:ARG:HD3	7	0.75
(1,2694)	1:438:A:LEU:HD11	1:434:A:GLU:HA	6	0.75
(1,2644)	1:402:A:ILE:HD11	1:397:A:TYR:HE1	1	0.75
(1,2633)	1:394:A:LEU:HD13	1:366:A:ILE:HD11	7	0.75
(1,2633)	1:394:A:LEU:HD12	1:366:A:ILE:HD12	17	0.75
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	9	0.75
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG22	10	0.75
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG21	17	0.75
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	3	0.75
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	12	0.75
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	2	0.75
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	19	0.75
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	3	0.75
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	4	0.75
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	7	0.75
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	12	0.75
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	19	0.75
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB1	5	0.75
(1,1804)	1:422:A:ILE:HD12	1:336:A:LEU:HD12	1	0.75
(1,1782)	1:337:A:LEU:HD11	1:397:A:TYR:HE2	2	0.75
(1,1723)	1:341:A:VAL:HG12	1:338:A:TRP:HE3	4	0.75
(1,1690)	1:402:A:ILE:HD13	1:400:A:LEU:HA	2	0.75
(1,1599)	1:412:A:LEU:HD22	1:364:A:PHE:H	12	0.75
(1,1599)	1:412:A:LEU:HD22	1:364:A:PHE:H	18	0.75
(1,1522)	1:422:A:ILE:HG21	1:430:A:LEU:HG	12	0.75
(1,1522)	1:422:A:ILE:HG22	1:430:A:LEU:HG	15	0.75
(1,1496)	1:430:A:LEU:HD22	1:427:A:THR:HA	12	0.75
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	5	0.75
(1,1357)	1:394:A:LEU:HD23	1:390:A:MET:HG3	11	0.75
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG21	14	0.75
(1,1142)	1:450:A:ILE:HD11	1:454:A:VAL:HA	8	0.75
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	7	0.75
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	7	0.75
(1,1024)	1:336:A:LEU:HD23	1:338:A:TRP:HZ2	4	0.75
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	8	0.75
(1,843)	1:430:A:LEU:HD23	1:336:A:LEU:HD12	6	0.75
(1,843)	1:430:A:LEU:HD21	1:336:A:LEU:HD11	16	0.75
(1,384)	1:344:A:LEU:HD13	1:375:A:LEU:HD23	13	0.75
(1,354)	1:393:A:ALA:HB3	1:438:A:LEU:HD23	15	0.75
(1,35)	1:341:A:VAL:HG13	1:345:A:LEU:HD13	6	0.75
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD22	6	0.74
(1,2876)	1:372:A:LEU:HD12	1:374:A:ARG:H	11	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2876)	1:372:A:LEU:HD12	1:374:A:ARG:H	14	0.74
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	3	0.74
(1,2841)	1:403:A:ILE:HD13	1:397:A:TYR:HA	5	0.74
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD12	13	0.74
(1,2806)	1:430:A:LEU:HD11	1:431:A:GLU:HG2	10	0.74
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB2	12	0.74
(1,2768)	1:394:A:LEU:HD13	1:387:A:TYR:HD1	10	0.74
(1,2762)	1:394:A:LEU:HD23	1:398:A:TYR:HE2	5	0.74
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD12	7	0.74
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD11	8	0.74
(1,2644)	1:402:A:ILE:HD11	1:397:A:TYR:HE1	14	0.74
(1,2644)	1:402:A:ILE:HD12	1:397:A:TYR:HE1	15	0.74
(1,2640)	1:400:A:LEU:HD23	1:402:A:ILE:HD11	9	0.74
(1,2633)	1:394:A:LEU:HD11	1:366:A:ILE:HD13	16	0.74
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG23	1	0.74
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD13	12	0.74
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	15	0.74
(1,2216)	1:408:A:GLY:H	1:409:A:GLN:HG3	14	0.74
(1,1917)	1:394:A:LEU:HD11	1:366:A:ILE:HD13	5	0.74
(1,1917)	1:394:A:LEU:HD12	1:366:A:ILE:HD11	6	0.74
(1,1774)	1:337:A:LEU:HD13	1:393:A:ALA:HB2	15	0.74
(1,1609)	1:411:A:LEU:HD22	1:387:A:TYR:HB2	7	0.74
(1,1599)	1:412:A:LEU:HD23	1:364:A:PHE:H	11	0.74
(1,1496)	1:430:A:LEU:HD22	1:427:A:THR:HA	7	0.74
(1,1495)	1:430:A:LEU:HD23	1:396:A:HIS:HA	15	0.74
(1,1430)	1:447:A:GLU:HB2	1:448:A:PRO:HD3	1	0.74
(1,1372)	1:390:A:MET:HG2	1:390:A:MET:H	12	0.74
(1,1357)	1:394:A:LEU:HD21	1:390:A:MET:HG3	9	0.74
(1,1357)	1:394:A:LEU:HD22	1:390:A:MET:HG3	16	0.74
(1,1357)	1:394:A:LEU:HD22	1:390:A:MET:HG3	17	0.74
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	19	0.74
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	5	0.74
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	18	0.74
(1,599)	1:401:A:ASN:H	1:401:A:ASN:HB3	13	0.74
(1,599)	1:401:A:ASN:H	1:401:A:ASN:HB3	15	0.74
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	9	0.74
(1,2984)	1:410:A:ARG:HE	1:366:A:ILE:HG21	6	0.73
(1,2932)	1:420:A:ASP:H	1:422:A:ILE:HB	7	0.73
(1,2879)	1:344:A:LEU:HD11	1:350:A:TYR:HE1	15	0.73
(1,2876)	1:372:A:LEU:HD12	1:374:A:ARG:H	2	0.73
(1,2876)	1:372:A:LEU:HD12	1:374:A:ARG:H	10	0.73
(1,2876)	1:372:A:LEU:HD12	1:374:A:ARG:H	19	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	15	0.73
(1,2841)	1:403:A:ILE:HD11	1:397:A:TYR:HA	3	0.73
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD12	11	0.73
(1,2826)	1:366:A:ILE:H	1:412:A:LEU:HD22	18	0.73
(1,2816)	1:422:A:ILE:HG21	1:417:A:LYS:HD3	9	0.73
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	18	0.73
(1,2726)	1:367:A:VAL:HG13	1:355:A:ARG:HD3	14	0.73
(1,2725)	1:367:A:VAL:HG21	1:365:A:ARG:HB3	16	0.73
(1,2708)	1:349:A:ARG:HD2	1:350:A:TYR:HE1	3	0.73
(1,2694)	1:438:A:LEU:HD13	1:434:A:GLU:HA	14	0.73
(1,2681)	1:418:A:THR:HG21	1:342:A:TYR:HD1	15	0.73
(1,2633)	1:394:A:LEU:HD11	1:366:A:ILE:HD12	10	0.73
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	15	0.73
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG22	19	0.73
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG22	8	0.73
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG21	12	0.73
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	7	0.73
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	11	0.73
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	5	0.73
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	7	0.73
(1,1917)	1:394:A:LEU:HD11	1:366:A:ILE:HD13	14	0.73
(1,1804)	1:422:A:ILE:HD13	1:336:A:LEU:HD12	15	0.73
(1,1774)	1:337:A:LEU:HD13	1:393:A:ALA:HB1	4	0.73
(1,1774)	1:337:A:LEU:HD11	1:393:A:ALA:HB2	5	0.73
(1,1774)	1:337:A:LEU:HD12	1:393:A:ALA:HB1	6	0.73
(1,1774)	1:337:A:LEU:HD13	1:393:A:ALA:HB3	9	0.73
(1,1609)	1:411:A:LEU:HD22	1:387:A:TYR:HB2	11	0.73
(1,1495)	1:430:A:LEU:HD21	1:396:A:HIS:HA	8	0.73
(1,1455)	1:437:A:VAL:H	1:436:A:GLN:HB2	19	0.73
(1,1403)	1:383:A:THR:HG23	1:382:A:ARG:HD2	1	0.73
(1,1357)	1:394:A:LEU:HD21	1:390:A:MET:HG3	10	0.73
(1,1182)	1:363:A:ILE:HD12	1:406:A:GLU:HG2	19	0.73
(1,1113)	1:411:A:LEU:HD11	1:369:A:PRO:HB2	9	0.73
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	15	0.73
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	9	0.73
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	12	0.73
(1,843)	1:430:A:LEU:HD22	1:336:A:LEU:HD11	19	0.73
(1,715)	1:414:A:ARG:HD2	1:414:A:ARG:HH12	16	0.73
(1,599)	1:401:A:ASN:H	1:401:A:ASN:HB3	9	0.73
(1,599)	1:401:A:ASN:H	1:401:A:ASN:HB3	10	0.73
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	8	0.73
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	15	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	17	0.73
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD12	6	0.73
(1,35)	1:341:A:VAL:HG12	1:345:A:LEU:HD11	5	0.73
(1,35)	1:341:A:VAL:HG13	1:345:A:LEU:HD11	7	0.73
(1,5)	1:337:A:LEU:HD21	1:390:A:MET:HG3	12	0.73
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD21	15	0.72
(1,2932)	1:420:A:ASP:H	1:422:A:ILE:HB	9	0.72
(1,2932)	1:420:A:ASP:H	1:422:A:ILE:HB	16	0.72
(1,2862)	1:379:A:HIS:HB3	1:340:A:TYR:HE1	9	0.72
(1,2862)	1:379:A:HIS:HB3	1:340:A:TYR:HE1	13	0.72
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	1	0.72
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD13	12	0.72
(1,2793)	1:433:A:LEU:HD22	1:429:A:ARG:HA	2	0.72
(1,2791)	1:438:A:LEU:HD22	1:385:A:MET:HG2	5	0.72
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD11	16	0.72
(1,2696)	1:438:A:LEU:HD23	1:382:A:ARG:HD2	19	0.72
(1,2694)	1:438:A:LEU:HD11	1:434:A:GLU:HA	15	0.72
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	4	0.72
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	10	0.72
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	8	0.72
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	9	0.72
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	15	0.72
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	17	0.72
(1,2149)	1:388:A:GLU:H	1:387:A:TYR:HD2	1	0.72
(1,1975)	1:349:A:ARG:H	1:349:A:ARG:HG3	13	0.72
(1,1917)	1:394:A:LEU:HD11	1:366:A:ILE:HD11	4	0.72
(1,1804)	1:422:A:ILE:HD12	1:336:A:LEU:HD12	2	0.72
(1,1804)	1:422:A:ILE:HD11	1:336:A:LEU:HD11	18	0.72
(1,1782)	1:337:A:LEU:HD11	1:397:A:TYR:HE2	10	0.72
(1,1774)	1:337:A:LEU:HD13	1:393:A:ALA:HB1	7	0.72
(1,1774)	1:337:A:LEU:HD12	1:393:A:ALA:HB1	11	0.72
(1,1723)	1:341:A:VAL:HG13	1:338:A:TRP:HE3	13	0.72
(1,1659)	1:404:A:ARG:HB2	1:404:A:ARG:HD3	6	0.72
(1,1609)	1:411:A:LEU:HD21	1:387:A:TYR:HB2	1	0.72
(1,1522)	1:422:A:ILE:HG21	1:430:A:LEU:HG	14	0.72
(1,1496)	1:430:A:LEU:HD21	1:427:A:THR:HA	17	0.72
(1,1495)	1:430:A:LEU:HD21	1:396:A:HIS:HA	3	0.72
(1,1471)	1:433:A:LEU:HA	1:436:A:GLN:HG3	19	0.72
(1,1407)	1:456:A:TRP:HB3	1:456:A:TRP:HZ3	18	0.72
(1,1392)	1:386:A:THR:HG22	1:389:A:LYS:HG2	7	0.72
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG23	15	0.72
(1,1113)	1:411:A:LEU:HD12	1:369:A:PRO:HB2	13	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	2	0.72
(1,843)	1:430:A:LEU:HD23	1:336:A:LEU:HD12	5	0.72
(1,843)	1:430:A:LEU:HD23	1:336:A:LEU:HD12	13	0.72
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	12	0.72
(1,715)	1:414:A:ARG:HD2	1:414:A:ARG:HH12	7	0.72
(1,624)	1:403:A:ILE:HG23	1:397:A:TYR:HB3	18	0.72
(1,599)	1:401:A:ASN:H	1:401:A:ASN:HB3	2	0.72
(1,599)	1:401:A:ASN:H	1:401:A:ASN:HB3	4	0.72
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	1	0.72
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	2	0.72
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	3	0.72
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	4	0.72
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	9	0.72
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	10	0.72
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	16	0.72
(1,457)	1:386:A:THR:HG23	1:389:A:LYS:HB2	12	0.72
(1,455)	1:386:A:THR:HG23	1:389:A:LYS:HE2	17	0.72
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD13	4	0.72
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD12	5	0.72
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD11	9	0.72
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD13	11	0.72
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD21	19	0.72
(1,2984)	1:410:A:ARG:HE	1:366:A:ILE:HG23	16	0.71
(1,2876)	1:372:A:LEU:HD13	1:374:A:ARG:H	15	0.71
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD13	1	0.71
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD13	8	0.71
(1,2826)	1:366:A:ILE:H	1:412:A:LEU:HD23	13	0.71
(1,2805)	1:372:A:LEU:HD23	1:373:A:ALA:H	9	0.71
(1,2799)	1:412:A:LEU:HD23	1:365:A:ARG:HD3	13	0.71
(1,2768)	1:394:A:LEU:HD12	1:387:A:TYR:HD1	9	0.71
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD11	13	0.71
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD11	14	0.71
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE3	16	0.71
(1,2694)	1:438:A:LEU:HD11	1:434:A:GLU:HA	8	0.71
(1,2681)	1:418:A:THR:HG21	1:342:A:TYR:HD1	18	0.71
(1,2633)	1:394:A:LEU:HD12	1:366:A:ILE:HD12	11	0.71
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG21	18	0.71
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD11	2	0.71
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	4	0.71
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD22	4	0.71
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD22	9	0.71
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	3	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	6	0.71
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	14	0.71
(1,2324)	1:352:A:ASN:HD21	1:367:A:VAL:HG22	5	0.71
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	17	0.71
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG21	13	0.71
(1,1804)	1:422:A:ILE:HD13	1:336:A:LEU:HD13	9	0.71
(1,1782)	1:337:A:LEU:HD13	1:397:A:TYR:HE2	12	0.71
(1,1690)	1:402:A:ILE:HD11	1:400:A:LEU:HA	4	0.71
(1,1690)	1:402:A:ILE:HD11	1:400:A:LEU:HA	13	0.71
(1,1495)	1:430:A:LEU:HD22	1:396:A:HIS:HA	11	0.71
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	10	0.71
(1,1393)	1:386:A:THR:HG23	1:388:A:GLU:HB3	14	0.71
(1,1372)	1:390:A:MET:HG2	1:390:A:MET:H	18	0.71
(1,1341)	1:399:A:LYS:HD2	1:400:A:LEU:H	5	0.71
(1,1330)	1:400:A:LEU:HD12	1:399:A:LYS:HB2	18	0.71
(1,1113)	1:411:A:LEU:HD12	1:369:A:PRO:HB2	12	0.71
(1,1024)	1:336:A:LEU:HD23	1:338:A:TRP:HZ2	8	0.71
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	4	0.71
(1,843)	1:430:A:LEU:HD21	1:336:A:LEU:HD11	1	0.71
(1,843)	1:430:A:LEU:HD23	1:336:A:LEU:HD11	17	0.71
(1,715)	1:414:A:ARG:HD2	1:414:A:ARG:HH12	4	0.71
(1,624)	1:403:A:ILE:HG22	1:397:A:TYR:HB3	4	0.71
(1,624)	1:403:A:ILE:HG21	1:397:A:TYR:HB3	11	0.71
(1,599)	1:401:A:ASN:H	1:401:A:ASN:HB3	8	0.71
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD11	13	0.71
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	6	0.71
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	18	0.71
(1,457)	1:386:A:THR:HG22	1:389:A:LYS:HB2	3	0.71
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD12	17	0.71
(1,35)	1:341:A:VAL:HG11	1:345:A:LEU:HD11	9	0.71
(1,35)	1:341:A:VAL:HG12	1:345:A:LEU:HD13	16	0.71
(1,2984)	1:410:A:ARG:HE	1:367:A:VAL:HG21	5	0.7
(1,2974)	1:433:A:LEU:H	1:431:A:GLU:HB2	11	0.7
(1,2879)	1:344:A:LEU:HD12	1:350:A:TYR:HE1	11	0.7
(1,2876)	1:372:A:LEU:HD12	1:374:A:ARG:H	9	0.7
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	2	0.7
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	7	0.7
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	9	0.7
(1,2840)	1:403:A:ILE:HG21	1:416:A:MET:H	5	0.7
(1,2840)	1:403:A:ILE:HG22	1:416:A:MET:H	16	0.7
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD11	18	0.7
(1,2789)	1:438:A:LEU:HD11	1:381:A:ASN:HD22	9	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD12	11	0.7
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	5	0.7
(1,2696)	1:438:A:LEU:HD21	1:382:A:ARG:HD2	3	0.7
(1,2633)	1:394:A:LEU:HD11	1:366:A:ILE:HD11	15	0.7
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG23	5	0.7
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG23	14	0.7
(1,2547)	1:442:A:THR:H	1:442:A:THR:HG21	8	0.7
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG23	15	0.7
(1,2447)	1:385:A:MET:H	1:444:A:GLN:HE21	4	0.7
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD21	16	0.7
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	4	0.7
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	12	0.7
(1,2258)	1:450:A:ILE:H	1:450:A:ILE:HG13	6	0.7
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG22	15	0.7
(1,1923)	1:344:A:LEU:HD21	1:375:A:LEU:HD22	8	0.7
(1,1917)	1:394:A:LEU:HD11	1:366:A:ILE:HD11	1	0.7
(1,1917)	1:394:A:LEU:HD13	1:366:A:ILE:HD13	3	0.7
(1,1917)	1:394:A:LEU:HD12	1:366:A:ILE:HD12	17	0.7
(1,1804)	1:422:A:ILE:HD13	1:336:A:LEU:HD12	17	0.7
(1,1774)	1:337:A:LEU:HD12	1:393:A:ALA:HB2	19	0.7
(1,1690)	1:402:A:ILE:HD13	1:400:A:LEU:HA	8	0.7
(1,1690)	1:402:A:ILE:HD13	1:400:A:LEU:HA	15	0.7
(1,1653)	1:404:A:ARG:HG2	1:414:A:ARG:HD3	11	0.7
(1,1495)	1:430:A:LEU:HD22	1:396:A:HIS:HA	1	0.7
(1,1444)	1:442:A:THR:HG21	1:443:A:TYR:HA	18	0.7
(1,1330)	1:400:A:LEU:HD13	1:399:A:LYS:HB2	16	0.7
(1,1133)	1:367:A:VAL:HG12	1:352:A:ASN:HB3	1	0.7
(1,1113)	1:411:A:LEU:HD13	1:369:A:PRO:HB2	11	0.7
(1,1113)	1:411:A:LEU:HD12	1:369:A:PRO:HB2	16	0.7
(1,1113)	1:411:A:LEU:HD12	1:369:A:PRO:HB2	17	0.7
(1,1025)	1:336:A:LEU:HD21	1:430:A:LEU:H	2	0.7
(1,1003)	1:409:A:GLN:HG2	1:406:A:GLU:HB2	11	0.7
(1,933)	1:443:A:TYR:HB3	1:443:A:TYR:HD1	13	0.7
(1,843)	1:430:A:LEU:HD23	1:336:A:LEU:HD13	14	0.7
(1,822)	1:429:A:ARG:HA	1:429:A:ARG:HG2	18	0.7
(1,624)	1:403:A:ILE:HG23	1:397:A:TYR:HB3	5	0.7
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD11	8	0.7
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD11	19	0.7
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD12	5	0.7
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD13	6	0.7
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD11	7	0.7
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD12	8	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,458)	1:386:A:THR:HG22	1:389:A:LYS:HD2	2	0.7
(1,458)	1:386:A:THR:HG22	1:389:A:LYS:HD2	15	0.7
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD13	1	0.7
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD13	8	0.7
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD12	12	0.7
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD11	15	0.7
(1,310)	1:450:A:ILE:HD13	1:450:A:ILE:HA	4	0.7
(1,265)	1:363:A:ILE:HG22	1:412:A:LEU:HA	14	0.7
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD22	18	0.7
(1,2984)	1:410:A:ARG:HE	1:367:A:VAL:HG23	4	0.69
(1,2932)	1:420:A:ASP:H	1:422:A:ILE:HB	2	0.69
(1,2932)	1:420:A:ASP:H	1:422:A:ILE:HB	8	0.69
(1,2932)	1:420:A:ASP:H	1:422:A:ILE:HB	18	0.69
(1,2909)	1:366:A:ILE:H	1:413:A:PHE:HZ	11	0.69
(1,2880)	1:402:A:ILE:HG22	1:397:A:TYR:HE2	2	0.69
(1,2879)	1:344:A:LEU:HD13	1:350:A:TYR:HE1	4	0.69
(1,2876)	1:372:A:LEU:HD11	1:374:A:ARG:H	3	0.69
(1,2843)	1:402:A:ILE:HG12	1:403:A:ILE:H	13	0.69
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD13	10	0.69
(1,2805)	1:372:A:LEU:HD21	1:373:A:ALA:H	11	0.69
(1,2799)	1:412:A:LEU:HD23	1:365:A:ARG:HD3	4	0.69
(1,2789)	1:438:A:LEU:HD12	1:381:A:ASN:HD22	13	0.69
(1,2768)	1:394:A:LEU:HD13	1:387:A:TYR:HD1	5	0.69
(1,2768)	1:394:A:LEU:HD13	1:387:A:TYR:HD1	15	0.69
(1,2762)	1:394:A:LEU:HD23	1:398:A:TYR:HE1	12	0.69
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD11	17	0.69
(1,2726)	1:367:A:VAL:HG12	1:365:A:ARG:HD2	9	0.69
(1,2726)	1:367:A:VAL:HG12	1:365:A:ARG:HD2	10	0.69
(1,2725)	1:354:A:ILE:HG13	1:367:A:VAL:HG23	6	0.69
(1,2645)	1:402:A:ILE:HD13	1:338:A:TRP:HB3	1	0.69
(1,2633)	1:394:A:LEU:HD12	1:366:A:ILE:HD12	19	0.69
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG23	18	0.69
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG23	16	0.69
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	1	0.69
(1,2472)	1:409:A:GLN:HE22	1:412:A:LEU:HD13	16	0.69
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	3	0.69
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD22	10	0.69
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	18	0.69
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	1	0.69
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	5	0.69
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	16	0.69
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	18	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2254)	1:443:A:TYR:H	1:443:A:TYR:HD2	1	0.69
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	18	0.69
(1,2167)	1:392:A:ARG:H	1:392:A:ARG:HG2	16	0.69
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG23	12	0.69
(1,1917)	1:394:A:LEU:HD13	1:366:A:ILE:HD11	7	0.69
(1,1917)	1:394:A:LEU:HD11	1:366:A:ILE:HD13	16	0.69
(1,1798)	1:336:A:LEU:H	1:336:A:LEU:HD11	12	0.69
(1,1774)	1:337:A:LEU:HD12	1:393:A:ALA:HB1	14	0.69
(1,1690)	1:402:A:ILE:HD11	1:400:A:LEU:HA	12	0.69
(1,1609)	1:411:A:LEU:HD22	1:387:A:TYR:HB2	8	0.69
(1,1495)	1:430:A:LEU:HD21	1:396:A:HIS:HA	6	0.69
(1,1495)	1:430:A:LEU:HD22	1:396:A:HIS:HA	16	0.69
(1,1455)	1:437:A:VAL:H	1:436:A:GLN:HB2	4	0.69
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	6	0.69
(1,1393)	1:386:A:THR:HG21	1:388:A:GLU:HB3	6	0.69
(1,1357)	1:394:A:LEU:HD22	1:390:A:MET:HG3	2	0.69
(1,1349)	1:443:A:TYR:HE1	1:445:A:GLU:HA	1	0.69
(1,1341)	1:399:A:LYS:HD2	1:400:A:LEU:H	1	0.69
(1,1341)	1:399:A:LYS:HD2	1:400:A:LEU:H	7	0.69
(1,1330)	1:400:A:LEU:HD11	1:399:A:LYS:HB2	15	0.69
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	18	0.69
(1,1113)	1:411:A:LEU:HD13	1:369:A:PRO:HB2	7	0.69
(1,1113)	1:411:A:LEU:HD11	1:369:A:PRO:HB2	10	0.69
(1,1113)	1:411:A:LEU:HD12	1:369:A:PRO:HB2	19	0.69
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	11	0.69
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	3	0.69
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	7	0.69
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	10	0.69
(1,933)	1:443:A:TYR:HB3	1:443:A:TYR:HD1	5	0.69
(1,843)	1:430:A:LEU:HD22	1:336:A:LEU:HD11	2	0.69
(1,806)	1:426:A:ARG:HD2	1:426:A:ARG:HA	3	0.69
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	15	0.69
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD13	9	0.69
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD12	12	0.69
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD12	1	0.69
(1,458)	1:386:A:THR:HG22	1:389:A:LYS:HD2	13	0.69
(1,458)	1:386:A:THR:HG21	1:389:A:LYS:HD2	16	0.69
(1,354)	1:393:A:ALA:HB3	1:438:A:LEU:HD23	5	0.69
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD13	7	0.69
(1,310)	1:450:A:ILE:HD12	1:450:A:ILE:HA	10	0.69
(1,267)	1:363:A:ILE:HG22	1:412:A:LEU:HG	3	0.69
(1,2932)	1:420:A:ASP:H	1:422:A:ILE:HB	1	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2932)	1:420:A:ASP:H	1:422:A:ILE:HB	15	0.68
(1,2884)	1:397:A:TYR:HE1	1:397:A:TYR:HA	3	0.68
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	13	0.68
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD11	7	0.68
(1,2805)	1:372:A:LEU:HD21	1:373:A:ALA:H	6	0.68
(1,2805)	1:372:A:LEU:HD21	1:373:A:ALA:H	14	0.68
(1,2805)	1:372:A:LEU:HD21	1:373:A:ALA:H	15	0.68
(1,2805)	1:372:A:LEU:HD21	1:373:A:ALA:H	19	0.68
(1,2793)	1:433:A:LEU:HD21	1:429:A:ARG:HA	18	0.68
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD13	3	0.68
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD12	12	0.68
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD13	18	0.68
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE3	8	0.68
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE3	9	0.68
(1,2694)	1:438:A:LEU:HD12	1:434:A:GLU:HA	7	0.68
(1,2645)	1:402:A:ILE:HD12	1:338:A:TRP:HB3	6	0.68
(1,2645)	1:402:A:ILE:HD13	1:338:A:TRP:HB3	16	0.68
(1,2644)	1:402:A:ILE:HD13	1:397:A:TYR:HE1	9	0.68
(1,2640)	1:400:A:LEU:HD21	1:402:A:ILE:HD12	1	0.68
(1,2640)	1:400:A:LEU:HD22	1:402:A:ILE:HD11	6	0.68
(1,2633)	1:394:A:LEU:HD13	1:366:A:ILE:HD12	2	0.68
(1,2618)	1:375:A:LEU:HD23	1:378:A:ASN:HB2	18	0.68
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	5	0.68
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	14	0.68
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	17	0.68
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	15	0.68
(1,2423)	1:441:A:GLN:H	1:441:A:GLN:HB2	7	0.68
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	2	0.68
(1,2324)	1:352:A:ASN:HD21	1:367:A:VAL:HG21	10	0.68
(1,2258)	1:450:A:ILE:H	1:450:A:ILE:HG13	8	0.68
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	10	0.68
(1,2167)	1:392:A:ARG:H	1:392:A:ARG:HG2	10	0.68
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG22	3	0.68
(1,1917)	1:394:A:LEU:HD11	1:366:A:ILE:HD12	10	0.68
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB1	2	0.68
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB2	12	0.68
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB3	14	0.68
(1,1774)	1:337:A:LEU:HD11	1:393:A:ALA:HB3	3	0.68
(1,1774)	1:337:A:LEU:HD11	1:393:A:ALA:HB3	13	0.68
(1,1402)	1:383:A:THR:HG22	1:384:A:ASN:HD21	16	0.68
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	5	0.68
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD23	2	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1356)	1:394:A:LEU:HD23	1:338:A:TRP:HB3	17	0.68
(1,1330)	1:400:A:LEU:HD11	1:399:A:LYS:HB2	3	0.68
(1,1330)	1:400:A:LEU:HD13	1:399:A:LYS:HB2	10	0.68
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG22	2	0.68
(1,1142)	1:450:A:ILE:HD13	1:454:A:VAL:HA	18	0.68
(1,1119)	1:367:A:VAL:HG23	1:355:A:ARG:HA	15	0.68
(1,1113)	1:411:A:LEU:HD11	1:369:A:PRO:HB2	6	0.68
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	10	0.68
(1,843)	1:430:A:LEU:HD21	1:336:A:LEU:HD13	12	0.68
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	1	0.68
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD11	4	0.68
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD12	14	0.68
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD11	9	0.68
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD12	14	0.68
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD12	14	0.68
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD12	16	0.68
(1,267)	1:363:A:ILE:HG22	1:412:A:LEU:HG	2	0.68
(1,265)	1:363:A:ILE:HG21	1:412:A:LEU:HA	15	0.68
(1,35)	1:341:A:VAL:HG11	1:345:A:LEU:HD12	2	0.68
(1,35)	1:341:A:VAL:HG11	1:345:A:LEU:HD13	15	0.68
(1,2879)	1:344:A:LEU:HD12	1:350:A:TYR:HE2	3	0.67
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	1	0.67
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	8	0.67
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	9	0.67
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD11	16	0.67
(1,2813)	1:418:A:THR:HG22	1:362:A:LYS:HD2	17	0.67
(1,2806)	1:430:A:LEU:HD13	1:431:A:GLU:HG2	19	0.67
(1,2805)	1:372:A:LEU:HD23	1:373:A:ALA:H	5	0.67
(1,2805)	1:372:A:LEU:HD22	1:373:A:ALA:H	7	0.67
(1,2805)	1:372:A:LEU:HD21	1:373:A:ALA:H	17	0.67
(1,2799)	1:412:A:LEU:HD22	1:365:A:ARG:HD3	3	0.67
(1,2768)	1:394:A:LEU:HD11	1:387:A:TYR:HD1	6	0.67
(1,2768)	1:394:A:LEU:HD11	1:387:A:TYR:HD1	17	0.67
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	15	0.67
(1,2748)	1:359:A:LYS:HA	1:358:A:ASP:HB3	15	0.67
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG21	1	0.67
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG23	3	0.67
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG22	8	0.67
(1,2555)	1:340:A:TYR:HA	1:343:A:GLN:HG2	10	0.67
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG21	4	0.67
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG21	4	0.67
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG22	5	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	1	0.67
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	18	0.67
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	19	0.67
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	3	0.67
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	4	0.67
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	13	0.67
(1,1923)	1:344:A:LEU:HD21	1:375:A:LEU:HD23	1	0.67
(1,1906)	1:451:A:ALA:HB3	1:449:A:THR:HG22	18	0.67
(1,1804)	1:422:A:ILE:HD11	1:336:A:LEU:HD13	13	0.67
(1,1776)	1:337:A:LEU:HD13	1:390:A:MET:HG3	7	0.67
(1,1774)	1:337:A:LEU:HD12	1:393:A:ALA:HB3	1	0.67
(1,1690)	1:402:A:ILE:HD11	1:400:A:LEU:HA	7	0.67
(1,1541)	1:445:A:GLU:HA	1:443:A:TYR:HD1	18	0.67
(1,1444)	1:442:A:THR:HG21	1:443:A:TYR:HA	7	0.67
(1,1393)	1:386:A:THR:HG22	1:388:A:GLU:HB3	8	0.67
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD22	9	0.67
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	11	0.67
(1,1330)	1:400:A:LEU:HD13	1:399:A:LYS:HB2	14	0.67
(1,1330)	1:400:A:LEU:HD13	1:399:A:LYS:HB2	17	0.67
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG23	12	0.67
(1,1113)	1:411:A:LEU:HD13	1:369:A:PRO:HB2	4	0.67
(1,1032)	1:348:A:SER:HB3	1:351:A:GLU:HG2	2	0.67
(1,933)	1:443:A:TYR:HB3	1:443:A:TYR:HD1	9	0.67
(1,933)	1:443:A:TYR:HB3	1:443:A:TYR:HD1	19	0.67
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	14	0.67
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD12	17	0.67
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD11	2	0.67
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD11	3	0.67
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD12	4	0.67
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD12	10	0.67
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD12	15	0.67
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD12	13	0.67
(1,267)	1:363:A:ILE:HG23	1:412:A:LEU:HG	9	0.67
(1,265)	1:363:A:ILE:HG21	1:412:A:LEU:HA	4	0.67
(1,232)	1:359:A:LYS:HG2	1:359:A:LYS:HE3	14	0.67
(1,172)	1:354:A:ILE:HG22	1:350:A:TYR:HD1	3	0.67
(1,172)	1:354:A:ILE:HG23	1:350:A:TYR:HD1	17	0.67
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	19	0.67
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	19	0.67
(1,35)	1:341:A:VAL:HG13	1:345:A:LEU:HD13	19	0.67
(1,2880)	1:402:A:ILE:HG23	1:397:A:TYR:HE2	18	0.66
(1,2876)	1:372:A:LEU:HD12	1:374:A:ARG:H	5	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	5	0.66
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	10	0.66
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	11	0.66
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	14	0.66
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	19	0.66
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD11	2	0.66
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD11	3	0.66
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD12	15	0.66
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD11	17	0.66
(1,2813)	1:418:A:THR:HG21	1:362:A:LYS:HD2	10	0.66
(1,2806)	1:430:A:LEU:HD13	1:431:A:GLU:HG2	11	0.66
(1,2806)	1:430:A:LEU:HD11	1:431:A:GLU:HG2	17	0.66
(1,2805)	1:372:A:LEU:HD21	1:373:A:ALA:H	1	0.66
(1,2805)	1:372:A:LEU:HD22	1:373:A:ALA:H	2	0.66
(1,2805)	1:372:A:LEU:HD23	1:373:A:ALA:H	8	0.66
(1,2805)	1:372:A:LEU:HD23	1:373:A:ALA:H	16	0.66
(1,2799)	1:412:A:LEU:HD23	1:365:A:ARG:HD3	1	0.66
(1,2793)	1:433:A:LEU:HD21	1:429:A:ARG:HA	10	0.66
(1,2768)	1:394:A:LEU:HD13	1:387:A:TYR:HD1	16	0.66
(1,2748)	1:359:A:LYS:HA	1:358:A:ASP:HB3	1	0.66
(1,2737)	1:361:A:SER:HB3	1:363:A:ILE:HG22	18	0.66
(1,2681)	1:418:A:THR:HG22	1:342:A:TYR:HD1	7	0.66
(1,2681)	1:418:A:THR:HG23	1:342:A:TYR:HD1	12	0.66
(1,2644)	1:402:A:ILE:HD12	1:397:A:TYR:HE1	5	0.66
(1,2640)	1:400:A:LEU:HD22	1:402:A:ILE:HD12	3	0.66
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	13	0.66
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG21	8	0.66
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG23	10	0.66
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG22	12	0.66
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG23	16	0.66
(1,2569)	1:349:A:ARG:HD3	1:350:A:TYR:HE2	6	0.66
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	4	0.66
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	8	0.66
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	6	0.66
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	7	0.66
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	12	0.66
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	8	0.66
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD23	17	0.66
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	10	0.66
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	13	0.66
(1,2258)	1:450:A:ILE:H	1:450:A:ILE:HG13	3	0.66
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	8	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD23	14	0.66
(1,1923)	1:344:A:LEU:HD21	1:375:A:LEU:HD23	2	0.66
(1,1923)	1:344:A:LEU:HD21	1:375:A:LEU:HD22	3	0.66
(1,1923)	1:344:A:LEU:HD21	1:375:A:LEU:HD23	10	0.66
(1,1804)	1:422:A:ILE:HD12	1:336:A:LEU:HD12	4	0.66
(1,1690)	1:402:A:ILE:HD13	1:400:A:LEU:HA	17	0.66
(1,1522)	1:422:A:ILE:HG23	1:430:A:LEU:HG	5	0.66
(1,1484)	1:432:A:HIS:HB3	1:430:A:LEU:H	2	0.66
(1,1424)	1:450:A:ILE:HG21	1:452:A:SER:HB2	2	0.66
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD22	7	0.66
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	3	0.66
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	9	0.66
(1,1182)	1:363:A:ILE:HD12	1:406:A:GLU:HG2	3	0.66
(1,1182)	1:363:A:ILE:HD11	1:406:A:GLU:HG2	16	0.66
(1,1133)	1:367:A:VAL:HG11	1:352:A:ASN:HB3	18	0.66
(1,1093)	1:369:A:PRO:HA	1:387:A:TYR:HB3	13	0.66
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	2	0.66
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	4	0.66
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	6	0.66
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	7	0.66
(1,1025)	1:336:A:LEU:HD23	1:430:A:LEU:H	4	0.66
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	16	0.66
(1,624)	1:403:A:ILE:HG21	1:397:A:TYR:HB3	3	0.66
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD12	1	0.66
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD11	3	0.66
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD12	5	0.66
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD12	6	0.66
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD13	7	0.66
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD12	10	0.66
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD12	11	0.66
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD12	13	0.66
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD12	16	0.66
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD12	18	0.66
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD13	11	0.66
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD12	16	0.66
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD13	19	0.66
(1,456)	1:386:A:THR:HG21	1:387:A:TYR:HB2	17	0.66
(1,332)	1:369:A:PRO:HD2	1:411:A:LEU:HD11	2	0.66
(1,267)	1:363:A:ILE:HG22	1:412:A:LEU:HG	5	0.66
(1,267)	1:363:A:ILE:HG23	1:412:A:LEU:HG	11	0.66
(1,267)	1:363:A:ILE:HG22	1:412:A:LEU:HG	13	0.66
(1,267)	1:363:A:ILE:HG23	1:412:A:LEU:HG	17	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:363:A:ILE:HG23	1:412:A:LEU:HG	19	0.66
(1,87)	1:346:A:SER:H	1:346:A:SER:HB2	9	0.66
(1,87)	1:346:A:SER:H	1:346:A:SER:HB2	10	0.66
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	3	0.66
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	4	0.66
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	5	0.66
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	6	0.66
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	7	0.66
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	8	0.66
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	9	0.66
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	10	0.66
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	11	0.66
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	12	0.66
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	13	0.66
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	14	0.66
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	15	0.66
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	16	0.66
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	18	0.66
(1,35)	1:341:A:VAL:HG12	1:345:A:LEU:HD13	8	0.66
(1,5)	1:337:A:LEU:HD21	1:390:A:MET:HG3	18	0.66
(1,2981)	1:413:A:PHE:H	1:412:A:LEU:HG	13	0.65
(1,2981)	1:413:A:PHE:H	1:412:A:LEU:HG	19	0.65
(1,2880)	1:402:A:ILE:HG21	1:397:A:TYR:HE2	15	0.65
(1,2876)	1:372:A:LEU:HD11	1:374:A:ARG:H	4	0.65
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	2	0.65
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	12	0.65
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	18	0.65
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD11	6	0.65
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD11	19	0.65
(1,2805)	1:372:A:LEU:HD22	1:373:A:ALA:H	10	0.65
(1,2805)	1:372:A:LEU:HD22	1:373:A:ALA:H	12	0.65
(1,2797)	1:433:A:LEU:HD11	1:434:A:GLU:HA	1	0.65
(1,2797)	1:433:A:LEU:HD12	1:434:A:GLU:HA	5	0.65
(1,2797)	1:433:A:LEU:HD12	1:434:A:GLU:HA	6	0.65
(1,2793)	1:433:A:LEU:HD22	1:429:A:ARG:HA	6	0.65
(1,2791)	1:380:A:LYS:HE3	1:438:A:LEU:HD23	15	0.65
(1,2768)	1:394:A:LEU:HD11	1:387:A:TYR:HD1	11	0.65
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD12	6	0.65
(1,2726)	1:367:A:VAL:HG11	1:365:A:ARG:HD2	15	0.65
(1,2725)	1:354:A:ILE:HG13	1:367:A:VAL:HG23	17	0.65
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG21	1	0.65
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG22	3	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG22	4	0.65
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG23	7	0.65
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG22	9	0.65
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB2	8	0.65
(1,2597)	1:358:A:ASP:HB3	1:363:A:ILE:HG23	15	0.65
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG21	9	0.65
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG22	14	0.65
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	5	0.65
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	6	0.65
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	7	0.65
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	14	0.65
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	15	0.65
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD11	7	0.65
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD13	8	0.65
(1,2473)	1:409:A:GLN:HE21	1:412:A:LEU:HD11	12	0.65
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	15	0.65
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	16	0.65
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD22	8	0.65
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	19	0.65
(1,2333)	1:364:A:PHE:H	1:364:A:PHE:HD2	8	0.65
(1,2325)	1:372:A:LEU:H	1:353:A:PHE:HE1	13	0.65
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	19	0.65
(1,1923)	1:344:A:LEU:HD21	1:375:A:LEU:HD21	18	0.65
(1,1917)	1:394:A:LEU:HD12	1:366:A:ILE:HD12	11	0.65
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB1	15	0.65
(1,1804)	1:422:A:ILE:HD13	1:336:A:LEU:HD12	3	0.65
(1,1782)	1:337:A:LEU:HD11	1:397:A:TYR:HE2	18	0.65
(1,1776)	1:337:A:LEU:HD12	1:390:A:MET:HG3	10	0.65
(1,1774)	1:337:A:LEU:HD13	1:393:A:ALA:HB2	2	0.65
(1,1774)	1:337:A:LEU:HD13	1:393:A:ALA:HB2	10	0.65
(1,1609)	1:411:A:LEU:HD21	1:387:A:TYR:HB2	3	0.65
(1,1523)	1:422:A:ILE:HG23	1:426:A:ARG:HG2	13	0.65
(1,1484)	1:432:A:HIS:HB3	1:430:A:LEU:H	1	0.65
(1,1476)	1:433:A:LEU:HD23	1:433:A:LEU:HA	17	0.65
(1,1448)	1:442:A:THR:HG21	1:456:A:TRP:HB3	4	0.65
(1,1424)	1:450:A:ILE:HG22	1:452:A:SER:HB2	3	0.65
(1,1357)	1:394:A:LEU:HD22	1:390:A:MET:HG3	3	0.65
(1,1357)	1:394:A:LEU:HD22	1:390:A:MET:HG3	14	0.65
(1,1330)	1:400:A:LEU:HD12	1:399:A:LYS:HB2	6	0.65
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD22	13	0.65
(1,1201)	1:363:A:ILE:HG13	1:361:A:SER:HB2	5	0.65
(1,1113)	1:411:A:LEU:HD13	1:369:A:PRO:HB2	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1025)	1:336:A:LEU:HD21	1:430:A:LEU:H	3	0.65
(1,1025)	1:336:A:LEU:HD22	1:430:A:LEU:H	13	0.65
(1,950)	1:448:A:PRO:HD2	1:448:A:PRO:HA	17	0.65
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	1	0.65
(1,932)	1:443:A:TYR:HB2	1:443:A:TYR:HD2	9	0.65
(1,927)	1:441:A:GLN:H	1:441:A:GLN:HG2	13	0.65
(1,843)	1:430:A:LEU:HD21	1:336:A:LEU:HD11	4	0.65
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	17	0.65
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD13	15	0.65
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD11	12	0.65
(1,458)	1:386:A:THR:HG23	1:389:A:LYS:HD2	14	0.65
(1,458)	1:386:A:THR:HG23	1:389:A:LYS:HD2	18	0.65
(1,455)	1:386:A:THR:HG21	1:389:A:LYS:HE3	19	0.65
(1,267)	1:363:A:ILE:HG23	1:412:A:LEU:HG	7	0.65
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	1	0.65
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	2	0.65
(1,56)	1:448:A:PRO:HG2	1:448:A:PRO:HD3	17	0.65
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	6	0.65
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	7	0.65
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD22	10	0.65
(1,2981)	1:413:A:PHE:H	1:412:A:LEU:HG	2	0.64
(1,2981)	1:413:A:PHE:H	1:412:A:LEU:HG	17	0.64
(1,2887)	1:336:A:LEU:H	1:336:A:LEU:HD11	12	0.64
(1,2884)	1:397:A:TYR:HE1	1:393:A:ALA:HA	12	0.64
(1,2880)	1:402:A:ILE:HG22	1:397:A:TYR:HE2	8	0.64
(1,2880)	1:402:A:ILE:HG22	1:397:A:TYR:HE2	9	0.64
(1,2880)	1:402:A:ILE:HG21	1:397:A:TYR:HE2	10	0.64
(1,2862)	1:379:A:HIS:HB3	1:340:A:TYR:HE1	2	0.64
(1,2858)	1:341:A:VAL:HG11	1:340:A:TYR:HD2	10	0.64
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	3	0.64
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	4	0.64
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	15	0.64
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD12	4	0.64
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD11	9	0.64
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD11	14	0.64
(1,2805)	1:372:A:LEU:HD23	1:373:A:ALA:H	3	0.64
(1,2805)	1:372:A:LEU:HD22	1:373:A:ALA:H	13	0.64
(1,2789)	1:438:A:LEU:HD12	1:381:A:ASN:HD22	8	0.64
(1,2789)	1:438:A:LEU:HD13	1:444:A:GLN:HE22	17	0.64
(1,2770)	1:373:A:ALA:HB3	1:371:A:GLY:H	7	0.64
(1,2770)	1:373:A:ALA:HB1	1:371:A:GLY:H	9	0.64
(1,2768)	1:394:A:LEU:HD12	1:387:A:TYR:HD1	3	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2644)	1:402:A:ILE:HD13	1:397:A:TYR:HE1	12	0.64
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG23	2	0.64
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG21	6	0.64
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG22	13	0.64
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG21	14	0.64
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG22	17	0.64
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG21	10	0.64
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG21	15	0.64
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	1	0.64
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	2	0.64
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	10	0.64
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	12	0.64
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	13	0.64
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	16	0.64
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD11	15	0.64
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	7	0.64
(1,2420)	1:443:A:TYR:H	1:443:A:TYR:HB2	9	0.64
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	8	0.64
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD23	15	0.64
(1,2258)	1:450:A:ILE:H	1:450:A:ILE:HG13	16	0.64
(1,2220)	1:413:A:PHE:H	1:413:A:PHE:HD2	13	0.64
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	1	0.64
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	6	0.64
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	8	0.64
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	18	0.64
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG22	3	0.64
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG21	9	0.64
(1,1923)	1:344:A:LEU:HD22	1:375:A:LEU:HD22	16	0.64
(1,1923)	1:344:A:LEU:HD23	1:375:A:LEU:HD23	17	0.64
(1,1917)	1:394:A:LEU:HD11	1:366:A:ILE:HD11	15	0.64
(1,1774)	1:337:A:LEU:HD13	1:393:A:ALA:HB2	8	0.64
(1,1774)	1:337:A:LEU:HD11	1:393:A:ALA:HB1	17	0.64
(1,1690)	1:402:A:ILE:HD13	1:400:A:LEU:HA	5	0.64
(1,1609)	1:411:A:LEU:HD22	1:387:A:TYR:HB2	6	0.64
(1,1609)	1:411:A:LEU:HD23	1:387:A:TYR:HB2	18	0.64
(1,1471)	1:433:A:LEU:HA	1:436:A:GLN:HG3	4	0.64
(1,1444)	1:442:A:THR:HG21	1:443:A:TYR:HA	16	0.64
(1,1360)	1:392:A:ARG:HD2	1:392:A:ARG:HB3	18	0.64
(1,1330)	1:400:A:LEU:HD13	1:399:A:LYS:HB2	8	0.64
(1,1133)	1:367:A:VAL:HG13	1:352:A:ASN:HB3	15	0.64
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	5	0.64
(1,1024)	1:336:A:LEU:HD22	1:338:A:TRP:HZ2	2	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,932)	1:443:A:TYR:HB2	1:443:A:TYR:HD2	19	0.64
(1,884)	1:437:A:VAL:HG21	1:392:A:ARG:HG3	18	0.64
(1,865)	1:438:A:LEU:HD12	1:380:A:LYS:HE3	2	0.64
(1,843)	1:430:A:LEU:HD21	1:336:A:LEU:HD13	7	0.64
(1,843)	1:430:A:LEU:HD22	1:336:A:LEU:HD11	15	0.64
(1,803)	1:426:A:ARG:H	1:426:A:ARG:HG2	5	0.64
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	5	0.64
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	6	0.64
(1,715)	1:414:A:ARG:HD2	1:414:A:ARG:HH12	11	0.64
(1,591)	1:400:A:LEU:HA	1:400:A:LEU:HD13	2	0.64
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD11	18	0.64
(1,265)	1:363:A:ILE:HG23	1:412:A:LEU:HA	13	0.64
(1,180)	1:355:A:ARG:HB2	1:355:A:ARG:HD2	12	0.64
(1,88)	1:346:A:SER:HB2	1:346:A:SER:HA	5	0.64
(1,88)	1:346:A:SER:HB2	1:346:A:SER:HA	18	0.64
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	16	0.64
(1,35)	1:341:A:VAL:HG12	1:345:A:LEU:HD12	14	0.64
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD23	6	0.64
(1,2981)	1:413:A:PHE:H	1:412:A:LEU:HG	9	0.63
(1,2981)	1:413:A:PHE:H	1:412:A:LEU:HG	10	0.63
(1,2981)	1:413:A:PHE:H	1:412:A:LEU:HG	11	0.63
(1,2981)	1:413:A:PHE:H	1:412:A:LEU:HG	18	0.63
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD23	4	0.63
(1,2884)	1:397:A:TYR:HE1	1:397:A:TYR:HA	9	0.63
(1,2880)	1:402:A:ILE:HG23	1:397:A:TYR:HE2	12	0.63
(1,2876)	1:372:A:LEU:HD13	1:374:A:ARG:H	17	0.63
(1,2857)	1:418:A:THR:HG21	1:342:A:TYR:HE1	16	0.63
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	7	0.63
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	16	0.63
(1,2829)	1:412:A:LEU:H	1:412:A:LEU:HD11	5	0.63
(1,2805)	1:372:A:LEU:HD21	1:373:A:ALA:H	4	0.63
(1,2770)	1:373:A:ALA:HB1	1:371:A:GLY:H	6	0.63
(1,2770)	1:373:A:ALA:HB3	1:371:A:GLY:H	10	0.63
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	11	0.63
(1,2729)	1:366:A:ILE:HG13	1:413:A:PHE:HZ	4	0.63
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG23	9	0.63
(1,2681)	1:418:A:THR:HG21	1:342:A:TYR:HD1	10	0.63
(1,2675)	1:417:A:LYS:HD2	1:402:A:ILE:HG13	14	0.63
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	1	0.63
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG21	19	0.63
(1,2547)	1:442:A:THR:H	1:442:A:THR:HG23	18	0.63
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	3	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	19	0.63
(1,2473)	1:409:A:GLN:HE21	1:412:A:LEU:HD12	2	0.63
(1,2437)	1:433:A:LEU:H	1:433:A:LEU:HB2	17	0.63
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	13	0.63
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	6	0.63
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	10	0.63
(1,2258)	1:450:A:ILE:H	1:450:A:ILE:HG13	2	0.63
(1,2254)	1:443:A:TYR:H	1:443:A:TYR:HD2	16	0.63
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG22	1	0.63
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG22	2	0.63
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	5	0.63
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	12	0.63
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	16	0.63
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG22	1	0.63
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG23	11	0.63
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG21	15	0.63
(1,1923)	1:344:A:LEU:HD21	1:375:A:LEU:HD22	4	0.63
(1,1923)	1:344:A:LEU:HD22	1:375:A:LEU:HD23	13	0.63
(1,1917)	1:394:A:LEU:HD12	1:366:A:ILE:HD12	19	0.63
(1,1906)	1:451:A:ALA:HB2	1:449:A:THR:HG22	16	0.63
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	16	0.63
(1,1774)	1:337:A:LEU:HD13	1:393:A:ALA:HB3	16	0.63
(1,1686)	1:402:A:ILE:HG23	1:403:A:ILE:HG12	16	0.63
(1,1653)	1:404:A:ARG:HG2	1:414:A:ARG:HD3	14	0.63
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	12	0.63
(1,1484)	1:432:A:HIS:HB2	1:430:A:LEU:H	12	0.63
(1,1442)	1:443:A:TYR:HE2	1:445:A:GLU:HG2	12	0.63
(1,1393)	1:386:A:THR:HG22	1:388:A:GLU:HB3	15	0.63
(1,1357)	1:394:A:LEU:HD21	1:390:A:MET:HG3	19	0.63
(1,1356)	1:394:A:LEU:HD23	1:338:A:TRP:HB3	16	0.63
(1,1330)	1:400:A:LEU:HD11	1:399:A:LYS:HB2	9	0.63
(1,1182)	1:363:A:ILE:HD11	1:406:A:GLU:HG2	8	0.63
(1,1119)	1:367:A:VAL:HG21	1:355:A:ARG:HA	8	0.63
(1,1101)	1:369:A:PRO:HB2	1:387:A:TYR:HD1	13	0.63
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	9	0.63
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	18	0.63
(1,1045)	1:349:A:ARG:HG2	1:349:A:ARG:HD2	1	0.63
(1,1045)	1:349:A:ARG:HG2	1:349:A:ARG:HD2	4	0.63
(1,1045)	1:349:A:ARG:HG2	1:349:A:ARG:HD2	8	0.63
(1,1045)	1:349:A:ARG:HG2	1:349:A:ARG:HD2	9	0.63
(1,1045)	1:349:A:ARG:HG2	1:349:A:ARG:HD2	14	0.63
(1,1045)	1:349:A:ARG:HG2	1:349:A:ARG:HD2	16	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:449:A:THR:H	1:449:A:THR:HG23	13	0.63
(1,958)	1:449:A:THR:H	1:449:A:THR:HG21	18	0.63
(1,843)	1:430:A:LEU:HD23	1:336:A:LEU:HD11	3	0.63
(1,512)	1:394:A:LEU:HA	1:394:A:LEU:HD13	17	0.63
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	1	0.63
(1,458)	1:386:A:THR:HG22	1:389:A:LYS:HD2	7	0.63
(1,458)	1:386:A:THR:HG22	1:389:A:LYS:HD2	9	0.63
(1,458)	1:386:A:THR:HG22	1:389:A:LYS:HD2	10	0.63
(1,458)	1:386:A:THR:HG23	1:389:A:LYS:HD2	19	0.63
(1,455)	1:386:A:THR:HG23	1:389:A:LYS:HE3	8	0.63
(1,267)	1:363:A:ILE:HG23	1:412:A:LEU:HG	4	0.63
(1,267)	1:363:A:ILE:HG21	1:412:A:LEU:HG	8	0.63
(1,267)	1:363:A:ILE:HG21	1:412:A:LEU:HG	12	0.63
(1,180)	1:355:A:ARG:HB2	1:355:A:ARG:HD2	6	0.63
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD12	1	0.63
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD12	3	0.63
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD11	5	0.63
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	12	0.63
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	17	0.63
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD22	2	0.63
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD22	14	0.63
(1,2981)	1:413:A:PHE:H	1:412:A:LEU:HG	4	0.62
(1,2981)	1:428:A:ASP:H	1:427:A:THR:HG21	6	0.62
(1,2981)	1:413:A:PHE:H	1:412:A:LEU:HG	15	0.62
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	2	0.62
(1,2880)	1:402:A:ILE:HG23	1:397:A:TYR:HE2	17	0.62
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	6	0.62
(1,2840)	1:403:A:ILE:HG23	1:416:A:MET:H	1	0.62
(1,2797)	1:433:A:LEU:HD12	1:434:A:GLU:HA	7	0.62
(1,2797)	1:433:A:LEU:HD13	1:434:A:GLU:HA	16	0.62
(1,2793)	1:433:A:LEU:HD21	1:429:A:ARG:HA	8	0.62
(1,2786)	1:446:A:ASP:H	1:445:A:GLU:HG2	3	0.62
(1,2770)	1:373:A:ALA:HB3	1:371:A:GLY:H	14	0.62
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	10	0.62
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD13	2	0.62
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD12	19	0.62
(1,2726)	1:367:A:VAL:HG13	1:355:A:ARG:HD3	3	0.62
(1,2683)	1:429:A:ARG:HG3	1:429:A:ARG:H	4	0.62
(1,2683)	1:429:A:ARG:HG3	1:429:A:ARG:H	16	0.62
(1,2681)	1:418:A:THR:HG21	1:342:A:TYR:HD1	3	0.62
(1,2681)	1:418:A:THR:HG22	1:342:A:TYR:HD1	4	0.62
(1,2644)	1:402:A:ILE:HD11	1:397:A:TYR:HE1	3	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2644)	1:402:A:ILE:HD12	1:397:A:TYR:HE1	19	0.62
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB2	10	0.62
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG21	7	0.62
(1,2550)	1:451:A:ALA:H	1:450:A:ILE:HG23	1	0.62
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	9	0.62
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD13	13	0.62
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	19	0.62
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	3	0.62
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	11	0.62
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	10	0.62
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	17	0.62
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD23	11	0.62
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG21	4	0.62
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG21	6	0.62
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG21	7	0.62
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG21	16	0.62
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG22	17	0.62
(1,1923)	1:344:A:LEU:HD23	1:375:A:LEU:HD21	7	0.62
(1,1923)	1:344:A:LEU:HD23	1:375:A:LEU:HD23	9	0.62
(1,1923)	1:344:A:LEU:HD21	1:375:A:LEU:HD22	14	0.62
(1,1923)	1:344:A:LEU:HD21	1:375:A:LEU:HD23	19	0.62
(1,1918)	1:354:A:ILE:HD12	1:366:A:ILE:HD12	18	0.62
(1,1917)	1:394:A:LEU:HD13	1:366:A:ILE:HD12	2	0.62
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	2	0.62
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	5	0.62
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	6	0.62
(1,1798)	1:336:A:LEU:H	1:336:A:LEU:HD13	10	0.62
(1,1671)	1:403:A:ILE:HG23	1:405:A:LYS:HA	18	0.62
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	7	0.62
(1,1609)	1:411:A:LEU:HD21	1:387:A:TYR:HB2	10	0.62
(1,1450)	1:442:A:THR:HG23	1:445:A:GLU:HB3	11	0.62
(1,1402)	1:383:A:THR:HG22	1:384:A:ASN:HD21	5	0.62
(1,1356)	1:394:A:LEU:HD23	1:338:A:TRP:HB3	8	0.62
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	2	0.62
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	3	0.62
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	9	0.62
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	12	0.62
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	16	0.62
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	17	0.62
(1,1330)	1:400:A:LEU:HD12	1:399:A:LYS:HB2	1	0.62
(1,1330)	1:400:A:LEU:HD11	1:399:A:LYS:HB2	7	0.62
(1,1330)	1:400:A:LEU:HD13	1:399:A:LYS:HB2	11	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1330)	1:400:A:LEU:HD13	1:399:A:LYS:HB2	12	0.62
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	3	0.62
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD21	15	0.62
(1,1201)	1:363:A:ILE:HG13	1:361:A:SER:HB2	13	0.62
(1,1201)	1:363:A:ILE:HG13	1:361:A:SER:HB2	17	0.62
(1,1182)	1:363:A:ILE:HD12	1:406:A:GLU:HG2	5	0.62
(1,1182)	1:363:A:ILE:HD13	1:406:A:GLU:HG2	13	0.62
(1,1164)	1:363:A:ILE:HG13	1:358:A:ASP:HB2	2	0.62
(1,1133)	1:367:A:VAL:HG11	1:352:A:ASN:HB3	9	0.62
(1,1133)	1:367:A:VAL:HG11	1:352:A:ASN:HB3	19	0.62
(1,1045)	1:349:A:ARG:HG2	1:349:A:ARG:HD2	5	0.62
(1,1045)	1:349:A:ARG:HG2	1:349:A:ARG:HD2	7	0.62
(1,1045)	1:349:A:ARG:HG2	1:349:A:ARG:HD2	10	0.62
(1,1045)	1:349:A:ARG:HG2	1:349:A:ARG:HD2	11	0.62
(1,1045)	1:349:A:ARG:HG2	1:349:A:ARG:HD2	18	0.62
(1,865)	1:438:A:LEU:HD13	1:380:A:LYS:HE3	9	0.62
(1,547)	1:395:A:ARG:HD2	1:395:A:ARG:H	3	0.62
(1,457)	1:386:A:THR:HG21	1:389:A:LYS:HB2	13	0.62
(1,358)	1:374:A:ARG:HA	1:374:A:ARG:HD2	6	0.62
(1,267)	1:363:A:ILE:HG23	1:412:A:LEU:HG	10	0.62
(1,265)	1:363:A:ILE:HG22	1:412:A:LEU:HA	6	0.62
(1,180)	1:355:A:ARG:HB2	1:355:A:ARG:HD2	2	0.62
(1,180)	1:355:A:ARG:HB2	1:355:A:ARG:HD2	10	0.62
(1,180)	1:355:A:ARG:HB2	1:355:A:ARG:HD2	11	0.62
(1,134)	1:351:A:GLU:HB3	1:351:A:GLU:HG2	17	0.62
(1,87)	1:346:A:SER:H	1:346:A:SER:HB2	19	0.62
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD11	17	0.62
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD22	3	0.62
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD22	8	0.62
(1,2984)	1:410:A:ARG:HE	1:367:A:VAL:HG21	14	0.61
(1,2981)	1:413:A:PHE:H	1:412:A:LEU:HG	7	0.61
(1,2981)	1:428:A:ASP:H	1:427:A:THR:HG23	8	0.61
(1,2981)	1:413:A:PHE:H	1:412:A:LEU:HG	14	0.61
(1,2981)	1:413:A:PHE:H	1:412:A:LEU:HG	16	0.61
(1,2884)	1:397:A:TYR:HE1	1:397:A:TYR:HA	11	0.61
(1,2880)	1:402:A:ILE:HG23	1:397:A:TYR:HE2	13	0.61
(1,2876)	1:372:A:LEU:HD13	1:374:A:ARG:H	7	0.61
(1,2855)	1:342:A:TYR:HE2	1:342:A:TYR:HB3	17	0.61
(1,2844)	1:402:A:ILE:HG23	1:397:A:TYR:HD2	11	0.61
(1,2828)	1:412:A:LEU:HD11	1:413:A:PHE:HD1	17	0.61
(1,2813)	1:418:A:THR:HG22	1:362:A:LYS:HD2	19	0.61
(1,2794)	1:433:A:LEU:HD23	1:429:A:ARG:HD3	14	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2793)	1:433:A:LEU:HD21	1:429:A:ARG:HA	5	0.61
(1,2770)	1:373:A:ALA:HB3	1:371:A:GLY:H	2	0.61
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB1	15	0.61
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB3	19	0.61
(1,2768)	1:394:A:LEU:HD13	1:387:A:TYR:HD1	14	0.61
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE2	19	0.61
(1,2726)	1:367:A:VAL:HG12	1:365:A:ARG:HD2	19	0.61
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG21	17	0.61
(1,2693)	1:437:A:VAL:HG11	1:396:A:HIS:HD2	17	0.61
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	11	0.61
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	16	0.61
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	19	0.61
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG22	11	0.61
(1,2606)	1:366:A:ILE:H	1:366:A:ILE:HG22	15	0.61
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG23	18	0.61
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	18	0.61
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	11	0.61
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	9	0.61
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	10	0.61
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	16	0.61
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD22	14	0.61
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	4	0.61
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	7	0.61
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG22	17	0.61
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	7	0.61
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	14	0.61
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD23	13	0.61
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG23	2	0.61
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG21	8	0.61
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG23	10	0.61
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG23	18	0.61
(1,1923)	1:344:A:LEU:HD23	1:375:A:LEU:HD23	15	0.61
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	8	0.61
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	11	0.61
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	12	0.61
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	19	0.61
(1,1776)	1:337:A:LEU:HD11	1:390:A:MET:HG3	1	0.61
(1,1671)	1:403:A:ILE:HG23	1:405:A:LYS:HA	3	0.61
(1,1484)	1:432:A:HIS:HB2	1:430:A:LEU:H	9	0.61
(1,1444)	1:442:A:THR:HG22	1:443:A:TYR:HA	8	0.61
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	9	0.61
(1,1430)	1:447:A:GLU:HB2	1:448:A:PRO:HD3	3	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	16	0.61
(1,1357)	1:394:A:LEU:HD23	1:390:A:MET:HG3	1	0.61
(1,1356)	1:394:A:LEU:HD21	1:338:A:TRP:HB3	1	0.61
(1,1356)	1:394:A:LEU:HD22	1:338:A:TRP:HB3	10	0.61
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	1	0.61
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	5	0.61
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	7	0.61
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	8	0.61
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	10	0.61
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	15	0.61
(1,1330)	1:400:A:LEU:HD13	1:399:A:LYS:HB2	13	0.61
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD23	19	0.61
(1,1133)	1:367:A:VAL:HG12	1:352:A:ASN:HB3	13	0.61
(1,1119)	1:367:A:VAL:HG22	1:355:A:ARG:HA	13	0.61
(1,1119)	1:367:A:VAL:HG21	1:355:A:ARG:HA	19	0.61
(1,1113)	1:411:A:LEU:HD11	1:369:A:PRO:HB2	2	0.61
(1,1113)	1:411:A:LEU:HD12	1:369:A:PRO:HB2	5	0.61
(1,1113)	1:411:A:LEU:HD12	1:369:A:PRO:HB2	14	0.61
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	8	0.61
(1,1045)	1:349:A:ARG:HG2	1:349:A:ARG:HD2	2	0.61
(1,1045)	1:349:A:ARG:HG2	1:349:A:ARG:HD2	6	0.61
(1,932)	1:443:A:TYR:HB2	1:443:A:TYR:HD2	5	0.61
(1,932)	1:443:A:TYR:HB2	1:443:A:TYR:HD2	13	0.61
(1,852)	1:431:A:GLU:H	1:431:A:GLU:HG2	13	0.61
(1,843)	1:430:A:LEU:HD23	1:336:A:LEU:HD13	8	0.61
(1,822)	1:429:A:ARG:HA	1:429:A:ARG:HG2	4	0.61
(1,822)	1:429:A:ARG:HA	1:429:A:ARG:HG2	16	0.61
(1,718)	1:414:A:ARG:HB3	1:414:A:ARG:HD3	7	0.61
(1,718)	1:414:A:ARG:HB2	1:414:A:ARG:HD3	11	0.61
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	15	0.61
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	17	0.61
(1,457)	1:386:A:THR:HG22	1:389:A:LYS:HB2	15	0.61
(1,267)	1:363:A:ILE:HG21	1:412:A:LEU:HG	6	0.61
(1,265)	1:363:A:ILE:HG23	1:412:A:LEU:HA	16	0.61
(1,134)	1:351:A:GLU:HB3	1:351:A:GLU:HG2	10	0.61
(1,87)	1:346:A:SER:H	1:346:A:SER:HB2	4	0.61
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD12	2	0.61
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD12	6	0.61
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD11	9	0.61
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	5	0.61
(1,35)	1:341:A:VAL:HG12	1:345:A:LEU:HD12	12	0.61
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD23	5	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD21	9	0.61
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD21	17	0.61
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	8	0.6
(1,2932)	1:420:A:ASP:H	1:422:A:ILE:HB	17	0.6
(1,2895)	1:353:A:PHE:H	1:367:A:VAL:HG21	18	0.6
(1,2884)	1:397:A:TYR:HE1	1:397:A:TYR:HA	4	0.6
(1,2828)	1:412:A:LEU:HD12	1:413:A:PHE:HD1	3	0.6
(1,2828)	1:412:A:LEU:HD11	1:413:A:PHE:HD1	19	0.6
(1,2799)	1:412:A:LEU:HD21	1:365:A:ARG:HD3	8	0.6
(1,2799)	1:412:A:LEU:HD23	1:365:A:ARG:HD3	10	0.6
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	2	0.6
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	4	0.6
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	7	0.6
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE2	2	0.6
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE3	3	0.6
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG23	16	0.6
(1,2696)	1:438:A:LEU:HD21	1:382:A:ARG:HD2	12	0.6
(1,2667)	1:414:A:ARG:HA	1:414:A:ARG:HD2	4	0.6
(1,2644)	1:402:A:ILE:HD12	1:397:A:TYR:HE1	8	0.6
(1,2618)	1:375:A:LEU:HD22	1:378:A:ASN:HB2	15	0.6
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	3	0.6
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG23	6	0.6
(1,2550)	1:451:A:ALA:H	1:450:A:ILE:HG23	13	0.6
(1,2547)	1:442:A:THR:H	1:442:A:THR:HG23	16	0.6
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG22	18	0.6
(1,2514)	1:444:A:GLN:H	1:444:A:GLN:HG3	11	0.6
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	11	0.6
(1,2507)	1:434:A:GLU:H	1:434:A:GLU:HB3	17	0.6
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	5	0.6
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	18	0.6
(1,2473)	1:409:A:GLN:HE21	1:412:A:LEU:HD13	13	0.6
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	15	0.6
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	19	0.6
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	2	0.6
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	9	0.6
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	18	0.6
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	12	0.6
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG21	5	0.6
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG23	12	0.6
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG21	13	0.6
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG23	14	0.6
(1,1923)	1:344:A:LEU:HD22	1:375:A:LEU:HD21	5	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1923)	1:344:A:LEU:HD23	1:375:A:LEU:HD22	12	0.6
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB3	6	0.6
(1,1873)	1:383:A:THR:HG22	1:384:A:ASN:HD22	11	0.6
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	1	0.6
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	3	0.6
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	4	0.6
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	18	0.6
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	1	0.6
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	9	0.6
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	11	0.6
(1,1523)	1:422:A:ILE:HG23	1:426:A:ARG:HG2	14	0.6
(1,1522)	1:422:A:ILE:HG22	1:430:A:LEU:HG	2	0.6
(1,1522)	1:422:A:ILE:HG22	1:430:A:LEU:HG	3	0.6
(1,1496)	1:430:A:LEU:HD23	1:427:A:THR:HA	2	0.6
(1,1393)	1:386:A:THR:HG22	1:388:A:GLU:HB3	17	0.6
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD23	15	0.6
(1,1357)	1:394:A:LEU:HD22	1:390:A:MET:HG3	7	0.6
(1,1349)	1:443:A:TYR:HE1	1:445:A:GLU:HA	14	0.6
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	6	0.6
(1,1330)	1:400:A:LEU:HD11	1:399:A:LYS:HB2	2	0.6
(1,1330)	1:400:A:LEU:HD13	1:399:A:LYS:HB2	5	0.6
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD21	17	0.6
(1,1133)	1:367:A:VAL:HG12	1:352:A:ASN:HB3	2	0.6
(1,1119)	1:367:A:VAL:HG22	1:355:A:ARG:HA	18	0.6
(1,1113)	1:411:A:LEU:HD12	1:369:A:PRO:HB2	3	0.6
(1,1113)	1:411:A:LEU:HD13	1:369:A:PRO:HB2	8	0.6
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	1	0.6
(1,820)	1:429:A:ARG:HA	1:432:A:HIS:HB2	6	0.6
(1,718)	1:414:A:ARG:HB3	1:414:A:ARG:HD3	4	0.6
(1,718)	1:414:A:ARG:HB2	1:414:A:ARG:HD3	5	0.6
(1,718)	1:414:A:ARG:HB3	1:414:A:ARG:HD3	10	0.6
(1,649)	1:405:A:LYS:HD2	1:405:A:LYS:HG3	1	0.6
(1,649)	1:405:A:LYS:HD2	1:405:A:LYS:HG3	2	0.6
(1,649)	1:405:A:LYS:HD2	1:405:A:LYS:HG3	4	0.6
(1,649)	1:405:A:LYS:HD2	1:405:A:LYS:HG3	6	0.6
(1,649)	1:405:A:LYS:HD2	1:405:A:LYS:HG3	12	0.6
(1,547)	1:395:A:ARG:HD2	1:395:A:ARG:H	10	0.6
(1,400)	1:377:A:GLY:HA3	1:382:A:ARG:HB3	8	0.6
(1,267)	1:363:A:ILE:HG23	1:412:A:LEU:HG	1	0.6
(1,267)	1:363:A:ILE:HG23	1:412:A:LEU:HG	15	0.6
(1,267)	1:363:A:ILE:HG22	1:412:A:LEU:HG	16	0.6
(1,265)	1:363:A:ILE:HG21	1:412:A:LEU:HA	19	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:355:A:ARG:HB2	1:355:A:ARG:HD2	19	0.6
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD13	8	0.6
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD13	10	0.6
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD11	12	0.6
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD11	14	0.6
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD11	15	0.6
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD13	16	0.6
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	13	0.6
(1,35)	1:341:A:VAL:HG11	1:345:A:LEU:HD13	11	0.6
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD21	7	0.6
(1,2981)	1:413:A:PHE:H	1:412:A:LEU:HG	12	0.59
(1,2974)	1:433:A:LEU:H	1:431:A:GLU:HB2	18	0.59
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	9	0.59
(1,2876)	1:372:A:LEU:HD12	1:374:A:ARG:H	12	0.59
(1,2813)	1:418:A:THR:HG21	1:362:A:LYS:HD2	18	0.59
(1,2806)	1:430:A:LEU:HD11	1:431:A:GLU:HG2	12	0.59
(1,2799)	1:412:A:LEU:HD21	1:365:A:ARG:HD3	19	0.59
(1,2770)	1:373:A:ALA:HB2	1:371:A:GLY:H	5	0.59
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	6	0.59
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE3	12	0.59
(1,2726)	1:367:A:VAL:HG13	1:355:A:ARG:HD3	8	0.59
(1,2667)	1:414:A:ARG:HA	1:414:A:ARG:HD2	10	0.59
(1,2640)	1:400:A:LEU:HD23	1:402:A:ILE:HD13	11	0.59
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	6	0.59
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG22	5	0.59
(1,2555)	1:340:A:TYR:HA	1:339:A:ASP:HB3	16	0.59
(1,2550)	1:451:A:ALA:H	1:450:A:ILE:HG22	10	0.59
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	2	0.59
(1,2423)	1:441:A:GLN:H	1:441:A:GLN:HB2	4	0.59
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	4	0.59
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD23	13	0.59
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	5	0.59
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG23	19	0.59
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	9	0.59
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	11	0.59
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD22	2	0.59
(1,1939)	1:341:A:VAL:H	1:341:A:VAL:HG22	19	0.59
(1,1923)	1:344:A:LEU:HD22	1:375:A:LEU:HD22	11	0.59
(1,1906)	1:451:A:ALA:HB1	1:449:A:THR:HG21	11	0.59
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	10	0.59
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	13	0.59
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	14	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1804)	1:422:A:ILE:HD12	1:336:A:LEU:HD12	16	0.59
(1,1776)	1:337:A:LEU:HD11	1:390:A:MET:HG3	6	0.59
(1,1661)	1:404:A:ARG:HG2	1:404:A:ARG:HD3	17	0.59
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	2	0.59
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD12	11	0.59
(1,1448)	1:442:A:THR:HG23	1:456:A:TRP:HB3	5	0.59
(1,1448)	1:442:A:THR:HG21	1:456:A:TRP:HB3	15	0.59
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD23	11	0.59
(1,1357)	1:394:A:LEU:HD21	1:390:A:MET:HG3	5	0.59
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	4	0.59
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	11	0.59
(1,1201)	1:363:A:ILE:HG13	1:361:A:SER:HB2	8	0.59
(1,1201)	1:363:A:ILE:HG13	1:361:A:SER:HB2	19	0.59
(1,1182)	1:363:A:ILE:HD13	1:406:A:GLU:HG2	10	0.59
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD13	18	0.59
(1,1119)	1:367:A:VAL:HG22	1:355:A:ARG:HA	1	0.59
(1,1119)	1:367:A:VAL:HG23	1:355:A:ARG:HA	5	0.59
(1,1119)	1:367:A:VAL:HG23	1:355:A:ARG:HA	9	0.59
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	12	0.59
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	16	0.59
(1,718)	1:414:A:ARG:HB3	1:414:A:ARG:HD3	1	0.59
(1,718)	1:414:A:ARG:HB2	1:414:A:ARG:HD3	14	0.59
(1,718)	1:414:A:ARG:HB3	1:414:A:ARG:HD3	16	0.59
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD12	17	0.59
(1,478)	1:389:A:LYS:HG3	1:389:A:LYS:HE2	4	0.59
(1,471)	1:388:A:GLU:HB3	1:388:A:GLU:HG2	2	0.59
(1,471)	1:388:A:GLU:HB3	1:388:A:GLU:HG2	6	0.59
(1,471)	1:388:A:GLU:HB3	1:388:A:GLU:HG2	10	0.59
(1,471)	1:388:A:GLU:HB3	1:388:A:GLU:HG2	15	0.59
(1,457)	1:386:A:THR:HG22	1:389:A:LYS:HB2	2	0.59
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD12	7	0.59
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD11	18	0.59
(1,35)	1:341:A:VAL:HG13	1:345:A:LEU:HD13	17	0.59
(1,2984)	1:410:A:ARG:HE	1:367:A:VAL:HG22	19	0.58
(1,2887)	1:336:A:LEU:H	1:336:A:LEU:HD13	10	0.58
(1,2884)	1:397:A:TYR:HE1	1:393:A:ALA:HA	2	0.58
(1,2806)	1:430:A:LEU:HD12	1:431:A:GLU:HG2	2	0.58
(1,2797)	1:433:A:LEU:HD11	1:434:A:GLU:HA	14	0.58
(1,2775)	1:387:A:TYR:HD2	1:390:A:MET:HG2	11	0.58
(1,2774)	1:443:A:TYR:HD1	1:445:A:GLU:HB2	7	0.58
(1,2770)	1:373:A:ALA:HB2	1:371:A:GLY:H	17	0.58
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	5	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2726)	1:367:A:VAL:HG11	1:355:A:ARG:HD3	18	0.58
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG23	5	0.58
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG23	15	0.58
(1,2667)	1:414:A:ARG:HA	1:414:A:ARG:HD2	1	0.58
(1,2667)	1:414:A:ARG:HA	1:414:A:ARG:HD2	3	0.58
(1,2667)	1:414:A:ARG:HA	1:414:A:ARG:HD2	5	0.58
(1,2640)	1:400:A:LEU:HD21	1:430:A:LEU:HD23	10	0.58
(1,2597)	1:358:A:ASP:HB3	1:363:A:ILE:HG22	7	0.58
(1,2597)	1:358:A:ASP:HB3	1:363:A:ILE:HG23	9	0.58
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG22	4	0.58
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG22	7	0.58
(1,2418)	1:444:A:GLN:H	1:441:A:GLN:HG2	11	0.58
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	17	0.58
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	8	0.58
(1,2275)	1:365:A:ARG:HE	1:412:A:LEU:HD11	7	0.58
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG21	4	0.58
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG22	9	0.58
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	15	0.58
(1,1906)	1:451:A:ALA:HB1	1:449:A:THR:HG23	17	0.58
(1,1885)	1:400:A:LEU:HD23	1:402:A:ILE:HD11	12	0.58
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	7	0.58
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	9	0.58
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	15	0.58
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD21	5	0.58
(1,1661)	1:404:A:ARG:HG2	1:404:A:ARG:HD3	1	0.58
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	17	0.58
(1,1522)	1:422:A:ILE:HG22	1:430:A:LEU:HG	9	0.58
(1,1502)	1:422:A:ILE:HA	1:427:A:THR:HG22	1	0.58
(1,1484)	1:432:A:HIS:HB2	1:430:A:LEU:H	10	0.58
(1,1402)	1:383:A:THR:HG23	1:384:A:ASN:HD21	13	0.58
(1,1357)	1:394:A:LEU:HD22	1:390:A:MET:HG3	15	0.58
(1,1356)	1:394:A:LEU:HD23	1:338:A:TRP:HB3	3	0.58
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	13	0.58
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	14	0.58
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	18	0.58
(1,1346)	1:398:A:TYR:HB2	1:398:A:TYR:HD1	19	0.58
(1,1330)	1:400:A:LEU:HD12	1:399:A:LYS:HB2	4	0.58
(1,1304)	1:376:A:TRP:HZ2	1:380:A:LYS:HE3	6	0.58
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD21	11	0.58
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD22	16	0.58
(1,1201)	1:363:A:ILE:HG13	1:361:A:SER:HB2	16	0.58
(1,1119)	1:367:A:VAL:HG22	1:355:A:ARG:HA	12	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1119)	1:367:A:VAL:HG23	1:355:A:ARG:HA	17	0.58
(1,1025)	1:336:A:LEU:HD22	1:430:A:LEU:H	1	0.58
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	9	0.58
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	19	0.58
(1,908)	1:411:A:LEU:HD21	1:366:A:ILE:H	5	0.58
(1,820)	1:429:A:ARG:HA	1:432:A:HIS:HB2	15	0.58
(1,806)	1:426:A:ARG:HD2	1:426:A:ARG:HA	5	0.58
(1,715)	1:414:A:ARG:HD2	1:414:A:ARG:HH12	3	0.58
(1,649)	1:405:A:LYS:HD2	1:405:A:LYS:HG3	11	0.58
(1,624)	1:403:A:ILE:HG23	1:397:A:TYR:HB3	17	0.58
(1,471)	1:388:A:GLU:HB3	1:388:A:GLU:HG2	7	0.58
(1,358)	1:374:A:ARG:HA	1:374:A:ARG:HD2	12	0.58
(1,267)	1:363:A:ILE:HG23	1:412:A:LEU:HG	18	0.58
(1,265)	1:363:A:ILE:HG22	1:412:A:LEU:HA	5	0.58
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	17	0.58
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD11	13	0.58
(1,35)	1:341:A:VAL:HG12	1:345:A:LEU:HD11	4	0.58
(1,35)	1:341:A:VAL:HG13	1:345:A:LEU:HD13	13	0.58
(1,2981)	1:428:A:ASP:H	1:427:A:THR:HG22	5	0.57
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	14	0.57
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	14	0.57
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	3	0.57
(1,2884)	1:397:A:TYR:HE1	1:393:A:ALA:HA	5	0.57
(1,2884)	1:397:A:TYR:HE1	1:397:A:TYR:HA	8	0.57
(1,2884)	1:397:A:TYR:HE1	1:397:A:TYR:HA	19	0.57
(1,2880)	1:402:A:ILE:HG23	1:397:A:TYR:HE2	11	0.57
(1,2876)	1:372:A:LEU:HD13	1:374:A:ARG:H	6	0.57
(1,2857)	1:418:A:THR:HG22	1:342:A:TYR:HE1	14	0.57
(1,2844)	1:403:A:ILE:H	1:402:A:ILE:HG22	17	0.57
(1,2828)	1:412:A:LEU:HD12	1:413:A:PHE:HD1	9	0.57
(1,2828)	1:412:A:LEU:HD13	1:413:A:PHE:HD1	13	0.57
(1,2799)	1:412:A:LEU:HD21	1:365:A:ARG:HD3	9	0.57
(1,2799)	1:412:A:LEU:HD22	1:365:A:ARG:HD3	18	0.57
(1,2770)	1:373:A:ALA:HB2	1:371:A:GLY:H	1	0.57
(1,2770)	1:373:A:ALA:HB2	1:371:A:GLY:H	3	0.57
(1,2770)	1:373:A:ALA:HB3	1:371:A:GLY:H	4	0.57
(1,2770)	1:373:A:ALA:HB2	1:371:A:GLY:H	8	0.57
(1,2770)	1:373:A:ALA:HB2	1:371:A:GLY:H	18	0.57
(1,2768)	1:394:A:LEU:HD12	1:387:A:TYR:HD1	2	0.57
(1,2768)	1:394:A:LEU:HD13	1:387:A:TYR:HD1	4	0.57
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	9	0.57
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	18	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG23	13	0.57
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG21	19	0.57
(1,2706)	1:349:A:ARG:HB3	1:350:A:TYR:HE2	19	0.57
(1,2683)	1:429:A:ARG:HG3	1:429:A:ARG:H	17	0.57
(1,2667)	1:414:A:ARG:HA	1:414:A:ARG:HD2	7	0.57
(1,2667)	1:414:A:ARG:HA	1:414:A:ARG:HD2	14	0.57
(1,2667)	1:414:A:ARG:HA	1:414:A:ARG:HD2	16	0.57
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	1	0.57
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	2	0.57
(1,2645)	1:402:A:ILE:HD11	1:338:A:TRP:HB3	5	0.57
(1,2644)	1:402:A:ILE:HD13	1:397:A:TYR:HE1	4	0.57
(1,2644)	1:402:A:ILE:HD11	1:397:A:TYR:HE1	10	0.57
(1,2640)	1:400:A:LEU:HD21	1:430:A:LEU:HD21	5	0.57
(1,2640)	1:400:A:LEU:HD21	1:430:A:LEU:HD21	8	0.57
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB2	2	0.57
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB3	3	0.57
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB3	5	0.57
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG21	17	0.57
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	14	0.57
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD22	2	0.57
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	3	0.57
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	6	0.57
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	11	0.57
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	13	0.57
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	18	0.57
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	19	0.57
(1,1776)	1:337:A:LEU:HD13	1:390:A:MET:HG3	5	0.57
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD11	3	0.57
(1,1356)	1:394:A:LEU:HD22	1:338:A:TRP:HB3	5	0.57
(1,1356)	1:394:A:LEU:HD22	1:338:A:TRP:HB3	13	0.57
(1,1344)	1:398:A:TYR:HD1	1:398:A:TYR:H	5	0.57
(1,1126)	1:355:A:ARG:HD2	1:367:A:VAL:HG23	2	0.57
(1,1121)	1:367:A:VAL:HG23	1:365:A:ARG:HA	17	0.57
(1,1119)	1:367:A:VAL:HG23	1:355:A:ARG:HA	14	0.57
(1,1113)	1:411:A:LEU:HD11	1:369:A:PRO:HB2	15	0.57
(1,1055)	1:350:A:TYR:H	1:350:A:TYR:HE1	14	0.57
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	5	0.57
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	11	0.57
(1,880)	1:437:A:VAL:HA	1:440:A:GLU:HB2	17	0.57
(1,852)	1:431:A:GLU:H	1:431:A:GLU:HG2	3	0.57
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	2	0.57
(1,458)	1:386:A:THR:HG21	1:389:A:LYS:HD2	5	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:386:A:THR:HG22	1:389:A:LYS:HE2	11	0.57
(1,267)	1:363:A:ILE:HG21	1:412:A:LEU:HG	14	0.57
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD13	4	0.57
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	15	0.57
(1,35)	1:341:A:VAL:HG13	1:345:A:LEU:HD11	1	0.57
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD22	1	0.57
(1,5)	1:337:A:LEU:HD23	1:390:A:MET:HG3	14	0.57
(1,5)	1:337:A:LEU:HD21	1:390:A:MET:HG3	16	0.57
(1,2981)	1:428:A:ASP:H	1:427:A:THR:HG23	3	0.56
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	9	0.56
(1,2880)	1:402:A:ILE:HG21	1:397:A:TYR:HE2	6	0.56
(1,2828)	1:412:A:LEU:HD11	1:413:A:PHE:HD1	6	0.56
(1,2789)	1:438:A:LEU:HD11	1:381:A:ASN:HD22	14	0.56
(1,2770)	1:373:A:ALA:HB2	1:371:A:GLY:H	11	0.56
(1,2770)	1:373:A:ALA:HB3	1:371:A:GLY:H	12	0.56
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE2	7	0.56
(1,2725)	1:367:A:VAL:HG21	1:365:A:ARG:HB3	7	0.56
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG21	3	0.56
(1,2683)	1:429:A:ARG:HG2	1:429:A:ARG:H	2	0.56
(1,2675)	1:417:A:LYS:HD2	1:402:A:ILE:HG13	18	0.56
(1,2667)	1:414:A:ARG:HA	1:414:A:ARG:HD2	11	0.56
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	3	0.56
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	6	0.56
(1,2645)	1:402:A:ILE:HD11	1:338:A:TRP:HB3	8	0.56
(1,2640)	1:400:A:LEU:HD23	1:430:A:LEU:HD22	7	0.56
(1,2633)	1:394:A:LEU:HD13	1:366:A:ILE:HD11	9	0.56
(1,2552)	1:452:A:SER:H	1:451:A:ALA:HB2	2	0.56
(1,2550)	1:451:A:ALA:H	1:450:A:ILE:HG23	14	0.56
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	13	0.56
(1,2423)	1:441:A:GLN:H	1:441:A:GLN:HB2	9	0.56
(1,2423)	1:441:A:GLN:H	1:441:A:GLN:HB2	11	0.56
(1,2423)	1:441:A:GLN:H	1:441:A:GLN:HB2	18	0.56
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	5	0.56
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	1	0.56
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG23	18	0.56
(1,2058)	1:363:A:ILE:H	1:358:A:ASP:HB2	15	0.56
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD23	4	0.56
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	4	0.56
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	7	0.56
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	8	0.56
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	14	0.56
(1,1918)	1:354:A:ILE:HD11	1:366:A:ILE:HD11	7	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB2	16	0.56
(1,1840)	1:374:A:ARG:HD3	1:374:A:ARG:HA	6	0.56
(1,1821)	1:386:A:THR:H	1:389:A:LYS:HD2	3	0.56
(1,1778)	1:337:A:LEU:HD12	1:376:A:TRP:HB3	19	0.56
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD22	7	0.56
(1,1690)	1:402:A:ILE:HD12	1:400:A:LEU:HA	14	0.56
(1,1661)	1:404:A:ARG:HG2	1:404:A:ARG:HD3	3	0.56
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD11	18	0.56
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD11	19	0.56
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD13	10	0.56
(1,1424)	1:450:A:ILE:HG22	1:452:A:SER:HB2	8	0.56
(1,1424)	1:450:A:ILE:HG23	1:452:A:SER:HB2	17	0.56
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	2	0.56
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	4	0.56
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	15	0.56
(1,1357)	1:394:A:LEU:HD22	1:390:A:MET:HG3	6	0.56
(1,1201)	1:363:A:ILE:HG13	1:361:A:SER:HB2	10	0.56
(1,1200)	1:361:A:SER:HA	1:361:A:SER:HB2	3	0.56
(1,1200)	1:361:A:SER:HA	1:361:A:SER:HB2	9	0.56
(1,1200)	1:361:A:SER:HA	1:361:A:SER:HB2	10	0.56
(1,1200)	1:361:A:SER:HA	1:361:A:SER:HB2	16	0.56
(1,1200)	1:361:A:SER:HA	1:361:A:SER:HB2	18	0.56
(1,1164)	1:363:A:ILE:HG13	1:358:A:ASP:HB2	14	0.56
(1,1133)	1:367:A:VAL:HG13	1:352:A:ASN:HB3	3	0.56
(1,1133)	1:367:A:VAL:HG12	1:352:A:ASN:HB3	6	0.56
(1,1121)	1:367:A:VAL:HG23	1:365:A:ARG:HA	16	0.56
(1,1033)	1:348:A:SER:HB3	1:351:A:GLU:HB3	12	0.56
(1,1025)	1:336:A:LEU:HD22	1:430:A:LEU:H	6	0.56
(1,1021)	1:437:A:VAL:HG12	1:396:A:HIS:HD2	2	0.56
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG23	18	0.56
(1,820)	1:429:A:ARG:HA	1:432:A:HIS:HB2	5	0.56
(1,718)	1:414:A:ARG:HB3	1:414:A:ARG:HD3	3	0.56
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	14	0.56
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD13	14	0.56
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD12	19	0.56
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	1	0.56
(1,5)	1:337:A:LEU:HD22	1:390:A:MET:HG3	5	0.56
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	18	0.55
(1,2884)	1:397:A:TYR:HE1	1:393:A:ALA:HA	1	0.55
(1,2880)	1:402:A:ILE:HG23	1:397:A:TYR:HE2	7	0.55
(1,2844)	1:403:A:ILE:H	1:402:A:ILE:HG22	18	0.55
(1,2813)	1:418:A:THR:HG23	1:362:A:LYS:HD2	16	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2797)	1:433:A:LEU:HD13	1:434:A:GLU:HA	3	0.55
(1,2797)	1:433:A:LEU:HD11	1:434:A:GLU:HA	13	0.55
(1,2770)	1:373:A:ALA:HB1	1:371:A:GLY:H	19	0.55
(1,2706)	1:349:A:ARG:HB3	1:350:A:TYR:HE1	12	0.55
(1,2683)	1:429:A:ARG:HG3	1:429:A:ARG:H	5	0.55
(1,2683)	1:429:A:ARG:HG2	1:429:A:ARG:H	19	0.55
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	14	0.55
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	16	0.55
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB3	1	0.55
(1,2555)	1:340:A:TYR:HA	1:339:A:ASP:HB3	3	0.55
(1,2555)	1:340:A:TYR:HA	1:339:A:ASP:HB3	6	0.55
(1,2550)	1:451:A:ALA:H	1:450:A:ILE:HG21	6	0.55
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG21	9	0.55
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	14	0.55
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD11	18	0.55
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD13	19	0.55
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	7	0.55
(1,2473)	1:409:A:GLN:HE21	1:412:A:LEU:HD11	8	0.55
(1,2423)	1:441:A:GLN:H	1:441:A:GLN:HB2	3	0.55
(1,2423)	1:441:A:GLN:H	1:441:A:GLN:HB2	5	0.55
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	9	0.55
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	11	0.55
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD22	5	0.55
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD21	7	0.55
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	14	0.55
(1,2258)	1:450:A:ILE:H	1:450:A:ILE:HG13	13	0.55
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	8	0.55
(1,2058)	1:363:A:ILE:H	1:358:A:ASP:HB2	9	0.55
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	2	0.55
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	9	0.55
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	10	0.55
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	16	0.55
(1,1918)	1:354:A:ILE:HD12	1:366:A:ILE:HD13	3	0.55
(1,1918)	1:354:A:ILE:HD11	1:366:A:ILE:HD11	4	0.55
(1,1918)	1:354:A:ILE:HD11	1:366:A:ILE:HD11	15	0.55
(1,1918)	1:354:A:ILE:HD13	1:366:A:ILE:HD12	17	0.55
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB2	13	0.55
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD21	5	0.55
(1,1798)	1:336:A:LEU:H	1:336:A:LEU:HD11	14	0.55
(1,1686)	1:402:A:ILE:HG21	1:403:A:ILE:HG12	9	0.55
(1,1671)	1:403:A:ILE:HG22	1:405:A:LYS:HA	5	0.55
(1,1671)	1:403:A:ILE:HG22	1:405:A:LYS:HA	17	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	18	0.55
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD11	2	0.55
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD11	6	0.55
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD11	9	0.55
(1,1430)	1:447:A:GLU:HB2	1:448:A:PRO:HD3	2	0.55
(1,1402)	1:383:A:THR:HG22	1:384:A:ASN:HD21	1	0.55
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	1	0.55
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	6	0.55
(1,1356)	1:394:A:LEU:HD22	1:338:A:TRP:HB3	4	0.55
(1,1356)	1:394:A:LEU:HD21	1:338:A:TRP:HB3	11	0.55
(1,1356)	1:394:A:LEU:HD23	1:338:A:TRP:HB3	18	0.55
(1,1356)	1:394:A:LEU:HD22	1:338:A:TRP:HB3	19	0.55
(1,1313)	1:375:A:LEU:HD13	1:376:A:TRP:H	13	0.55
(1,1201)	1:363:A:ILE:HG13	1:361:A:SER:HB2	11	0.55
(1,1200)	1:361:A:SER:HA	1:361:A:SER:HB2	1	0.55
(1,1200)	1:361:A:SER:HA	1:361:A:SER:HB2	7	0.55
(1,1200)	1:361:A:SER:HA	1:361:A:SER:HB2	8	0.55
(1,1200)	1:361:A:SER:HA	1:361:A:SER:HB2	11	0.55
(1,1200)	1:361:A:SER:HA	1:361:A:SER:HB2	13	0.55
(1,1200)	1:361:A:SER:HA	1:361:A:SER:HB2	17	0.55
(1,1200)	1:361:A:SER:HA	1:361:A:SER:HB2	19	0.55
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD11	8	0.55
(1,1119)	1:367:A:VAL:HG21	1:355:A:ARG:HA	3	0.55
(1,1033)	1:348:A:SER:HB3	1:351:A:GLU:HB3	7	0.55
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	7	0.55
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	17	0.55
(1,908)	1:411:A:LEU:HD21	1:366:A:ILE:H	11	0.55
(1,908)	1:411:A:LEU:HD22	1:366:A:ILE:H	12	0.55
(1,843)	1:430:A:LEU:HD23	1:336:A:LEU:HD12	9	0.55
(1,843)	1:430:A:LEU:HD21	1:336:A:LEU:HD12	11	0.55
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	7	0.55
(1,456)	1:386:A:THR:HG21	1:387:A:TYR:HB2	9	0.55
(1,443)	1:384:A:ASN:H	1:384:A:ASN:HB2	11	0.55
(1,265)	1:363:A:ILE:HG21	1:412:A:LEU:HA	10	0.55
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD11	1	0.55
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD11	12	0.55
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	2	0.55
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	14	0.55
(1,35)	1:341:A:VAL:HG13	1:345:A:LEU:HD12	10	0.55
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD21	12	0.55
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	1	0.54
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	3	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	7	0.54
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	11	0.54
(1,2884)	1:397:A:TYR:HE1	1:393:A:ALA:HA	7	0.54
(1,2880)	1:402:A:ILE:HG23	1:397:A:TYR:HE2	14	0.54
(1,2858)	1:341:A:VAL:HG11	1:340:A:TYR:HD2	1	0.54
(1,2858)	1:341:A:VAL:HG12	1:340:A:TYR:HD2	2	0.54
(1,2858)	1:341:A:VAL:HG13	1:340:A:TYR:HD2	8	0.54
(1,2828)	1:412:A:LEU:HD12	1:413:A:PHE:HD1	15	0.54
(1,2828)	1:412:A:LEU:HD12	1:413:A:PHE:HD1	16	0.54
(1,2828)	1:412:A:LEU:HD12	1:413:A:PHE:HD1	18	0.54
(1,2808)	1:427:A:THR:HA	1:430:A:LEU:HG	18	0.54
(1,2806)	1:430:A:LEU:HD12	1:431:A:GLU:HG2	7	0.54
(1,2775)	1:387:A:TYR:HD2	1:390:A:MET:HG2	14	0.54
(1,2774)	1:443:A:TYR:HD2	1:445:A:GLU:HB2	1	0.54
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	1	0.54
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	8	0.54
(1,2724)	1:367:A:VAL:HG21	1:352:A:ASN:HA	1	0.54
(1,2688)	1:440:A:GLU:HG2	1:440:A:GLU:HB3	7	0.54
(1,2688)	1:440:A:GLU:HG2	1:440:A:GLU:HB3	12	0.54
(1,2688)	1:440:A:GLU:HG2	1:440:A:GLU:HB3	18	0.54
(1,2688)	1:440:A:GLU:HG2	1:440:A:GLU:HB3	19	0.54
(1,2683)	1:429:A:ARG:HG2	1:429:A:ARG:H	6	0.54
(1,2683)	1:429:A:ARG:HG3	1:429:A:ARG:H	11	0.54
(1,2683)	1:429:A:ARG:HG2	1:429:A:ARG:H	12	0.54
(1,2683)	1:429:A:ARG:HG3	1:429:A:ARG:H	18	0.54
(1,2675)	1:417:A:LYS:HD2	1:402:A:ILE:HG13	7	0.54
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD13	3	0.54
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	7	0.54
(1,2640)	1:400:A:LEU:HD22	1:430:A:LEU:HD21	13	0.54
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	17	0.54
(1,2597)	1:358:A:ASP:HB2	1:363:A:ILE:HG22	3	0.54
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG21	2	0.54
(1,2569)	1:349:A:ARG:HD3	1:350:A:TYR:HE1	9	0.54
(1,2569)	1:349:A:ARG:HD3	1:350:A:TYR:HE1	11	0.54
(1,2547)	1:442:A:THR:H	1:442:A:THR:HG23	7	0.54
(1,2508)	1:434:A:GLU:H	1:434:A:GLU:HG2	17	0.54
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	19	0.54
(1,2472)	1:409:A:GLN:HE22	1:412:A:LEU:HD12	1	0.54
(1,2415)	1:447:A:GLU:H	1:448:A:PRO:HD3	17	0.54
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	2	0.54
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD21	7	0.54
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD21	8	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD22	12	0.54
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD22	15	0.54
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	1	0.54
(1,1918)	1:354:A:ILE:HD11	1:366:A:ILE:HD11	6	0.54
(1,1776)	1:337:A:LEU:HD12	1:390:A:MET:HG3	4	0.54
(1,1776)	1:337:A:LEU:HD12	1:390:A:MET:HG3	8	0.54
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD23	14	0.54
(1,1690)	1:402:A:ILE:HD13	1:400:A:LEU:HA	19	0.54
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD13	11	0.54
(1,1671)	1:403:A:ILE:HG23	1:405:A:LYS:HA	16	0.54
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD12	13	0.54
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD11	17	0.54
(1,1512)	1:424:A:SER:HA	1:424:A:SER:HB2	2	0.54
(1,1512)	1:424:A:SER:HA	1:424:A:SER:HB2	5	0.54
(1,1512)	1:424:A:SER:HA	1:424:A:SER:HB2	7	0.54
(1,1512)	1:424:A:SER:HA	1:424:A:SER:HB2	14	0.54
(1,1512)	1:424:A:SER:HA	1:424:A:SER:HB2	15	0.54
(1,1485)	1:432:A:HIS:HD2	1:433:A:LEU:HD21	12	0.54
(1,1484)	1:432:A:HIS:HB3	1:430:A:LEU:H	7	0.54
(1,1484)	1:432:A:HIS:HB3	1:430:A:LEU:H	16	0.54
(1,1480)	1:412:A:LEU:HD23	1:357:A:GLU:HG2	2	0.54
(1,1472)	1:434:A:GLU:H	1:433:A:LEU:HB2	17	0.54
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	4	0.54
(1,1356)	1:394:A:LEU:HD23	1:338:A:TRP:HB3	7	0.54
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD22	10	0.54
(1,1200)	1:361:A:SER:HA	1:361:A:SER:HB2	5	0.54
(1,1182)	1:363:A:ILE:HD11	1:406:A:GLU:HG2	17	0.54
(1,1113)	1:411:A:LEU:HD12	1:369:A:PRO:HB2	18	0.54
(1,1025)	1:336:A:LEU:HD21	1:430:A:LEU:H	5	0.54
(1,1025)	1:336:A:LEU:HD22	1:430:A:LEU:H	16	0.54
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	16	0.54
(1,908)	1:411:A:LEU:HD21	1:366:A:ILE:H	7	0.54
(1,908)	1:411:A:LEU:HD21	1:366:A:ILE:H	8	0.54
(1,865)	1:438:A:LEU:HD11	1:380:A:LYS:HE3	16	0.54
(1,852)	1:431:A:GLU:H	1:431:A:GLU:HG2	5	0.54
(1,852)	1:431:A:GLU:H	1:431:A:GLU:HG2	6	0.54
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	8	0.54
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	18	0.54
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	19	0.54
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD21	6	0.54
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	10	0.54
(1,458)	1:386:A:THR:HG22	1:389:A:LYS:HD2	8	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,265)	1:363:A:ILE:HG21	1:412:A:LEU:HA	12	0.54
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	6	0.54
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	10	0.54
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	16	0.54
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD11	7	0.54
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	10	0.54
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	16	0.53
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	10	0.53
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	13	0.53
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	16	0.53
(1,2884)	1:397:A:TYR:HE1	1:393:A:ALA:HA	14	0.53
(1,2884)	1:397:A:TYR:HE1	1:397:A:TYR:HA	18	0.53
(1,2880)	1:402:A:ILE:HG22	1:397:A:TYR:HE2	5	0.53
(1,2858)	1:341:A:VAL:HG13	1:340:A:TYR:HD2	14	0.53
(1,2828)	1:412:A:LEU:HD11	1:413:A:PHE:HD1	10	0.53
(1,2806)	1:430:A:LEU:HD12	1:431:A:GLU:HG2	15	0.53
(1,2775)	1:387:A:TYR:HD2	1:390:A:MET:HG2	2	0.53
(1,2770)	1:373:A:ALA:HB2	1:371:A:GLY:H	16	0.53
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	12	0.53
(1,2754)	1:355:A:ARG:H	1:354:A:ILE:HD12	10	0.53
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE3	13	0.53
(1,2726)	1:367:A:VAL:HG13	1:355:A:ARG:HD3	1	0.53
(1,2726)	1:367:A:VAL:HG13	1:365:A:ARG:HD2	2	0.53
(1,2697)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	11	0.53
(1,2693)	1:437:A:VAL:HG21	1:441:A:GLN:HE22	16	0.53
(1,2688)	1:440:A:GLU:HG2	1:440:A:GLU:HB3	2	0.53
(1,2681)	1:418:A:THR:HG22	1:342:A:TYR:HD1	14	0.53
(1,2675)	1:417:A:LYS:HD2	1:402:A:ILE:HG13	5	0.53
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	9	0.53
(1,2643)	1:402:A:ILE:HD12	1:397:A:TYR:HD1	2	0.53
(1,2643)	1:402:A:ILE:HD11	1:397:A:TYR:HD1	16	0.53
(1,2640)	1:400:A:LEU:HD21	1:430:A:LEU:HD22	4	0.53
(1,2640)	1:400:A:LEU:HD21	1:402:A:ILE:HD13	18	0.53
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB3	13	0.53
(1,2579)	1:358:A:ASP:HB2	1:363:A:ILE:HG23	9	0.53
(1,2569)	1:349:A:ARG:HD3	1:350:A:TYR:HE1	2	0.53
(1,2552)	1:452:A:SER:H	1:451:A:ALA:HB2	18	0.53
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG21	15	0.53
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	16	0.53
(1,2423)	1:441:A:GLN:H	1:441:A:GLN:HB2	16	0.53
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	6	0.53
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	16	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	3	0.53
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	17	0.53
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD23	1	0.53
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD21	17	0.53
(1,1918)	1:354:A:ILE:HD12	1:366:A:ILE:HD12	2	0.53
(1,1918)	1:354:A:ILE:HD11	1:366:A:ILE:HD13	5	0.53
(1,1918)	1:354:A:ILE:HD13	1:366:A:ILE:HD12	8	0.53
(1,1918)	1:354:A:ILE:HD13	1:366:A:ILE:HD13	13	0.53
(1,1906)	1:451:A:ALA:HB3	1:449:A:THR:HG22	3	0.53
(1,1798)	1:336:A:LEU:H	1:336:A:LEU:HD11	8	0.53
(1,1776)	1:337:A:LEU:HD12	1:390:A:MET:HG3	14	0.53
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD21	3	0.53
(1,1709)	1:344:A:LEU:HD23	1:345:A:LEU:H	13	0.53
(1,1671)	1:403:A:ILE:HG23	1:405:A:LYS:HA	13	0.53
(1,1671)	1:403:A:ILE:HG21	1:405:A:LYS:HA	14	0.53
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD11	7	0.53
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD13	12	0.53
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	9	0.53
(1,1523)	1:422:A:ILE:HG23	1:426:A:ARG:HG2	4	0.53
(1,1484)	1:432:A:HIS:HB3	1:430:A:LEU:H	3	0.53
(1,1484)	1:432:A:HIS:HB3	1:430:A:LEU:H	18	0.53
(1,1427)	1:447:A:GLU:HA	1:448:A:PRO:HD3	17	0.53
(1,1393)	1:386:A:THR:HG22	1:388:A:GLU:HB3	1	0.53
(1,1356)	1:394:A:LEU:HD22	1:338:A:TRP:HB3	9	0.53
(1,1356)	1:394:A:LEU:HD22	1:338:A:TRP:HB3	12	0.53
(1,1356)	1:394:A:LEU:HD23	1:338:A:TRP:HB3	14	0.53
(1,1316)	1:433:A:LEU:HD23	1:396:A:HIS:HD2	11	0.53
(1,1316)	1:433:A:LEU:HD23	1:396:A:HIS:HD2	18	0.53
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD12	12	0.53
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD11	3	0.53
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD12	6	0.53
(1,1142)	1:450:A:ILE:HD12	1:454:A:VAL:HA	19	0.53
(1,1135)	1:367:A:VAL:HG13	1:352:A:ASN:H	15	0.53
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	12	0.53
(1,908)	1:411:A:LEU:HD23	1:366:A:ILE:H	2	0.53
(1,908)	1:411:A:LEU:HD21	1:366:A:ILE:H	6	0.53
(1,908)	1:411:A:LEU:HD23	1:366:A:ILE:H	9	0.53
(1,908)	1:411:A:LEU:HD23	1:366:A:ILE:H	10	0.53
(1,908)	1:411:A:LEU:HD21	1:366:A:ILE:H	13	0.53
(1,908)	1:411:A:LEU:HD23	1:366:A:ILE:H	15	0.53
(1,908)	1:411:A:LEU:HD23	1:366:A:ILE:H	17	0.53
(1,852)	1:431:A:GLU:H	1:431:A:GLU:HG2	16	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,843)	1:430:A:LEU:HD22	1:336:A:LEU:HD12	10	0.53
(1,834)	1:430:A:LEU:HD13	1:397:A:TYR:HD1	6	0.53
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD23	1	0.53
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD21	3	0.53
(1,530)	1:394:A:LEU:HD22	1:397:A:TYR:HB3	13	0.53
(1,456)	1:386:A:THR:HG22	1:387:A:TYR:HB2	2	0.53
(1,455)	1:386:A:THR:HG23	1:389:A:LYS:HE3	9	0.53
(1,265)	1:363:A:ILE:HG23	1:412:A:LEU:HA	2	0.53
(1,265)	1:363:A:ILE:HG23	1:412:A:LEU:HA	11	0.53
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	19	0.53
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD11	4	0.53
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD13	8	0.53
(1,75)	1:344:A:LEU:HA	1:344:A:LEU:HD12	11	0.53
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	3	0.53
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	18	0.53
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD23	16	0.53
(1,5)	1:337:A:LEU:HD22	1:390:A:MET:HG3	6	0.53
(1,2947)	1:362:A:LYS:H	1:362:A:LYS:HD2	13	0.52
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	15	0.52
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG23	14	0.52
(1,2884)	1:397:A:TYR:HE1	1:393:A:ALA:HA	15	0.52
(1,2880)	1:402:A:ILE:HG23	1:397:A:TYR:HE2	4	0.52
(1,2860)	1:340:A:TYR:HD1	1:340:A:TYR:H	14	0.52
(1,2858)	1:341:A:VAL:HG12	1:340:A:TYR:HD2	11	0.52
(1,2844)	1:402:A:ILE:HG22	1:397:A:TYR:HD2	9	0.52
(1,2837)	1:410:A:ARG:HB2	1:410:A:ARG:HD3	1	0.52
(1,2828)	1:412:A:LEU:HD12	1:413:A:PHE:HD1	4	0.52
(1,2799)	1:412:A:LEU:HD23	1:365:A:ARG:HD3	11	0.52
(1,2798)	1:412:A:LEU:HD22	1:365:A:ARG:HD2	12	0.52
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	4	0.52
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	15	0.52
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB2	10	0.52
(1,2768)	1:394:A:LEU:HD12	1:387:A:TYR:HD1	18	0.52
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	16	0.52
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE2	4	0.52
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE2	11	0.52
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE2	18	0.52
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG21	1	0.52
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG23	6	0.52
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG22	11	0.52
(1,2696)	1:438:A:LEU:HD21	1:382:A:ARG:HD2	9	0.52
(1,2688)	1:431:A:GLU:HG2	1:431:A:GLU:HB2	11	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2683)	1:429:A:ARG:HG3	1:429:A:ARG:H	1	0.52
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	4	0.52
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	19	0.52
(1,2644)	1:402:A:ILE:HD12	1:397:A:TYR:HE1	11	0.52
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB2	11	0.52
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG23	11	0.52
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	17	0.52
(1,2423)	1:441:A:GLN:H	1:441:A:GLN:HB2	8	0.52
(1,2359)	1:382:A:ARG:H	1:382:A:ARG:HG3	17	0.52
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	9	0.52
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	5	0.52
(1,2011)	1:355:A:ARG:H	1:355:A:ARG:HB2	17	0.52
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	17	0.52
(1,1974)	1:349:A:ARG:H	1:349:A:ARG:HB2	12	0.52
(1,1918)	1:354:A:ILE:HD11	1:366:A:ILE:HD11	1	0.52
(1,1899)	1:430:A:LEU:HD12	1:400:A:LEU:HD23	9	0.52
(1,1802)	1:336:A:LEU:HD13	1:431:A:GLU:HA	17	0.52
(1,1776)	1:337:A:LEU:HD12	1:390:A:MET:HG3	15	0.52
(1,1776)	1:337:A:LEU:HD13	1:390:A:MET:HG3	16	0.52
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD22	19	0.52
(1,1671)	1:403:A:ILE:HG23	1:405:A:LYS:HA	2	0.52
(1,1671)	1:403:A:ILE:HG22	1:405:A:LYS:HA	15	0.52
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD13	1	0.52
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD12	4	0.52
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD13	8	0.52
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD13	10	0.52
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD11	16	0.52
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD11	12	0.52
(1,1522)	1:422:A:ILE:HG22	1:430:A:LEU:HG	10	0.52
(1,1507)	1:426:A:ARG:HG2	1:426:A:ARG:HA	5	0.52
(1,1484)	1:432:A:HIS:HB3	1:430:A:LEU:H	14	0.52
(1,1422)	1:451:A:ALA:HB3	1:450:A:ILE:HA	17	0.52
(1,1392)	1:386:A:THR:HG22	1:389:A:LYS:HG2	1	0.52
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	11	0.52
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD2	14	0.52
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD13	7	0.52
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD12	9	0.52
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD12	17	0.52
(1,1135)	1:367:A:VAL:HG11	1:352:A:ASN:H	18	0.52
(1,1126)	1:355:A:ARG:HD2	1:367:A:VAL:HG23	10	0.52
(1,1119)	1:367:A:VAL:HG21	1:355:A:ARG:HA	2	0.52
(1,1119)	1:367:A:VAL:HG22	1:355:A:ARG:HA	10	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1033)	1:348:A:SER:HB3	1:351:A:GLU:HB3	15	0.52
(1,1025)	1:336:A:LEU:HD22	1:430:A:LEU:H	10	0.52
(1,1006)	1:380:A:LYS:HA	1:380:A:LYS:HD3	11	0.52
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	2	0.52
(1,908)	1:411:A:LEU:HD23	1:366:A:ILE:H	1	0.52
(1,908)	1:411:A:LEU:HD21	1:366:A:ILE:H	4	0.52
(1,908)	1:411:A:LEU:HD23	1:366:A:ILE:H	14	0.52
(1,834)	1:430:A:LEU:HD13	1:397:A:TYR:HD1	16	0.52
(1,820)	1:429:A:ARG:HA	1:432:A:HIS:HB2	16	0.52
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD23	18	0.52
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	16	0.52
(1,457)	1:386:A:THR:HG21	1:389:A:LYS:HB2	4	0.52
(1,457)	1:386:A:THR:HG22	1:389:A:LYS:HB2	17	0.52
(1,457)	1:386:A:THR:HG23	1:389:A:LYS:HB2	18	0.52
(1,456)	1:386:A:THR:HG21	1:387:A:TYR:HB2	1	0.52
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	4	0.52
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	6	0.52
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	11	0.52
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	12	0.52
(1,384)	1:344:A:LEU:HD13	1:375:A:LEU:HD22	4	0.52
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD12	4	0.52
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD11	13	0.52
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD11	17	0.52
(1,265)	1:363:A:ILE:HG23	1:412:A:LEU:HA	1	0.52
(1,265)	1:363:A:ILE:HG23	1:412:A:LEU:HA	3	0.52
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD12	2	0.52
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD11	5	0.52
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD13	13	0.52
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD13	16	0.52
(1,136)	1:351:A:GLU:H	1:351:A:GLU:HG2	10	0.52
(1,5)	1:337:A:LEU:HD23	1:390:A:MET:HG3	7	0.52
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	10	0.51
(1,2887)	1:336:A:LEU:H	1:336:A:LEU:HD11	14	0.51
(1,2880)	1:402:A:ILE:HG21	1:397:A:TYR:HE2	16	0.51
(1,2860)	1:340:A:TYR:HD1	1:340:A:TYR:H	3	0.51
(1,2858)	1:341:A:VAL:HG13	1:340:A:TYR:HD2	16	0.51
(1,2858)	1:341:A:VAL:HG11	1:340:A:TYR:HD2	17	0.51
(1,2837)	1:410:A:ARG:HB2	1:410:A:ARG:HD3	10	0.51
(1,2828)	1:412:A:LEU:HD12	1:413:A:PHE:HD1	5	0.51
(1,2828)	1:412:A:LEU:HD11	1:413:A:PHE:HD1	8	0.51
(1,2828)	1:412:A:LEU:HD11	1:413:A:PHE:HD1	14	0.51
(1,2813)	1:418:A:THR:HG21	1:362:A:LYS:HD2	3	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2813)	1:418:A:THR:HG22	1:362:A:LYS:HD2	9	0.51
(1,2794)	1:433:A:LEU:HD21	1:429:A:ARG:HD3	8	0.51
(1,2791)	1:438:A:LEU:HD23	1:385:A:MET:HG2	1	0.51
(1,2789)	1:438:A:LEU:HD13	1:444:A:GLN:HE22	4	0.51
(1,2786)	1:447:A:GLU:HG2	1:446:A:ASP:H	5	0.51
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	9	0.51
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	16	0.51
(1,2775)	1:387:A:TYR:HD2	1:390:A:MET:HG2	9	0.51
(1,2768)	1:394:A:LEU:HD13	1:387:A:TYR:HD1	8	0.51
(1,2764)	1:350:A:TYR:H	1:350:A:TYR:HE1	14	0.51
(1,2726)	1:367:A:VAL:HG11	1:355:A:ARG:HD2	12	0.51
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG22	12	0.51
(1,2683)	1:429:A:ARG:HG3	1:429:A:ARG:H	14	0.51
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD12	10	0.51
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	12	0.51
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	15	0.51
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	17	0.51
(1,2645)	1:402:A:ILE:HD11	1:338:A:TRP:HB3	11	0.51
(1,2645)	1:402:A:ILE:HD12	1:338:A:TRP:HB3	13	0.51
(1,2643)	1:402:A:ILE:HD12	1:397:A:TYR:HD1	19	0.51
(1,2640)	1:400:A:LEU:HD22	1:430:A:LEU:HD23	15	0.51
(1,2550)	1:451:A:ALA:H	1:450:A:ILE:HG23	3	0.51
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD13	11	0.51
(1,2432)	1:435:A:SER:H	1:436:A:GLN:HB2	19	0.51
(1,2423)	1:441:A:GLN:H	1:441:A:GLN:HB2	12	0.51
(1,2423)	1:441:A:GLN:H	1:441:A:GLN:HB2	14	0.51
(1,2423)	1:441:A:GLN:H	1:441:A:GLN:HB2	15	0.51
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	1	0.51
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG2	7	0.51
(1,2324)	1:352:A:ASN:HD21	1:367:A:VAL:HG21	1	0.51
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	7	0.51
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB3	8	0.51
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	2	0.51
(1,2159)	1:389:A:LYS:H	1:388:A:GLU:HG2	1	0.51
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD23	6	0.51
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD22	16	0.51
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD22	18	0.51
(1,1918)	1:354:A:ILE:HD11	1:366:A:ILE:HD12	10	0.51
(1,1918)	1:354:A:ILE:HD11	1:366:A:ILE:HD12	11	0.51
(1,1918)	1:354:A:ILE:HD13	1:366:A:ILE:HD13	16	0.51
(1,1918)	1:354:A:ILE:HD11	1:366:A:ILE:HD12	19	0.51
(1,1917)	1:394:A:LEU:HD13	1:366:A:ILE:HD11	9	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1771)	1:341:A:VAL:HG12	1:337:A:LEU:HD11	15	0.51
(1,1771)	1:341:A:VAL:HG11	1:337:A:LEU:HD13	19	0.51
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD21	1	0.51
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD21	6	0.51
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD21	16	0.51
(1,1690)	1:402:A:ILE:HD11	1:400:A:LEU:HA	9	0.51
(1,1686)	1:402:A:ILE:HG23	1:403:A:ILE:HG12	3	0.51
(1,1671)	1:403:A:ILE:HG21	1:405:A:LYS:HA	19	0.51
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	16	0.51
(1,1356)	1:394:A:LEU:HD23	1:338:A:TRP:HB3	2	0.51
(1,1356)	1:394:A:LEU:HD23	1:338:A:TRP:HB3	6	0.51
(1,1349)	1:443:A:TYR:HE1	1:445:A:GLU:HA	8	0.51
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD21	8	0.51
(1,1201)	1:363:A:ILE:HG13	1:361:A:SER:HB2	1	0.51
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD13	1	0.51
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD13	2	0.51
(1,1142)	1:450:A:ILE:HD12	1:454:A:VAL:HA	16	0.51
(1,1135)	1:367:A:VAL:HG11	1:352:A:ASN:H	16	0.51
(1,1133)	1:367:A:VAL:HG12	1:352:A:ASN:HB3	4	0.51
(1,1126)	1:355:A:ARG:HD2	1:367:A:VAL:HG21	6	0.51
(1,1126)	1:355:A:ARG:HD2	1:367:A:VAL:HG23	19	0.51
(1,1121)	1:367:A:VAL:HG22	1:365:A:ARG:HA	12	0.51
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	16	0.51
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	19	0.51
(1,1033)	1:348:A:SER:HB3	1:351:A:GLU:HB3	16	0.51
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	19	0.51
(1,457)	1:386:A:THR:HG21	1:389:A:LYS:HB2	11	0.51
(1,456)	1:386:A:THR:HG21	1:387:A:TYR:HB2	10	0.51
(1,455)	1:386:A:THR:HG21	1:389:A:LYS:HE3	14	0.51
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	1	0.51
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	2	0.51
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	3	0.51
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	5	0.51
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	7	0.51
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	9	0.51
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	10	0.51
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	14	0.51
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	15	0.51
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	16	0.51
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	17	0.51
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	18	0.51
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	19	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,445)	1:384:A:ASN:HD22	1:384:A:ASN:HB2	18	0.51
(1,444)	1:384:A:ASN:HD21	1:384:A:ASN:HB2	18	0.51
(1,400)	1:377:A:GLY:HA3	1:382:A:ARG:HB3	11	0.51
(1,365)	1:374:A:ARG:H	1:374:A:ARG:HD2	1	0.51
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD12	3	0.51
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD11	6	0.51
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD13	11	0.51
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD11	15	0.51
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD12	16	0.51
(1,265)	1:363:A:ILE:HG23	1:412:A:LEU:HA	7	0.51
(1,265)	1:363:A:ILE:HG22	1:412:A:LEU:HA	8	0.51
(1,265)	1:363:A:ILE:HG21	1:412:A:LEU:HA	9	0.51
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	6	0.51
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD13	9	0.51
(1,2974)	1:433:A:LEU:H	1:431:A:GLU:HB2	3	0.5
(1,2947)	1:362:A:LYS:H	1:363:A:ILE:HB	8	0.5
(1,2947)	1:362:A:LYS:H	1:362:A:LYS:HD2	16	0.5
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG21	4	0.5
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG23	10	0.5
(1,2884)	1:397:A:TYR:HE1	1:393:A:ALA:HA	6	0.5
(1,2884)	1:397:A:TYR:HE1	1:393:A:ALA:HA	13	0.5
(1,2860)	1:340:A:TYR:HD1	1:340:A:TYR:H	4	0.5
(1,2860)	1:340:A:TYR:HD1	1:340:A:TYR:H	8	0.5
(1,2860)	1:340:A:TYR:H	1:340:A:TYR:HD2	9	0.5
(1,2860)	1:340:A:TYR:H	1:340:A:TYR:HD2	12	0.5
(1,2858)	1:341:A:VAL:HG13	1:340:A:TYR:HD2	3	0.5
(1,2828)	1:412:A:LEU:HD11	1:413:A:PHE:HD1	2	0.5
(1,2813)	1:418:A:THR:HG23	1:362:A:LYS:HD2	12	0.5
(1,2797)	1:433:A:LEU:HD12	1:434:A:GLU:HA	12	0.5
(1,2791)	1:438:A:LEU:HD21	1:385:A:MET:HG2	16	0.5
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	14	0.5
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	17	0.5
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	19	0.5
(1,2770)	1:373:A:ALA:HB3	1:371:A:GLY:H	13	0.5
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG23	4	0.5
(1,2693)	1:437:A:VAL:HG23	1:441:A:GLN:HE22	3	0.5
(1,2683)	1:429:A:ARG:HG3	1:429:A:ARG:H	3	0.5
(1,2681)	1:418:A:THR:HG23	1:342:A:TYR:HD1	6	0.5
(1,2681)	1:418:A:THR:HG23	1:342:A:TYR:HD1	17	0.5
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD13	19	0.5
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	10	0.5
(1,2618)	1:375:A:LEU:HD22	1:378:A:ASN:HB2	10	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB2	19	0.5
(1,2552)	1:452:A:SER:H	1:451:A:ALA:HB3	7	0.5
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD21	12	0.5
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD22	13	0.5
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD23	19	0.5
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD12	11	0.5
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB3	19	0.5
(1,2423)	1:441:A:GLN:H	1:441:A:GLN:HB2	10	0.5
(1,2415)	1:447:A:GLU:H	1:448:A:PRO:HD3	9	0.5
(1,2258)	1:450:A:ILE:H	1:450:A:ILE:HG13	1	0.5
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	7	0.5
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG21	11	0.5
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD23	10	0.5
(1,1798)	1:336:A:LEU:H	1:336:A:LEU:HD11	7	0.5
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD12	11	0.5
(1,1771)	1:341:A:VAL:HG11	1:337:A:LEU:HD11	7	0.5
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD22	4	0.5
(1,1709)	1:344:A:LEU:HD22	1:345:A:LEU:H	19	0.5
(1,1671)	1:403:A:ILE:HG21	1:405:A:LYS:HA	8	0.5
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD11	5	0.5
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD11	14	0.5
(1,1596)	1:412:A:LEU:HB2	1:412:A:LEU:HD12	15	0.5
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	3	0.5
(1,1485)	1:432:A:HIS:HD2	1:433:A:LEU:HD21	3	0.5
(1,1393)	1:386:A:THR:HG22	1:388:A:GLU:HB3	10	0.5
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	14	0.5
(1,1357)	1:394:A:LEU:HD21	1:390:A:MET:HG3	4	0.5
(1,1356)	1:394:A:LEU:HD23	1:338:A:TRP:HB3	15	0.5
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD21	1	0.5
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD22	18	0.5
(1,1201)	1:363:A:ILE:HG13	1:361:A:SER:HB2	7	0.5
(1,1193)	1:362:A:LYS:HE2	1:362:A:LYS:HA	8	0.5
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD12	6	0.5
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD12	5	0.5
(1,1121)	1:367:A:VAL:HG22	1:365:A:ARG:HA	10	0.5
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	1	0.5
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	2	0.5
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	5	0.5
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	9	0.5
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	10	0.5
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	11	0.5
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	14	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1006)	1:380:A:LYS:HA	1:380:A:LYS:HD3	16	0.5
(1,1006)	1:380:A:LYS:HA	1:380:A:LYS:HD3	17	0.5
(1,1006)	1:380:A:LYS:HA	1:380:A:LYS:HD3	19	0.5
(1,908)	1:411:A:LEU:HD22	1:366:A:ILE:H	16	0.5
(1,908)	1:411:A:LEU:HD22	1:366:A:ILE:H	18	0.5
(1,852)	1:431:A:GLU:H	1:431:A:GLU:HG2	1	0.5
(1,834)	1:430:A:LEU:HD11	1:397:A:TYR:HD1	5	0.5
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD22	11	0.5
(1,547)	1:395:A:ARG:HD2	1:395:A:ARG:H	12	0.5
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	11	0.5
(1,457)	1:386:A:THR:HG22	1:389:A:LYS:HB2	9	0.5
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	8	0.5
(1,445)	1:384:A:ASN:HD22	1:384:A:ASN:HB2	11	0.5
(1,445)	1:384:A:ASN:HD22	1:384:A:ASN:HB2	14	0.5
(1,444)	1:384:A:ASN:HD21	1:384:A:ASN:HB2	11	0.5
(1,400)	1:377:A:GLY:HA3	1:382:A:ARG:HB3	3	0.5
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD11	1	0.5
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD13	2	0.5
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD13	5	0.5
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD11	7	0.5
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD12	8	0.5
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD13	9	0.5
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD13	12	0.5
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD12	18	0.5
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD13	19	0.5
(1,265)	1:363:A:ILE:HG21	1:412:A:LEU:HA	17	0.5
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	10	0.5
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	17	0.5
(1,230)	1:356:A:TRP:HE1	1:359:A:LYS:HD2	17	0.5
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD12	3	0.5
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD11	6	0.5
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD11	10	0.5
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD11	19	0.5
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD21	15	0.5
(1,5)	1:337:A:LEU:HD22	1:390:A:MET:HG3	1	0.5
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	4	0.49
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD22	17	0.49
(1,2887)	1:336:A:LEU:H	1:336:A:LEU:HD11	8	0.49
(1,2884)	1:397:A:TYR:HE1	1:393:A:ALA:HA	10	0.49
(1,2880)	1:402:A:ILE:HG21	1:397:A:TYR:HE2	1	0.49
(1,2880)	1:402:A:ILE:HG22	1:397:A:TYR:HE2	19	0.49
(1,2876)	1:372:A:LEU:HD13	1:374:A:ARG:H	13	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2872)	1:444:A:GLN:HG2	1:444:A:GLN:HB3	11	0.49
(1,2860)	1:340:A:TYR:HD1	1:340:A:TYR:H	19	0.49
(1,2858)	1:341:A:VAL:HG12	1:340:A:TYR:HD2	9	0.49
(1,2858)	1:341:A:VAL:HG12	1:340:A:TYR:HD2	18	0.49
(1,2858)	1:341:A:VAL:HG11	1:340:A:TYR:HD2	19	0.49
(1,2799)	1:412:A:LEU:HD23	1:365:A:ARG:HD3	14	0.49
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	2	0.49
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	5	0.49
(1,2683)	1:429:A:ARG:HG3	1:429:A:ARG:H	8	0.49
(1,2683)	1:429:A:ARG:HG3	1:429:A:ARG:H	9	0.49
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	18	0.49
(1,2645)	1:402:A:ILE:HD12	1:338:A:TRP:HB3	7	0.49
(1,2643)	1:402:A:ILE:HD11	1:397:A:TYR:HD1	14	0.49
(1,2640)	1:400:A:LEU:HD21	1:430:A:LEU:HD23	19	0.49
(1,2612)	1:393:A:ALA:HB3	1:376:A:TRP:HZ3	5	0.49
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB3	7	0.49
(1,2569)	1:349:A:ARG:HD3	1:350:A:TYR:HE1	7	0.49
(1,2550)	1:451:A:ALA:H	1:450:A:ILE:HG21	4	0.49
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG22	7	0.49
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD21	13	0.49
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD21	15	0.49
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	15	0.49
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD11	1	0.49
(1,2423)	1:441:A:GLN:H	1:441:A:GLN:HB2	6	0.49
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD22	19	0.49
(1,2275)	1:365:A:ARG:HE	1:412:A:LEU:HD11	16	0.49
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB3	1	0.49
(1,2159)	1:389:A:LYS:H	1:388:A:GLU:HG2	5	0.49
(1,2058)	1:363:A:ILE:H	1:358:A:ASP:HB2	7	0.49
(1,1918)	1:354:A:ILE:HD11	1:366:A:ILE:HD12	12	0.49
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD21	8	0.49
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD22	15	0.49
(1,1800)	1:336:A:LEU:HD12	1:338:A:TRP:HD1	5	0.49
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD13	2	0.49
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD21	8	0.49
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD21	9	0.49
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD21	15	0.49
(1,1690)	1:402:A:ILE:HD11	1:400:A:LEU:HA	6	0.49
(1,1686)	1:402:A:ILE:HG21	1:403:A:ILE:HG12	19	0.49
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD11	19	0.49
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD13	19	0.49
(1,1523)	1:422:A:ILE:HG23	1:426:A:ARG:HG2	12	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1484)	1:432:A:HIS:HB3	1:430:A:LEU:H	19	0.49
(1,1480)	1:412:A:LEU:HD23	1:357:A:GLU:HG2	3	0.49
(1,1480)	1:412:A:LEU:HD22	1:357:A:GLU:HG2	8	0.49
(1,1475)	1:433:A:LEU:HD23	1:434:A:GLU:H	2	0.49
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	10	0.49
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD23	5	0.49
(1,1316)	1:433:A:LEU:HD21	1:396:A:HIS:HD2	9	0.49
(1,1316)	1:433:A:LEU:HD23	1:396:A:HIS:HD2	10	0.49
(1,1266)	1:354:A:ILE:HD12	1:365:A:ARG:H	7	0.49
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD22	2	0.49
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD13	4	0.49
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD11	15	0.49
(1,1135)	1:367:A:VAL:HG13	1:352:A:ASN:H	3	0.49
(1,1119)	1:367:A:VAL:HG21	1:355:A:ARG:HA	7	0.49
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	4	0.49
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	6	0.49
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	7	0.49
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	8	0.49
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	13	0.49
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	18	0.49
(1,1025)	1:336:A:LEU:HD22	1:430:A:LEU:H	7	0.49
(1,1006)	1:380:A:LYS:HA	1:380:A:LYS:HD3	6	0.49
(1,1006)	1:380:A:LYS:HA	1:380:A:LYS:HD3	14	0.49
(1,973)	1:452:A:SER:H	1:452:A:SER:HB2	8	0.49
(1,937)	1:444:A:GLN:HE22	1:444:A:GLN:HG2	18	0.49
(1,908)	1:411:A:LEU:HD22	1:366:A:ILE:H	19	0.49
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB3	8	0.49
(1,834)	1:430:A:LEU:HD13	1:397:A:TYR:HD1	12	0.49
(1,834)	1:430:A:LEU:HD12	1:397:A:TYR:HD1	19	0.49
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD11	15	0.49
(1,456)	1:386:A:THR:HG23	1:387:A:TYR:HB2	4	0.49
(1,456)	1:386:A:THR:HG21	1:387:A:TYR:HB2	13	0.49
(1,456)	1:386:A:THR:HG22	1:387:A:TYR:HB2	14	0.49
(1,452)	1:423:A:MET:HG2	1:423:A:MET:HB2	13	0.49
(1,445)	1:384:A:ASN:HD22	1:384:A:ASN:HB2	4	0.49
(1,445)	1:384:A:ASN:HD22	1:384:A:ASN:HB2	8	0.49
(1,445)	1:384:A:ASN:HD22	1:384:A:ASN:HB2	15	0.49
(1,444)	1:384:A:ASN:HD21	1:384:A:ASN:HB2	4	0.49
(1,444)	1:384:A:ASN:HD21	1:384:A:ASN:HB2	14	0.49
(1,444)	1:384:A:ASN:HD21	1:384:A:ASN:HB2	15	0.49
(1,400)	1:377:A:GLY:HA3	1:382:A:ARG:HB3	19	0.49
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD13	10	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:366:A:ILE:HG22	1:411:A:LEU:HB3	3	0.49
(1,300)	1:366:A:ILE:HG21	1:411:A:LEU:HB3	19	0.49
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	9	0.49
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	14	0.49
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD11	11	0.49
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD12	18	0.49
(1,35)	1:341:A:VAL:HG12	1:345:A:LEU:HD12	3	0.49
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	10	0.48
(1,2947)	1:362:A:LYS:H	1:363:A:ILE:HB	4	0.48
(1,2947)	1:362:A:LYS:H	1:363:A:ILE:HB	10	0.48
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	6	0.48
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	19	0.48
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	17	0.48
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG22	1	0.48
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG21	3	0.48
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG21	8	0.48
(1,2884)	1:397:A:TYR:HE1	1:393:A:ALA:HA	16	0.48
(1,2884)	1:397:A:TYR:HE1	1:397:A:TYR:HA	17	0.48
(1,2860)	1:340:A:TYR:H	1:340:A:TYR:HD2	2	0.48
(1,2860)	1:340:A:TYR:HD1	1:340:A:TYR:H	10	0.48
(1,2860)	1:340:A:TYR:H	1:340:A:TYR:HD2	13	0.48
(1,2858)	1:341:A:VAL:HG13	1:340:A:TYR:HD2	4	0.48
(1,2858)	1:341:A:VAL:HG11	1:340:A:TYR:HD2	7	0.48
(1,2828)	1:412:A:LEU:HD11	1:413:A:PHE:HD1	12	0.48
(1,2799)	1:412:A:LEU:HD22	1:365:A:ARG:HD3	2	0.48
(1,2797)	1:433:A:LEU:HD13	1:434:A:GLU:HA	9	0.48
(1,2789)	1:438:A:LEU:HD11	1:381:A:ASN:HD22	11	0.48
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	10	0.48
(1,2775)	1:387:A:TYR:HD1	1:390:A:MET:HG2	1	0.48
(1,2770)	1:373:A:ALA:HB2	1:371:A:GLY:H	15	0.48
(1,2726)	1:367:A:VAL:HG12	1:355:A:ARG:HD3	13	0.48
(1,2724)	1:367:A:VAL:HG23	1:352:A:ASN:HA	8	0.48
(1,2688)	1:440:A:GLU:HG2	1:440:A:GLU:HB3	9	0.48
(1,2681)	1:418:A:THR:HG22	1:342:A:TYR:HD1	13	0.48
(1,2675)	1:417:A:LYS:HD2	1:402:A:ILE:HG13	6	0.48
(1,2675)	1:417:A:LYS:HD2	1:402:A:ILE:HG13	11	0.48
(1,2675)	1:417:A:LYS:HD2	1:402:A:ILE:HG13	19	0.48
(1,2658)	1:366:A:ILE:HG23	1:411:A:LEU:HB2	10	0.48
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	5	0.48
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	13	0.48
(1,2649)	1:403:A:ILE:HG23	1:364:A:PHE:HZ	17	0.48
(1,2643)	1:402:A:ILE:HD13	1:397:A:TYR:HD1	7	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2640)	1:400:A:LEU:HD21	1:430:A:LEU:HD21	14	0.48
(1,2617)	1:375:A:LEU:HB2	1:376:A:TRP:HB3	18	0.48
(1,2607)	1:367:A:VAL:HA	1:365:A:ARG:HD2	17	0.48
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB2	18	0.48
(1,2597)	1:358:A:ASP:HB3	1:363:A:ILE:HG21	14	0.48
(1,2555)	1:340:A:TYR:HA	1:339:A:ASP:HB3	1	0.48
(1,2550)	1:451:A:ALA:H	1:450:A:ILE:HG22	5	0.48
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG22	2	0.48
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG22	9	0.48
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG23	14	0.48
(1,2527)	1:367:A:VAL:HG13	1:368:A:ASP:H	5	0.48
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	10	0.48
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD13	14	0.48
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD13	16	0.48
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	2	0.48
(1,2415)	1:447:A:GLU:H	1:448:A:PRO:HD3	15	0.48
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB2	5	0.48
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB3	15	0.48
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB2	17	0.48
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB3	19	0.48
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	4	0.48
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG23	14	0.48
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG21	16	0.48
(1,1918)	1:354:A:ILE:HD13	1:366:A:ILE:HD11	9	0.48
(1,1918)	1:354:A:ILE:HD13	1:366:A:ILE:HD13	14	0.48
(1,1904)	1:437:A:VAL:HG13	1:438:A:LEU:HD21	8	0.48
(1,1899)	1:430:A:LEU:HD12	1:400:A:LEU:HD22	16	0.48
(1,1895)	1:411:A:LEU:HD21	1:366:A:ILE:HD11	19	0.48
(1,1885)	1:400:A:LEU:HD23	1:402:A:ILE:HD13	2	0.48
(1,1885)	1:400:A:LEU:HD23	1:402:A:ILE:HD11	4	0.48
(1,1885)	1:400:A:LEU:HD23	1:402:A:ILE:HD12	14	0.48
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB1	10	0.48
(1,1873)	1:383:A:THR:HG23	1:384:A:ASN:HD22	10	0.48
(1,1855)	1:430:A:LEU:HD23	1:397:A:TYR:HE1	18	0.48
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD22	6	0.48
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD23	13	0.48
(1,1800)	1:336:A:LEU:HD12	1:338:A:TRP:HD1	3	0.48
(1,1800)	1:336:A:LEU:HD11	1:338:A:TRP:HD1	17	0.48
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD12	1	0.48
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD13	4	0.48
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD12	6	0.48
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD13	7	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD13	9	0.48
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD13	10	0.48
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD11	13	0.48
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD13	16	0.48
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD11	17	0.48
(1,1771)	1:341:A:VAL:HG11	1:337:A:LEU:HD13	1	0.48
(1,1771)	1:341:A:VAL:HG13	1:337:A:LEU:HD11	4	0.48
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD23	2	0.48
(1,1709)	1:344:A:LEU:HD23	1:345:A:LEU:H	3	0.48
(1,1709)	1:344:A:LEU:HD22	1:345:A:LEU:H	9	0.48
(1,1709)	1:344:A:LEU:HD22	1:345:A:LEU:H	17	0.48
(1,1686)	1:402:A:ILE:HG22	1:403:A:ILE:HG12	18	0.48
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD22	6	0.48
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD23	19	0.48
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD12	3	0.48
(1,1523)	1:422:A:ILE:HG22	1:426:A:ARG:HG2	7	0.48
(1,1484)	1:432:A:HIS:HB3	1:430:A:LEU:H	13	0.48
(1,1480)	1:412:A:LEU:HD23	1:357:A:GLU:HG2	18	0.48
(1,1424)	1:450:A:ILE:HG21	1:452:A:SER:HB2	4	0.48
(1,1392)	1:386:A:THR:HG21	1:389:A:LYS:HG2	16	0.48
(1,1201)	1:363:A:ILE:HG13	1:361:A:SER:HB2	3	0.48
(1,1201)	1:363:A:ILE:HG13	1:361:A:SER:HB2	18	0.48
(1,1193)	1:362:A:LYS:HE2	1:362:A:LYS:HA	13	0.48
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD11	11	0.48
(1,1135)	1:367:A:VAL:HG12	1:352:A:ASN:H	4	0.48
(1,1135)	1:367:A:VAL:HG13	1:352:A:ASN:H	14	0.48
(1,1135)	1:367:A:VAL:HG11	1:352:A:ASN:H	17	0.48
(1,1133)	1:367:A:VAL:HG11	1:352:A:ASN:HB3	12	0.48
(1,1126)	1:355:A:ARG:HD2	1:367:A:VAL:HG22	11	0.48
(1,1121)	1:367:A:VAL:HG23	1:365:A:ARG:HA	6	0.48
(1,1119)	1:367:A:VAL:HG22	1:355:A:ARG:HA	4	0.48
(1,1006)	1:380:A:LYS:HA	1:380:A:LYS:HD3	1	0.48
(1,1006)	1:380:A:LYS:HA	1:380:A:LYS:HD3	13	0.48
(1,954)	1:450:A:ILE:H	1:449:A:THR:HA	18	0.48
(1,620)	1:403:A:ILE:HG21	1:403:A:ILE:H	1	0.48
(1,620)	1:403:A:ILE:HG21	1:403:A:ILE:H	6	0.48
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	2	0.48
(1,478)	1:389:A:LYS:HG3	1:389:A:LYS:HE2	14	0.48
(1,457)	1:386:A:THR:HG23	1:389:A:LYS:HB2	19	0.48
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	1	0.48
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	2	0.48
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	5	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	11	0.48
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	16	0.48
(1,205)	1:357:A:GLU:HB3	1:363:A:ILE:HG22	15	0.48
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD13	17	0.48
(1,127)	1:349:A:ARG:HD2	1:350:A:TYR:HE1	18	0.48
(1,55)	1:344:A:LEU:H	1:343:A:GLN:HB2	8	0.48
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB2	8	0.47
(1,2981)	1:428:A:ASP:H	1:427:A:THR:HG22	1	0.47
(1,2947)	1:362:A:LYS:H	1:363:A:ILE:HB	5	0.47
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	5	0.47
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	6	0.47
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD23	11	0.47
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG23	6	0.47
(1,2880)	1:402:A:ILE:HG21	1:397:A:TYR:HE2	3	0.47
(1,2860)	1:340:A:TYR:H	1:340:A:TYR:HD2	6	0.47
(1,2860)	1:340:A:TYR:H	1:340:A:TYR:HD2	7	0.47
(1,2860)	1:340:A:TYR:H	1:340:A:TYR:HD2	11	0.47
(1,2860)	1:340:A:TYR:H	1:340:A:TYR:HD2	15	0.47
(1,2797)	1:433:A:LEU:HD12	1:434:A:GLU:HA	11	0.47
(1,2797)	1:433:A:LEU:HD12	1:434:A:GLU:HA	15	0.47
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	1	0.47
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	11	0.47
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	13	0.47
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE3	5	0.47
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG22	18	0.47
(1,2688)	1:440:A:GLU:HG2	1:440:A:GLU:HB3	14	0.47
(1,2681)	1:418:A:THR:HG23	1:342:A:TYR:HD1	2	0.47
(1,2658)	1:366:A:ILE:HG22	1:411:A:LEU:HB2	13	0.47
(1,2657)	1:411:A:LEU:HB2	1:413:A:PHE:HZ	8	0.47
(1,2645)	1:402:A:ILE:HD13	1:338:A:TRP:HB3	3	0.47
(1,2645)	1:402:A:ILE:HD12	1:338:A:TRP:HB3	12	0.47
(1,2645)	1:402:A:ILE:HD11	1:338:A:TRP:HB3	18	0.47
(1,2643)	1:402:A:ILE:HD13	1:397:A:TYR:HD1	6	0.47
(1,2618)	1:375:A:LEU:HD21	1:378:A:ASN:HB2	3	0.47
(1,2618)	1:375:A:LEU:HD21	1:378:A:ASN:HB2	8	0.47
(1,2587)	1:362:A:LYS:HA	1:415:A:PHE:HD2	9	0.47
(1,2569)	1:349:A:ARG:HD3	1:350:A:TYR:HE1	5	0.47
(1,2557)	1:341:A:VAL:HG12	1:403:A:ILE:HD13	17	0.47
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	9	0.47
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD12	9	0.47
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	1	0.47
(1,2447)	1:385:A:MET:H	1:444:A:GLN:HE21	16	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	11	0.47
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB3	12	0.47
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	8	0.47
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	14	0.47
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	17	0.47
(1,2129)	1:447:A:GLU:H	1:447:A:GLU:HB3	11	0.47
(1,1837)	1:448:A:PRO:HD2	1:448:A:PRO:HB2	17	0.47
(1,1802)	1:336:A:LEU:HD11	1:431:A:GLU:HA	13	0.47
(1,1800)	1:336:A:LEU:HD12	1:338:A:TRP:HD1	2	0.47
(1,1800)	1:336:A:LEU:HD13	1:338:A:TRP:HD1	7	0.47
(1,1800)	1:336:A:LEU:HD11	1:338:A:TRP:HD1	15	0.47
(1,1776)	1:337:A:LEU:HD13	1:390:A:MET:HG3	9	0.47
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD13	8	0.47
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD12	14	0.47
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD13	15	0.47
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD12	19	0.47
(1,1709)	1:344:A:LEU:HD21	1:345:A:LEU:H	5	0.47
(1,1709)	1:344:A:LEU:HD21	1:345:A:LEU:H	6	0.47
(1,1686)	1:402:A:ILE:HG22	1:403:A:ILE:HG12	11	0.47
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG21	9	0.47
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD12	17	0.47
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD12	18	0.47
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD21	2	0.47
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD22	11	0.47
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD21	18	0.47
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD13	5	0.47
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	5	0.47
(1,1484)	1:432:A:HIS:HB3	1:430:A:LEU:H	15	0.47
(1,1427)	1:447:A:GLU:HA	1:448:A:PRO:HD3	9	0.47
(1,1424)	1:450:A:ILE:HG23	1:452:A:SER:HB2	19	0.47
(1,1393)	1:386:A:THR:HG22	1:388:A:GLU:HB3	7	0.47
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	3	0.47
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	18	0.47
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD22	14	0.47
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD22	18	0.47
(1,1330)	1:400:A:LEU:HD12	1:399:A:LYS:HB2	19	0.47
(1,1304)	1:376:A:TRP:HZ2	1:380:A:LYS:HE3	16	0.47
(1,1266)	1:354:A:ILE:HD11	1:365:A:ARG:H	9	0.47
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD22	4	0.47
(1,1201)	1:363:A:ILE:HG13	1:361:A:SER:HB2	9	0.47
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD11	16	0.47
(1,1135)	1:367:A:VAL:HG12	1:352:A:ASN:H	7	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	17	0.47
(1,1025)	1:336:A:LEU:HD21	1:430:A:LEU:H	17	0.47
(1,1021)	1:437:A:VAL:HG12	1:396:A:HIS:HD2	8	0.47
(1,1021)	1:437:A:VAL:HG11	1:396:A:HIS:HD2	16	0.47
(1,1006)	1:380:A:LYS:HA	1:380:A:LYS:HD3	4	0.47
(1,1005)	1:382:A:ARG:HD2	1:382:A:ARG:HA	10	0.47
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	12	0.47
(1,973)	1:452:A:SER:H	1:452:A:SER:HB2	16	0.47
(1,937)	1:444:A:GLN:HE22	1:444:A:GLN:HG2	7	0.47
(1,908)	1:411:A:LEU:HD23	1:366:A:ILE:H	3	0.47
(1,620)	1:403:A:ILE:HG21	1:403:A:ILE:H	14	0.47
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD12	19	0.47
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	8	0.47
(1,478)	1:389:A:LYS:HG3	1:389:A:LYS:HE2	3	0.47
(1,444)	1:384:A:ASN:HD21	1:384:A:ASN:HB2	8	0.47
(1,346)	1:372:A:LEU:HB2	1:372:A:LEU:HD13	14	0.47
(1,297)	1:366:A:ILE:HG21	1:368:A:ASP:HA	8	0.47
(1,297)	1:366:A:ILE:HG21	1:368:A:ASP:HA	14	0.47
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	4	0.47
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	7	0.47
(1,204)	1:357:A:GLU:HB3	1:412:A:LEU:HD12	12	0.47
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	15	0.47
(1,127)	1:349:A:ARG:HD2	1:350:A:TYR:HE1	19	0.47
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG21	4	0.46
(1,2974)	1:433:A:LEU:H	1:436:A:GLN:HB2	13	0.46
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	9	0.46
(1,2887)	1:336:A:LEU:H	1:336:A:LEU:HD11	7	0.46
(1,2872)	1:447:A:GLU:HG3	1:447:A:GLU:HB2	13	0.46
(1,2860)	1:340:A:TYR:H	1:340:A:TYR:HD2	17	0.46
(1,2858)	1:341:A:VAL:HG11	1:340:A:TYR:HD2	6	0.46
(1,2858)	1:341:A:VAL:HG13	1:340:A:TYR:HD2	12	0.46
(1,2850)	1:344:A:LEU:HD12	1:350:A:TYR:HD2	19	0.46
(1,2844)	1:402:A:ILE:HG21	1:397:A:TYR:HD2	10	0.46
(1,2844)	1:402:A:ILE:HG22	1:397:A:TYR:HD2	19	0.46
(1,2828)	1:412:A:LEU:HD12	1:413:A:PHE:HD1	7	0.46
(1,2813)	1:418:A:THR:HG23	1:362:A:LYS:HD2	8	0.46
(1,2797)	1:433:A:LEU:HD13	1:434:A:GLU:HA	18	0.46
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	6	0.46
(1,2762)	1:394:A:LEU:HD21	1:398:A:TYR:HE1	2	0.46
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG23	8	0.46
(1,2696)	1:438:A:LEU:HD23	1:382:A:ARG:HD2	16	0.46
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG3	11	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2688)	1:440:A:GLU:HG2	1:440:A:GLU:HB3	10	0.46
(1,2688)	1:440:A:GLU:HG2	1:440:A:GLU:HB3	15	0.46
(1,2688)	1:440:A:GLU:HG2	1:440:A:GLU:HB3	17	0.46
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD13	4	0.46
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD12	6	0.46
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD11	9	0.46
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD13	11	0.46
(1,2658)	1:366:A:ILE:HG21	1:411:A:LEU:HB2	1	0.46
(1,2658)	1:366:A:ILE:HG21	1:411:A:LEU:HB2	8	0.46
(1,2612)	1:393:A:ALA:HB3	1:376:A:TRP:HZ3	15	0.46
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB3	16	0.46
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB3	17	0.46
(1,2556)	1:341:A:VAL:HG12	1:364:A:PHE:HZ	7	0.46
(1,2550)	1:451:A:ALA:H	1:450:A:ILE:HG23	17	0.46
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD22	3	0.46
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD23	4	0.46
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD23	17	0.46
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD11	4	0.46
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD13	19	0.46
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD13	6	0.46
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	11	0.46
(1,2423)	1:441:A:GLN:H	1:441:A:GLN:HB2	17	0.46
(1,2415)	1:447:A:GLU:H	1:448:A:PRO:HD3	19	0.46
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	3	0.46
(1,2275)	1:365:A:ARG:HE	1:412:A:LEU:HD11	17	0.46
(1,2258)	1:450:A:ILE:H	1:450:A:ILE:HG13	14	0.46
(1,2252)	1:442:A:THR:H	1:441:A:GLN:HB3	5	0.46
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB2	4	0.46
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB3	7	0.46
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB3	11	0.46
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	2	0.46
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	5	0.46
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	7	0.46
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	12	0.46
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	19	0.46
(1,2058)	1:363:A:ILE:H	1:358:A:ASP:HB2	2	0.46
(1,1919)	1:367:A:VAL:HG23	1:367:A:VAL:HG13	3	0.46
(1,1919)	1:367:A:VAL:HG23	1:367:A:VAL:HG12	7	0.46
(1,1919)	1:367:A:VAL:HG21	1:367:A:VAL:HG11	10	0.46
(1,1919)	1:367:A:VAL:HG22	1:367:A:VAL:HG13	14	0.46
(1,1919)	1:367:A:VAL:HG22	1:367:A:VAL:HG11	16	0.46
(1,1919)	1:367:A:VAL:HG22	1:367:A:VAL:HG11	17	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1906)	1:451:A:ALA:HB2	1:449:A:THR:HG23	1	0.46
(1,1904)	1:437:A:VAL:HG11	1:438:A:LEU:HD23	9	0.46
(1,1904)	1:437:A:VAL:HG13	1:438:A:LEU:HD22	19	0.46
(1,1895)	1:411:A:LEU:HD23	1:366:A:ILE:HD12	13	0.46
(1,1885)	1:400:A:LEU:HD22	1:402:A:ILE:HD11	7	0.46
(1,1871)	1:426:A:ARG:HD2	1:426:A:ARG:HB3	18	0.46
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD23	7	0.46
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD21	10	0.46
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD23	16	0.46
(1,1800)	1:336:A:LEU:HD12	1:338:A:TRP:HD1	16	0.46
(1,1771)	1:341:A:VAL:HG13	1:337:A:LEU:HD13	14	0.46
(1,1771)	1:341:A:VAL:HG11	1:337:A:LEU:HD12	17	0.46
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD22	11	0.46
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD21	13	0.46
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD22	17	0.46
(1,1709)	1:344:A:LEU:HD23	1:345:A:LEU:H	1	0.46
(1,1709)	1:344:A:LEU:HD23	1:345:A:LEU:H	8	0.46
(1,1709)	1:344:A:LEU:HD22	1:345:A:LEU:H	15	0.46
(1,1709)	1:344:A:LEU:HD21	1:345:A:LEU:H	16	0.46
(1,1690)	1:402:A:ILE:HD12	1:400:A:LEU:HA	1	0.46
(1,1686)	1:402:A:ILE:HG21	1:403:A:ILE:HG12	2	0.46
(1,1686)	1:402:A:ILE:HG21	1:403:A:ILE:HG12	5	0.46
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG23	16	0.46
(1,1671)	1:403:A:ILE:HG21	1:405:A:LYS:HA	6	0.46
(1,1653)	1:404:A:ARG:HG2	1:414:A:ARG:HD3	7	0.46
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD21	3	0.46
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD23	9	0.46
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD21	12	0.46
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	1	0.46
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	4	0.46
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	10	0.46
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD11	4	0.46
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD12	8	0.46
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	1	0.46
(1,1509)	1:426:A:ARG:HG3	1:426:A:ARG:HB2	3	0.46
(1,1509)	1:426:A:ARG:HG3	1:426:A:ARG:HB2	11	0.46
(1,1509)	1:426:A:ARG:HG3	1:426:A:ARG:HB2	18	0.46
(1,1509)	1:426:A:ARG:HG3	1:426:A:ARG:HB2	19	0.46
(1,1484)	1:432:A:HIS:HB3	1:430:A:LEU:H	6	0.46
(1,1480)	1:412:A:LEU:HD21	1:357:A:GLU:HG2	5	0.46
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	7	0.46
(1,1427)	1:447:A:GLU:HA	1:448:A:PRO:HD3	15	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1424)	1:450:A:ILE:HG22	1:452:A:SER:HB2	13	0.46
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD21	4	0.46
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD23	13	0.46
(1,1316)	1:433:A:LEU:HD22	1:396:A:HIS:HD2	3	0.46
(1,1266)	1:354:A:ILE:HD12	1:365:A:ARG:H	1	0.46
(1,1266)	1:354:A:ILE:HD11	1:365:A:ARG:H	16	0.46
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD21	6	0.46
(1,1193)	1:362:A:LYS:HE2	1:362:A:LYS:HA	14	0.46
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD13	10	0.46
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD12	13	0.46
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD13	14	0.46
(1,1142)	1:450:A:ILE:HD13	1:454:A:VAL:HA	3	0.46
(1,1135)	1:367:A:VAL:HG13	1:352:A:ASN:H	8	0.46
(1,1135)	1:367:A:VAL:HG11	1:352:A:ASN:H	19	0.46
(1,1133)	1:367:A:VAL:HG12	1:352:A:ASN:HB3	7	0.46
(1,1006)	1:380:A:LYS:HA	1:380:A:LYS:HD3	5	0.46
(1,1006)	1:380:A:LYS:HA	1:380:A:LYS:HD3	7	0.46
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	8	0.46
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	15	0.46
(1,958)	1:449:A:THR:H	1:449:A:THR:HG23	6	0.46
(1,945)	1:447:A:GLU:H	1:447:A:GLU:HG2	11	0.46
(1,834)	1:430:A:LEU:HD11	1:397:A:TYR:HD1	7	0.46
(1,834)	1:430:A:LEU:HD11	1:397:A:TYR:HD1	15	0.46
(1,620)	1:403:A:ILE:HG22	1:403:A:ILE:H	7	0.46
(1,620)	1:403:A:ILE:HG21	1:403:A:ILE:H	12	0.46
(1,620)	1:403:A:ILE:HG23	1:403:A:ILE:H	13	0.46
(1,620)	1:403:A:ILE:HG22	1:403:A:ILE:H	15	0.46
(1,549)	1:396:A:HIS:HB3	1:430:A:LEU:HD22	17	0.46
(1,544)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	5	0.46
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD13	3	0.46
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	3	0.46
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	9	0.46
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	12	0.46
(1,457)	1:386:A:THR:HG22	1:389:A:LYS:HB2	1	0.46
(1,457)	1:386:A:THR:HG22	1:389:A:LYS:HB2	8	0.46
(1,456)	1:386:A:THR:HG22	1:387:A:TYR:HB2	15	0.46
(1,297)	1:366:A:ILE:HG22	1:368:A:ASP:HA	13	0.46
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	12	0.46
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	15	0.46
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	18	0.46
(1,5)	1:337:A:LEU:HD22	1:390:A:MET:HG3	3	0.46
(1,2947)	1:362:A:LYS:H	1:363:A:ILE:HB	14	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	17	0.45
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	3	0.45
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD21	10	0.45
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG21	5	0.45
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG21	16	0.45
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG22	18	0.45
(1,2860)	1:340:A:TYR:H	1:340:A:TYR:HD2	18	0.45
(1,2858)	1:341:A:VAL:HG12	1:340:A:TYR:HD2	15	0.45
(1,2794)	1:433:A:LEU:HD23	1:429:A:ARG:HD2	16	0.45
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	3	0.45
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	7	0.45
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	8	0.45
(1,2775)	1:387:A:TYR:HD2	1:390:A:MET:HG2	6	0.45
(1,2774)	1:443:A:TYR:HD1	1:445:A:GLU:HB2	8	0.45
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD12	17	0.45
(1,2658)	1:366:A:ILE:HG23	1:411:A:LEU:HB2	7	0.45
(1,2658)	1:366:A:ILE:HG22	1:411:A:LEU:HB2	12	0.45
(1,2658)	1:366:A:ILE:HG23	1:411:A:LEU:HB2	18	0.45
(1,2643)	1:402:A:ILE:HD11	1:397:A:TYR:HD1	1	0.45
(1,2618)	1:375:A:LEU:HD22	1:378:A:ASN:HB2	19	0.45
(1,2612)	1:393:A:ALA:HB2	1:376:A:TRP:HZ3	4	0.45
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB3	6	0.45
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB2	15	0.45
(1,2587)	1:361:A:SER:H	1:362:A:LYS:HA	15	0.45
(1,2555)	1:340:A:TYR:HA	1:339:A:ASP:HB3	2	0.45
(1,2551)	1:451:A:ALA:H	1:451:A:ALA:HB2	15	0.45
(1,2550)	1:451:A:ALA:H	1:450:A:ILE:HG21	12	0.45
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG21	3	0.45
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG23	5	0.45
(1,2493)	1:440:A:GLU:H	1:439:A:ASP:HB3	17	0.45
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	16	0.45
(1,2473)	1:409:A:GLN:HE21	1:412:A:LEU:HD12	18	0.45
(1,2423)	1:441:A:GLN:H	1:441:A:GLN:HB2	1	0.45
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	6	0.45
(1,2359)	1:382:A:ARG:H	1:382:A:ARG:HG3	4	0.45
(1,2321)	1:350:A:TYR:H	1:350:A:TYR:HD1	12	0.45
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB3	9	0.45
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB3	16	0.45
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	9	0.45
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	10	0.45
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	13	0.45
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	15	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	16	0.45
(1,2058)	1:363:A:ILE:H	1:358:A:ASP:HB2	1	0.45
(1,1980)	1:350:A:TYR:H	1:348:A:SER:HA	19	0.45
(1,1919)	1:367:A:VAL:HG22	1:367:A:VAL:HG13	2	0.45
(1,1919)	1:367:A:VAL:HG21	1:367:A:VAL:HG13	6	0.45
(1,1919)	1:367:A:VAL:HG22	1:367:A:VAL:HG11	9	0.45
(1,1906)	1:451:A:ALA:HB1	1:449:A:THR:HG21	13	0.45
(1,1904)	1:437:A:VAL:HG11	1:438:A:LEU:HD23	11	0.45
(1,1899)	1:430:A:LEU:HD13	1:400:A:LEU:HD22	3	0.45
(1,1899)	1:430:A:LEU:HD13	1:400:A:LEU:HD22	7	0.45
(1,1885)	1:400:A:LEU:HD23	1:402:A:ILE:HD13	5	0.45
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD23	3	0.45
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD23	12	0.45
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD23	14	0.45
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD21	18	0.45
(1,1800)	1:336:A:LEU:HD11	1:338:A:TRP:HD1	1	0.45
(1,1780)	1:337:A:LEU:HD13	1:376:A:TRP:HA	19	0.45
(1,1778)	1:337:A:LEU:HD11	1:376:A:TRP:HB3	3	0.45
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD11	3	0.45
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD13	18	0.45
(1,1771)	1:341:A:VAL:HG12	1:337:A:LEU:HD11	9	0.45
(1,1709)	1:344:A:LEU:HD23	1:345:A:LEU:H	18	0.45
(1,1686)	1:402:A:ILE:HG23	1:403:A:ILE:HG12	10	0.45
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG23	3	0.45
(1,1609)	1:411:A:LEU:HD22	1:387:A:TYR:HB2	5	0.45
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD23	17	0.45
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	2	0.45
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	5	0.45
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	6	0.45
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	7	0.45
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	8	0.45
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	11	0.45
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	12	0.45
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	13	0.45
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	14	0.45
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	15	0.45
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	17	0.45
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	18	0.45
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD11	6	0.45
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD11	11	0.45
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD12	14	0.45
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG21	19	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1480)	1:412:A:LEU:HD21	1:357:A:GLU:HG2	6	0.45
(1,1430)	1:447:A:GLU:HB2	1:448:A:PRO:HD3	13	0.45
(1,1422)	1:451:A:ALA:HB3	1:450:A:ILE:HA	7	0.45
(1,1422)	1:451:A:ALA:HB3	1:450:A:ILE:HA	10	0.45
(1,1422)	1:451:A:ALA:HB3	1:450:A:ILE:HA	13	0.45
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	6	0.45
(1,1266)	1:354:A:ILE:HD11	1:365:A:ARG:H	8	0.45
(1,1266)	1:354:A:ILE:HD12	1:365:A:ARG:H	11	0.45
(1,1266)	1:354:A:ILE:HD12	1:365:A:ARG:H	15	0.45
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD21	7	0.45
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD22	14	0.45
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD3	2	0.45
(1,1182)	1:363:A:ILE:HD13	1:406:A:GLU:HG2	12	0.45
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD13	12	0.45
(1,1135)	1:367:A:VAL:HG11	1:352:A:ASN:H	10	0.45
(1,1135)	1:367:A:VAL:HG11	1:352:A:ASN:H	12	0.45
(1,1135)	1:367:A:VAL:HG12	1:352:A:ASN:H	13	0.45
(1,1051)	1:350:A:TYR:HB2	1:350:A:TYR:HD1	15	0.45
(1,1021)	1:437:A:VAL:HG13	1:396:A:HIS:HD2	1	0.45
(1,1021)	1:437:A:VAL:HG11	1:396:A:HIS:HD2	5	0.45
(1,1021)	1:437:A:VAL:HG11	1:396:A:HIS:HD2	12	0.45
(1,1006)	1:380:A:LYS:HA	1:380:A:LYS:HD3	8	0.45
(1,1006)	1:380:A:LYS:HA	1:380:A:LYS:HD3	15	0.45
(1,998)	1:375:A:LEU:H	1:374:A:ARG:HB2	3	0.45
(1,884)	1:437:A:VAL:HG22	1:392:A:ARG:HG3	4	0.45
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB2	14	0.45
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB3	15	0.45
(1,825)	1:392:A:ARG:HD3	1:392:A:ARG:HB3	16	0.45
(1,690)	1:411:A:LEU:HD22	1:369:A:PRO:HB2	7	0.45
(1,690)	1:411:A:LEU:HD23	1:369:A:PRO:HB2	12	0.45
(1,620)	1:403:A:ILE:HG21	1:403:A:ILE:H	4	0.45
(1,620)	1:403:A:ILE:HG21	1:403:A:ILE:H	11	0.45
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD23	15	0.45
(1,457)	1:386:A:THR:HG22	1:389:A:LYS:HB2	10	0.45
(1,456)	1:386:A:THR:HG23	1:387:A:TYR:HB2	12	0.45
(1,297)	1:366:A:ILE:HG23	1:368:A:ASP:HA	5	0.45
(1,297)	1:366:A:ILE:HG22	1:368:A:ASP:HA	11	0.45
(1,297)	1:366:A:ILE:HG22	1:368:A:ASP:HA	12	0.45
(1,297)	1:366:A:ILE:HG21	1:368:A:ASP:HA	19	0.45
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	3	0.45
(1,155)	1:354:A:ILE:HA	1:354:A:ILE:HD11	15	0.45
(1,85)	1:344:A:LEU:HD21	1:350:A:TYR:HD1	18	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,57)	1:343:A:GLN:HG3	1:344:A:LEU:HD23	8	0.45
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB2	18	0.44
(1,2972)	1:435:A:SER:H	1:436:A:GLN:HG3	6	0.44
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	15	0.44
(1,2895)	1:353:A:PHE:H	1:367:A:VAL:HG22	14	0.44
(1,2895)	1:353:A:PHE:H	1:367:A:VAL:HG23	15	0.44
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG22	17	0.44
(1,2872)	1:447:A:GLU:HG3	1:447:A:GLU:HB2	9	0.44
(1,2872)	1:445:A:GLU:HB2	1:445:A:GLU:HG2	14	0.44
(1,2860)	1:340:A:TYR:H	1:340:A:TYR:HD2	5	0.44
(1,2860)	1:340:A:TYR:H	1:340:A:TYR:HD2	16	0.44
(1,2850)	1:344:A:LEU:HD11	1:350:A:TYR:HD1	18	0.44
(1,2837)	1:410:A:ARG:HB2	1:410:A:ARG:HD3	7	0.44
(1,2837)	1:404:A:ARG:HD3	1:404:A:ARG:HB3	8	0.44
(1,2799)	1:412:A:LEU:HD22	1:365:A:ARG:HD3	15	0.44
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	7	0.44
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG23	7	0.44
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG22	14	0.44
(1,2697)	1:447:A:GLU:HG3	1:447:A:GLU:HB2	13	0.44
(1,2688)	1:440:A:GLU:HG2	1:440:A:GLU:HB3	8	0.44
(1,2683)	1:429:A:ARG:HG2	1:429:A:ARG:H	15	0.44
(1,2681)	1:418:A:THR:HG22	1:342:A:TYR:HD1	9	0.44
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD13	1	0.44
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD13	8	0.44
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD12	12	0.44
(1,2649)	1:403:A:ILE:HG21	1:364:A:PHE:HZ	3	0.44
(1,2640)	1:400:A:LEU:HD21	1:430:A:LEU:HD22	12	0.44
(1,2618)	1:375:A:LEU:HD21	1:378:A:ASN:HB2	16	0.44
(1,2607)	1:367:A:VAL:HA	1:365:A:ARG:HD2	6	0.44
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB2	9	0.44
(1,2556)	1:341:A:VAL:HG12	1:364:A:PHE:HZ	1	0.44
(1,2552)	1:452:A:SER:H	1:451:A:ALA:HB2	16	0.44
(1,2552)	1:452:A:SER:H	1:451:A:ALA:HB3	17	0.44
(1,2527)	1:367:A:VAL:HG13	1:368:A:ASP:H	10	0.44
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD12	13	0.44
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	2	0.44
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	5	0.44
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB2	14	0.44
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	13	0.44
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	15	0.44
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG21	6	0.44
(1,2048)	1:361:A:SER:H	1:358:A:ASP:HB2	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	15	0.44
(1,1980)	1:350:A:TYR:H	1:348:A:SER:HA	13	0.44
(1,1919)	1:367:A:VAL:HG22	1:367:A:VAL:HG13	11	0.44
(1,1919)	1:367:A:VAL:HG21	1:367:A:VAL:HG11	12	0.44
(1,1906)	1:451:A:ALA:HB1	1:449:A:THR:HG21	2	0.44
(1,1906)	1:451:A:ALA:HB2	1:449:A:THR:HG23	8	0.44
(1,1904)	1:437:A:VAL:HG12	1:438:A:LEU:HD22	10	0.44
(1,1885)	1:400:A:LEU:HD21	1:402:A:ILE:HD13	17	0.44
(1,1871)	1:426:A:ARG:HD2	1:426:A:ARG:HB3	19	0.44
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD22	19	0.44
(1,1840)	1:374:A:ARG:HA	1:374:A:ARG:HD2	2	0.44
(1,1802)	1:336:A:LEU:HD11	1:431:A:GLU:HA	9	0.44
(1,1802)	1:336:A:LEU:HD12	1:431:A:GLU:HA	18	0.44
(1,1800)	1:336:A:LEU:HD12	1:338:A:TRP:HD1	10	0.44
(1,1776)	1:337:A:LEU:HD13	1:390:A:MET:HG3	2	0.44
(1,1776)	1:337:A:LEU:HD13	1:390:A:MET:HG3	3	0.44
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD11	5	0.44
(1,1771)	1:341:A:VAL:HG11	1:337:A:LEU:HD13	6	0.44
(1,1771)	1:341:A:VAL:HG11	1:337:A:LEU:HD11	10	0.44
(1,1771)	1:341:A:VAL:HG11	1:337:A:LEU:HD12	13	0.44
(1,1709)	1:344:A:LEU:HD23	1:345:A:LEU:H	2	0.44
(1,1709)	1:344:A:LEU:HD23	1:345:A:LEU:H	10	0.44
(1,1709)	1:344:A:LEU:HD23	1:345:A:LEU:H	14	0.44
(1,1690)	1:402:A:ILE:HD12	1:400:A:LEU:HA	3	0.44
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG22	14	0.44
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG23	15	0.44
(1,1671)	1:403:A:ILE:HG22	1:405:A:LYS:HA	10	0.44
(1,1660)	1:404:A:ARG:HG3	1:404:A:ARG:HD2	4	0.44
(1,1653)	1:404:A:ARG:HG2	1:414:A:ARG:HD3	4	0.44
(1,1607)	1:411:A:LEU:HD11	1:366:A:ILE:H	2	0.44
(1,1600)	1:412:A:LEU:HD21	1:412:A:LEU:H	8	0.44
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD22	1	0.44
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD22	4	0.44
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD23	7	0.44
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD22	10	0.44
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD22	13	0.44
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD21	16	0.44
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	3	0.44
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	9	0.44
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	16	0.44
(1,1587)	1:412:A:LEU:HB2	1:413:A:PHE:H	19	0.44
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD13	13	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	8	0.44
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG22	6	0.44
(1,1513)	1:424:A:SER:HB2	1:424:A:SER:H	4	0.44
(1,1486)	1:432:A:HIS:HD2	1:436:A:GLN:HB2	6	0.44
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	1	0.44
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	3	0.44
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	8	0.44
(1,1449)	1:442:A:THR:HG22	1:445:A:GLU:HB2	11	0.44
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD21	1	0.44
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD23	8	0.44
(1,1316)	1:433:A:LEU:HD21	1:396:A:HIS:HD2	2	0.44
(1,1313)	1:375:A:LEU:HD11	1:376:A:TRP:H	19	0.44
(1,1266)	1:354:A:ILE:HD13	1:365:A:ARG:H	3	0.44
(1,1193)	1:362:A:LYS:HE2	1:362:A:LYS:HA	5	0.44
(1,1182)	1:363:A:ILE:HD11	1:406:A:GLU:HG2	4	0.44
(1,1182)	1:363:A:ILE:HD13	1:406:A:GLU:HG2	14	0.44
(1,1135)	1:367:A:VAL:HG12	1:352:A:ASN:H	2	0.44
(1,1133)	1:367:A:VAL:HG11	1:352:A:ASN:HB3	17	0.44
(1,1121)	1:367:A:VAL:HG21	1:365:A:ARG:HA	11	0.44
(1,1033)	1:348:A:SER:HB3	1:351:A:GLU:HB3	19	0.44
(1,1006)	1:380:A:LYS:HA	1:380:A:LYS:HD3	2	0.44
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	18	0.44
(1,978)	1:453:A:PRO:HA	1:450:A:ILE:HD13	7	0.44
(1,941)	1:447:A:GLU:H	1:446:A:ASP:HB2	18	0.44
(1,888)	1:437:A:VAL:HG21	1:441:A:GLN:HE22	16	0.44
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB2	7	0.44
(1,834)	1:430:A:LEU:HD11	1:397:A:TYR:HD1	13	0.44
(1,834)	1:430:A:LEU:HD13	1:397:A:TYR:HD1	14	0.44
(1,822)	1:429:A:ARG:HA	1:429:A:ARG:HG2	19	0.44
(1,690)	1:411:A:LEU:HD21	1:369:A:PRO:HB2	2	0.44
(1,690)	1:411:A:LEU:HD22	1:369:A:PRO:HB2	11	0.44
(1,690)	1:411:A:LEU:HD21	1:369:A:PRO:HB2	14	0.44
(1,644)	1:405:A:LYS:H	1:405:A:LYS:HG3	6	0.44
(1,620)	1:403:A:ILE:HG23	1:403:A:ILE:H	3	0.44
(1,620)	1:403:A:ILE:HG22	1:403:A:ILE:H	5	0.44
(1,620)	1:403:A:ILE:HG21	1:403:A:ILE:H	8	0.44
(1,620)	1:403:A:ILE:HG22	1:403:A:ILE:H	10	0.44
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	5	0.44
(1,457)	1:386:A:THR:HG21	1:389:A:LYS:HB2	16	0.44
(1,384)	1:344:A:LEU:HD12	1:375:A:LEU:HD22	11	0.44
(1,300)	1:366:A:ILE:HG23	1:411:A:LEU:HB3	5	0.44
(1,300)	1:366:A:ILE:HG23	1:411:A:LEU:HB3	10	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:366:A:ILE:HG23	1:411:A:LEU:HB3	18	0.44
(1,297)	1:366:A:ILE:HG21	1:368:A:ASP:HA	1	0.44
(1,297)	1:366:A:ILE:HG23	1:368:A:ASP:HA	2	0.44
(1,297)	1:366:A:ILE:HG22	1:368:A:ASP:HA	4	0.44
(1,297)	1:366:A:ILE:HG21	1:368:A:ASP:HA	6	0.44
(1,297)	1:366:A:ILE:HG22	1:368:A:ASP:HA	15	0.44
(1,297)	1:366:A:ILE:HG23	1:368:A:ASP:HA	18	0.44
(1,265)	1:363:A:ILE:HG23	1:412:A:LEU:HA	18	0.44
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	2	0.44
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	3	0.44
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	11	0.44
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG23	11	0.43
(1,2974)	1:433:A:LEU:H	1:431:A:GLU:HB2	7	0.43
(1,2974)	1:433:A:LEU:H	1:431:A:GLU:HB2	12	0.43
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	15	0.43
(1,2947)	1:362:A:LYS:H	1:363:A:ILE:HB	9	0.43
(1,2947)	1:362:A:LYS:H	1:363:A:ILE:HB	19	0.43
(1,2931)	1:420:A:ASP:H	1:421:A:GLU:HG3	9	0.43
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG21	7	0.43
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	10	0.43
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	9	0.43
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	13	0.43
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	16	0.43
(1,2860)	1:340:A:TYR:H	1:340:A:TYR:HD2	1	0.43
(1,2858)	1:341:A:VAL:HG13	1:340:A:TYR:HD2	5	0.43
(1,2858)	1:341:A:VAL:HG11	1:340:A:TYR:HD2	13	0.43
(1,2844)	1:402:A:ILE:HG23	1:397:A:TYR:HD2	4	0.43
(1,2837)	1:404:A:ARG:HD3	1:404:A:ARG:HB3	12	0.43
(1,2837)	1:410:A:ARG:HB2	1:410:A:ARG:HD3	17	0.43
(1,2828)	1:412:A:LEU:HD11	1:413:A:PHE:HD1	1	0.43
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	18	0.43
(1,2775)	1:443:A:TYR:HD2	1:445:A:GLU:HB2	5	0.43
(1,2774)	1:443:A:TYR:HD2	1:445:A:GLU:HB2	5	0.43
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB1	5	0.43
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB2	14	0.43
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE2	10	0.43
(1,2730)	1:366:A:ILE:HG22	1:370:A:ASN:H	11	0.43
(1,2730)	1:366:A:ILE:HG22	1:370:A:ASN:H	12	0.43
(1,2697)	1:445:A:GLU:HB2	1:445:A:GLU:HG2	14	0.43
(1,2693)	1:437:A:VAL:HG23	1:441:A:GLN:HE22	15	0.43
(1,2693)	1:437:A:VAL:HG21	1:441:A:GLN:HE22	19	0.43
(1,2688)	1:431:A:GLU:HG2	1:431:A:GLU:HB3	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2675)	1:417:A:LYS:HD2	1:402:A:ILE:HG13	2	0.43
(1,2675)	1:417:A:LYS:HD2	1:402:A:ILE:HG13	17	0.43
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD13	7	0.43
(1,2658)	1:366:A:ILE:HG22	1:411:A:LEU:HB2	4	0.43
(1,2658)	1:366:A:ILE:HG22	1:411:A:LEU:HB2	11	0.43
(1,2655)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	8	0.43
(1,2611)	1:393:A:ALA:HB1	1:397:A:TYR:HE1	8	0.43
(1,2611)	1:393:A:ALA:HB3	1:397:A:TYR:HE1	17	0.43
(1,2607)	1:367:A:VAL:HA	1:365:A:ARG:HD2	16	0.43
(1,2587)	1:362:A:LYS:HA	1:415:A:PHE:HD2	14	0.43
(1,2569)	1:349:A:ARG:HD3	1:350:A:TYR:HE1	1	0.43
(1,2556)	1:341:A:VAL:HG13	1:364:A:PHE:HZ	9	0.43
(1,2556)	1:341:A:VAL:HG11	1:364:A:PHE:HZ	16	0.43
(1,2245)	1:430:A:LEU:H	1:430:A:LEU:HG	18	0.43
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB2	3	0.43
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB2	6	0.43
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB2	13	0.43
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD13	11	0.43
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD23	5	0.43
(1,1919)	1:367:A:VAL:HG23	1:367:A:VAL:HG13	8	0.43
(1,1919)	1:367:A:VAL:HG22	1:367:A:VAL:HG11	15	0.43
(1,1906)	1:451:A:ALA:HB1	1:449:A:THR:HG21	4	0.43
(1,1906)	1:451:A:ALA:HB1	1:449:A:THR:HG22	19	0.43
(1,1895)	1:411:A:LEU:HD23	1:366:A:ILE:HD11	11	0.43
(1,1885)	1:400:A:LEU:HD23	1:402:A:ILE:HD13	19	0.43
(1,1861)	1:436:A:GLN:HG2	1:436:A:GLN:HA	4	0.43
(1,1840)	1:374:A:ARG:HD3	1:374:A:ARG:HA	12	0.43
(1,1802)	1:336:A:LEU:HD12	1:431:A:GLU:HA	7	0.43
(1,1802)	1:336:A:LEU:HD11	1:431:A:GLU:HA	11	0.43
(1,1802)	1:336:A:LEU:HD12	1:431:A:GLU:HA	12	0.43
(1,1800)	1:336:A:LEU:HD11	1:338:A:TRP:HD1	8	0.43
(1,1800)	1:336:A:LEU:HD13	1:338:A:TRP:HD1	14	0.43
(1,1778)	1:337:A:LEU:HD13	1:376:A:TRP:HB3	16	0.43
(1,1776)	1:337:A:LEU:HD12	1:390:A:MET:HG3	11	0.43
(1,1773)	1:337:A:LEU:HB3	1:337:A:LEU:HD12	12	0.43
(1,1771)	1:341:A:VAL:HG13	1:337:A:LEU:HD12	5	0.43
(1,1761)	1:340:A:TYR:HB2	1:337:A:LEU:HA	17	0.43
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD23	10	0.43
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG21	2	0.43
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG22	13	0.43
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG21	19	0.43
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD22	14	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD21	15	0.43
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	4	0.43
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	10	0.43
(1,1522)	1:422:A:ILE:HG21	1:430:A:LEU:HG	13	0.43
(1,1509)	1:426:A:ARG:HG3	1:426:A:ARG:HB2	5	0.43
(1,1484)	1:432:A:HIS:HB3	1:430:A:LEU:H	4	0.43
(1,1480)	1:412:A:LEU:HD21	1:357:A:GLU:HG2	10	0.43
(1,1480)	1:412:A:LEU:HD22	1:357:A:GLU:HG2	17	0.43
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	4	0.43
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	5	0.43
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	6	0.43
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	7	0.43
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	12	0.43
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	14	0.43
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	15	0.43
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	16	0.43
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	18	0.43
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	19	0.43
(1,1432)	1:445:A:GLU:HG2	1:445:A:GLU:HA	16	0.43
(1,1424)	1:450:A:ILE:HG23	1:452:A:SER:HB2	9	0.43
(1,1422)	1:451:A:ALA:HB2	1:450:A:ILE:HA	16	0.43
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	9	0.43
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	18	0.43
(1,1340)	1:399:A:LYS:HD3	1:396:A:HIS:HA	5	0.43
(1,1340)	1:399:A:LYS:HD3	1:396:A:HIS:HA	7	0.43
(1,1316)	1:433:A:LEU:HD22	1:396:A:HIS:HD2	7	0.43
(1,1313)	1:375:A:LEU:HD13	1:376:A:TRP:H	2	0.43
(1,1313)	1:375:A:LEU:HD12	1:376:A:TRP:H	8	0.43
(1,1266)	1:354:A:ILE:HD12	1:365:A:ARG:H	5	0.43
(1,1266)	1:354:A:ILE:HD11	1:365:A:ARG:H	13	0.43
(1,1266)	1:354:A:ILE:HD11	1:365:A:ARG:H	14	0.43
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD22	3	0.43
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD21	9	0.43
(1,1142)	1:450:A:ILE:HD12	1:454:A:VAL:HA	1	0.43
(1,1135)	1:367:A:VAL:HG12	1:352:A:ASN:H	6	0.43
(1,1121)	1:367:A:VAL:HG23	1:365:A:ARG:HA	5	0.43
(1,1084)	1:372:A:LEU:HD13	1:344:A:LEU:HD11	4	0.43
(1,1084)	1:372:A:LEU:HD12	1:344:A:LEU:HD13	6	0.43
(1,1025)	1:336:A:LEU:HD21	1:430:A:LEU:H	18	0.43
(1,1021)	1:437:A:VAL:HG11	1:396:A:HIS:HD2	3	0.43
(1,978)	1:453:A:PRO:HA	1:450:A:ILE:HD11	17	0.43
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB3	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,834)	1:430:A:LEU:HD12	1:397:A:TYR:HD1	1	0.43
(1,825)	1:392:A:ARG:HD3	1:392:A:ARG:HB3	10	0.43
(1,690)	1:411:A:LEU:HD22	1:369:A:PRO:HB2	4	0.43
(1,690)	1:411:A:LEU:HD22	1:369:A:PRO:HB2	13	0.43
(1,620)	1:403:A:ILE:HG21	1:403:A:ILE:H	9	0.43
(1,620)	1:403:A:ILE:HG23	1:403:A:ILE:H	16	0.43
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD22	10	0.43
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD22	5	0.43
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD23	7	0.43
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD23	14	0.43
(1,495)	1:392:A:ARG:HA	1:392:A:ARG:HG2	16	0.43
(1,456)	1:386:A:THR:HG23	1:387:A:TYR:HB2	5	0.43
(1,400)	1:377:A:GLY:HA3	1:382:A:ARG:HB3	6	0.43
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG22	10	0.43
(1,297)	1:366:A:ILE:HG22	1:368:A:ASP:HA	3	0.43
(1,297)	1:366:A:ILE:HG23	1:368:A:ASP:HA	7	0.43
(1,297)	1:366:A:ILE:HG23	1:368:A:ASP:HA	10	0.43
(1,297)	1:366:A:ILE:HG22	1:368:A:ASP:HA	17	0.43
(1,187)	1:356:A:TRP:HB2	1:359:A:LYS:HD3	14	0.43
(1,2974)	1:433:A:LEU:H	1:431:A:GLU:HB2	1	0.42
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	4	0.42
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	7	0.42
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	9	0.42
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	19	0.42
(1,2947)	1:362:A:LYS:H	1:363:A:ILE:HB	3	0.42
(1,2947)	1:362:A:LYS:H	1:363:A:ILE:HB	12	0.42
(1,2947)	1:362:A:LYS:H	1:363:A:ILE:HB	18	0.42
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	8	0.42
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	16	0.42
(1,2895)	1:353:A:PHE:H	1:367:A:VAL:HG23	8	0.42
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG22	12	0.42
(1,2872)	1:447:A:GLU:HG3	1:447:A:GLU:HB2	8	0.42
(1,2872)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	10	0.42
(1,2872)	1:444:A:GLN:HG2	1:444:A:GLN:HB3	12	0.42
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	5	0.42
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	1	0.42
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	6	0.42
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	17	0.42
(1,2850)	1:344:A:LEU:HD11	1:350:A:TYR:HD1	9	0.42
(1,2828)	1:412:A:LEU:HD13	1:413:A:PHE:HD1	11	0.42
(1,2797)	1:433:A:LEU:HD13	1:434:A:GLU:HA	2	0.42
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	2	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	9	0.42
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	11	0.42
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	12	0.42
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	17	0.42
(1,2776)	1:387:A:TYR:HA	1:387:A:TYR:HE2	12	0.42
(1,2725)	1:367:A:VAL:HG21	1:365:A:ARG:HB3	5	0.42
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG22	2	0.42
(1,2697)	1:447:A:GLU:HG3	1:447:A:GLU:HB2	9	0.42
(1,2697)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	12	0.42
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG3	13	0.42
(1,2688)	1:431:A:GLU:HG2	1:431:A:GLU:HB3	13	0.42
(1,2684)	1:429:A:ARG:HG2	1:433:A:LEU:HD22	9	0.42
(1,2683)	1:429:A:ARG:HG2	1:429:A:ARG:H	13	0.42
(1,2675)	1:417:A:LYS:HD2	1:402:A:ILE:HG13	1	0.42
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD12	16	0.42
(1,2643)	1:402:A:ILE:HD13	1:397:A:TYR:HD1	13	0.42
(1,2587)	1:362:A:LYS:HA	1:415:A:PHE:HD2	11	0.42
(1,2586)	1:431:A:GLU:H	1:431:A:GLU:HG2	5	0.42
(1,2579)	1:358:A:ASP:HB2	1:363:A:ILE:HG22	7	0.42
(1,2569)	1:349:A:ARG:HD3	1:350:A:TYR:HE1	4	0.42
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG22	19	0.42
(1,2527)	1:367:A:VAL:HG11	1:368:A:ASP:H	11	0.42
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD23	3	0.42
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD22	3	0.42
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD21	12	0.42
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD11	10	0.42
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD12	14	0.42
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	8	0.42
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	6	0.42
(1,2447)	1:385:A:MET:H	1:444:A:GLN:HE21	7	0.42
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB2	15	0.42
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB2	16	0.42
(1,2418)	1:444:A:GLN:H	1:441:A:GLN:HG3	14	0.42
(1,2405)	1:384:A:ASN:H	1:385:A:MET:HB2	19	0.42
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	10	0.42
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	1	0.42
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	3	0.42
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	6	0.42
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	11	0.42
(1,2182)	1:400:A:LEU:H	1:400:A:LEU:HB3	18	0.42
(1,2058)	1:363:A:ILE:H	1:358:A:ASP:HB2	4	0.42
(1,1974)	1:349:A:ARG:H	1:349:A:ARG:HB2	13	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1919)	1:367:A:VAL:HG22	1:367:A:VAL:HG11	5	0.42
(1,1909)	1:344:A:LEU:HD12	1:354:A:ILE:HG21	18	0.42
(1,1906)	1:451:A:ALA:HB1	1:449:A:THR:HG23	14	0.42
(1,1899)	1:430:A:LEU:HD13	1:400:A:LEU:HD23	2	0.42
(1,1899)	1:430:A:LEU:HD12	1:400:A:LEU:HD22	6	0.42
(1,1897)	1:430:A:LEU:HD13	1:430:A:LEU:HD21	3	0.42
(1,1897)	1:430:A:LEU:HD13	1:430:A:LEU:HD23	9	0.42
(1,1885)	1:400:A:LEU:HD23	1:402:A:ILE:HD12	10	0.42
(1,1871)	1:426:A:ARG:HD2	1:426:A:ARG:HB3	11	0.42
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD22	1	0.42
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD22	9	0.42
(1,1778)	1:337:A:LEU:HD13	1:376:A:TRP:HB3	15	0.42
(1,1771)	1:341:A:VAL:HG13	1:337:A:LEU:HD12	3	0.42
(1,1771)	1:341:A:VAL:HG12	1:337:A:LEU:HD13	11	0.42
(1,1726)	1:341:A:VAL:HG21	1:338:A:TRP:HA	18	0.42
(1,1709)	1:344:A:LEU:HD22	1:345:A:LEU:H	7	0.42
(1,1709)	1:344:A:LEU:HD22	1:345:A:LEU:H	12	0.42
(1,1686)	1:402:A:ILE:HG23	1:403:A:ILE:HG12	1	0.42
(1,1686)	1:402:A:ILE:HG22	1:403:A:ILE:HG12	4	0.42
(1,1686)	1:402:A:ILE:HG23	1:403:A:ILE:HG12	6	0.42
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG22	4	0.42
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG22	11	0.42
(1,1671)	1:403:A:ILE:HG21	1:405:A:LYS:HA	1	0.42
(1,1671)	1:403:A:ILE:HG21	1:405:A:LYS:HA	4	0.42
(1,1660)	1:404:A:ARG:HG3	1:404:A:ARG:HD2	10	0.42
(1,1653)	1:404:A:ARG:HG2	1:414:A:ARG:HD3	5	0.42
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	4	0.42
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	13	0.42
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD22	5	0.42
(1,1594)	1:412:A:LEU:HB3	1:412:A:LEU:HD23	8	0.42
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD12	17	0.42
(1,1554)	1:417:A:LYS:HE3	1:402:A:ILE:HG13	16	0.42
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG22	12	0.42
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG21	13	0.42
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	9	0.42
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	10	0.42
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	13	0.42
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD22	3	0.42
(1,1315)	1:375:A:LEU:HD22	1:376:A:TRP:H	15	0.42
(1,1304)	1:376:A:TRP:HZ2	1:380:A:LYS:HE3	14	0.42
(1,1266)	1:354:A:ILE:HD13	1:365:A:ARG:H	2	0.42
(1,1266)	1:354:A:ILE:HD12	1:365:A:ARG:H	4	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1266)	1:354:A:ILE:HD12	1:365:A:ARG:H	6	0.42
(1,1266)	1:354:A:ILE:HD12	1:365:A:ARG:H	19	0.42
(1,1130)	1:365:A:ARG:HG2	1:367:A:VAL:HG21	2	0.42
(1,1130)	1:365:A:ARG:HG2	1:367:A:VAL:HG21	14	0.42
(1,1121)	1:367:A:VAL:HG21	1:365:A:ARG:HA	7	0.42
(1,1025)	1:336:A:LEU:HD22	1:430:A:LEU:H	9	0.42
(1,1006)	1:380:A:LYS:HA	1:380:A:LYS:HD3	10	0.42
(1,978)	1:453:A:PRO:HA	1:450:A:ILE:HD13	16	0.42
(1,927)	1:441:A:GLN:H	1:441:A:GLN:HG2	19	0.42
(1,888)	1:437:A:VAL:HG23	1:441:A:GLN:HE22	3	0.42
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	11	0.42
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	15	0.42
(1,690)	1:411:A:LEU:HD22	1:369:A:PRO:HB2	6	0.42
(1,690)	1:411:A:LEU:HD23	1:369:A:PRO:HB2	18	0.42
(1,620)	1:403:A:ILE:HG23	1:403:A:ILE:H	18	0.42
(1,620)	1:403:A:ILE:HG21	1:403:A:ILE:H	19	0.42
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD22	9	0.42
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD22	4	0.42
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD23	6	0.42
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	6	0.42
(1,495)	1:392:A:ARG:HA	1:392:A:ARG:HG2	10	0.42
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	7	0.42
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	18	0.42
(1,478)	1:389:A:LYS:HG3	1:389:A:LYS:HE2	12	0.42
(1,458)	1:386:A:THR:HG21	1:389:A:LYS:HD2	4	0.42
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	3	0.42
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	4	0.42
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	5	0.42
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	6	0.42
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	7	0.42
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	8	0.42
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	9	0.42
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	10	0.42
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	11	0.42
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	12	0.42
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	13	0.42
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	14	0.42
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	15	0.42
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	16	0.42
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	17	0.42
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	19	0.42
(1,306)	1:354:A:ILE:HD11	1:366:A:ILE:HG21	12	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG22	5	0.42
(1,300)	1:366:A:ILE:HG23	1:411:A:LEU:HB3	7	0.42
(1,5)	1:337:A:LEU:HD23	1:390:A:MET:HG3	19	0.42
(1,2974)	1:433:A:LEU:H	1:436:A:GLN:HB2	10	0.41
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	5	0.41
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	12	0.41
(1,2944)	1:365:A:ARG:H	1:356:A:TRP:HE3	13	0.41
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	7	0.41
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	18	0.41
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	19	0.41
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD21	19	0.41
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG23	2	0.41
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG21	15	0.41
(1,2872)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	3	0.41
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	5	0.41
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	11	0.41
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	14	0.41
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	14	0.41
(1,2837)	1:410:A:ARG:HB2	1:410:A:ARG:HD3	3	0.41
(1,2784)	1:457:A:PRO:HB3	1:457:A:PRO:HD2	1	0.41
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	18	0.41
(1,2775)	1:387:A:TYR:HD1	1:390:A:MET:HG2	8	0.41
(1,2775)	1:387:A:TYR:HD2	1:390:A:MET:HG2	17	0.41
(1,2767)	1:396:A:HIS:HB3	1:393:A:ALA:HA	17	0.41
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG21	8	0.41
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG3	9	0.41
(1,2681)	1:418:A:THR:HG23	1:342:A:TYR:HD1	8	0.41
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD12	13	0.41
(1,2640)	1:400:A:LEU:HD21	1:430:A:LEU:HD23	2	0.41
(1,2618)	1:375:A:LEU:HD21	1:378:A:ASN:HB2	11	0.41
(1,2556)	1:341:A:VAL:HG11	1:364:A:PHE:HZ	12	0.41
(1,2556)	1:341:A:VAL:HG11	1:364:A:PHE:HZ	14	0.41
(1,2551)	1:451:A:ALA:H	1:451:A:ALA:HB1	7	0.41
(1,2548)	1:443:A:TYR:H	1:442:A:THR:HG22	14	0.41
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD13	9	0.41
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD21	11	0.41
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD21	18	0.41
(1,2508)	1:434:A:GLU:H	1:434:A:GLU:HG2	11	0.41
(1,2438)	1:432:A:HIS:H	1:433:A:LEU:HB2	17	0.41
(1,2380)	1:399:A:LYS:H	1:400:A:LEU:HD22	12	0.41
(1,2359)	1:382:A:ARG:H	1:382:A:ARG:HG3	11	0.41
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	3	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	4	0.41
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	4	0.41
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	5	0.41
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	2	0.41
(1,1919)	1:367:A:VAL:HG21	1:367:A:VAL:HG11	18	0.41
(1,1904)	1:437:A:VAL:HG12	1:438:A:LEU:HD21	5	0.41
(1,1904)	1:437:A:VAL:HG12	1:438:A:LEU:HD22	17	0.41
(1,1897)	1:430:A:LEU:HD13	1:430:A:LEU:HD23	6	0.41
(1,1895)	1:411:A:LEU:HD22	1:366:A:ILE:HD11	17	0.41
(1,1892)	1:403:A:ILE:HD12	1:402:A:ILE:HG23	16	0.41
(1,1885)	1:400:A:LEU:HD21	1:402:A:ILE:HD11	13	0.41
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB2	1	0.41
(1,1802)	1:336:A:LEU:HD12	1:431:A:GLU:HA	8	0.41
(1,1802)	1:336:A:LEU:HD13	1:431:A:GLU:HA	15	0.41
(1,1800)	1:336:A:LEU:HD12	1:338:A:TRP:HD1	6	0.41
(1,1771)	1:341:A:VAL:HG12	1:337:A:LEU:HD11	2	0.41
(1,1761)	1:340:A:TYR:HB2	1:337:A:LEU:HA	8	0.41
(1,1761)	1:340:A:TYR:HB2	1:337:A:LEU:HA	12	0.41
(1,1726)	1:341:A:VAL:HG23	1:338:A:TRP:HA	3	0.41
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG22	7	0.41
(1,1670)	1:403:A:ILE:HG23	1:397:A:TYR:HB2	18	0.41
(1,1600)	1:412:A:LEU:HD22	1:412:A:LEU:H	12	0.41
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	6	0.41
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	14	0.41
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	17	0.41
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	1	0.41
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	2	0.41
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	4	0.41
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	5	0.41
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	6	0.41
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	7	0.41
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	9	0.41
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	10	0.41
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	12	0.41
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	14	0.41
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	15	0.41
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	17	0.41
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	19	0.41
(1,1484)	1:432:A:HIS:HB3	1:430:A:LEU:H	5	0.41
(1,1480)	1:412:A:LEU:HD22	1:357:A:GLU:HG2	9	0.41
(1,1475)	1:433:A:LEU:HD22	1:434:A:GLU:H	10	0.41
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	2	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	11	0.41
(1,1452)	1:361:A:SER:H	1:360:A:GLU:HG3	4	0.41
(1,1427)	1:447:A:GLU:HA	1:448:A:PRO:HD3	14	0.41
(1,1392)	1:386:A:THR:HG21	1:389:A:LYS:HG2	5	0.41
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	17	0.41
(1,1340)	1:399:A:LYS:HD3	1:396:A:HIS:HA	1	0.41
(1,1316)	1:433:A:LEU:HD23	1:396:A:HIS:HD2	5	0.41
(1,1316)	1:433:A:LEU:HD21	1:396:A:HIS:HD2	6	0.41
(1,1313)	1:375:A:LEU:HD13	1:376:A:TRP:H	1	0.41
(1,1313)	1:375:A:LEU:HD13	1:376:A:TRP:H	11	0.41
(1,1266)	1:354:A:ILE:HD12	1:365:A:ARG:H	10	0.41
(1,1266)	1:354:A:ILE:HD12	1:365:A:ARG:H	12	0.41
(1,1266)	1:354:A:ILE:HD13	1:365:A:ARG:H	18	0.41
(1,1193)	1:362:A:LYS:HE2	1:362:A:LYS:HA	10	0.41
(1,1135)	1:367:A:VAL:HG13	1:352:A:ASN:H	1	0.41
(1,1135)	1:367:A:VAL:HG11	1:352:A:ASN:H	5	0.41
(1,1135)	1:367:A:VAL:HG12	1:352:A:ASN:H	11	0.41
(1,1133)	1:367:A:VAL:HG12	1:352:A:ASN:HB3	11	0.41
(1,1128)	1:355:A:ARG:HB3	1:367:A:VAL:HG22	9	0.41
(1,1119)	1:367:A:VAL:HG23	1:355:A:ARG:HA	16	0.41
(1,1025)	1:336:A:LEU:HD22	1:430:A:LEU:H	11	0.41
(1,1021)	1:437:A:VAL:HG13	1:396:A:HIS:HD2	11	0.41
(1,834)	1:430:A:LEU:HD13	1:397:A:TYR:HD1	9	0.41
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	7	0.41
(1,620)	1:403:A:ILE:HG23	1:403:A:ILE:H	2	0.41
(1,594)	1:400:A:LEU:HD23	1:426:A:ARG:HG3	13	0.41
(1,577)	1:399:A:LYS:HA	1:399:A:LYS:HG3	3	0.41
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD12	11	0.41
(1,458)	1:386:A:THR:HG21	1:389:A:LYS:HD2	6	0.41
(1,457)	1:386:A:THR:HG21	1:389:A:LYS:HB2	6	0.41
(1,457)	1:386:A:THR:HG22	1:389:A:LYS:HB2	7	0.41
(1,456)	1:386:A:THR:HG23	1:387:A:TYR:HB2	16	0.41
(1,456)	1:386:A:THR:HG22	1:387:A:TYR:HB2	18	0.41
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	18	0.41
(1,400)	1:377:A:GLY:HA3	1:382:A:ARG:HB3	1	0.41
(1,365)	1:374:A:ARG:H	1:374:A:ARG:HD2	6	0.41
(1,297)	1:366:A:ILE:HG22	1:368:A:ASP:HA	9	0.41
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	19	0.41
(1,136)	1:351:A:GLU:H	1:351:A:GLU:HG2	17	0.41
(1,85)	1:344:A:LEU:HD21	1:350:A:TYR:HD1	3	0.41
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG21	12	0.4
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG21	19	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	1	0.4
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	3	0.4
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	18	0.4
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	2	0.4
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	11	0.4
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD21	10	0.4
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD21	16	0.4
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD22	17	0.4
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	2	0.4
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	3	0.4
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	8	0.4
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	12	0.4
(1,2818)	1:417:A:LYS:HG2	1:416:A:MET:HB2	9	0.4
(1,2789)	1:438:A:LEU:HD13	1:444:A:GLN:HE22	3	0.4
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	4	0.4
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	8	0.4
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	14	0.4
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	15	0.4
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	19	0.4
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB3	9	0.4
(1,2762)	1:394:A:LEU:HD21	1:398:A:TYR:HE1	7	0.4
(1,2725)	1:367:A:VAL:HG22	1:365:A:ARG:HB3	1	0.4
(1,2697)	1:447:A:GLU:HG3	1:447:A:GLU:HB2	8	0.4
(1,2697)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	10	0.4
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG3	12	0.4
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG3	14	0.4
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG3	16	0.4
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG3	18	0.4
(1,2675)	1:417:A:LYS:HD2	1:402:A:ILE:HG13	12	0.4
(1,2661)	1:369:A:PRO:HD2	1:411:A:LEU:HD11	2	0.4
(1,2645)	1:402:A:ILE:HD13	1:338:A:TRP:HB3	10	0.4
(1,2644)	1:402:A:ILE:HD12	1:397:A:TYR:HE1	17	0.4
(1,2643)	1:402:A:ILE:HD11	1:397:A:TYR:HD1	3	0.4
(1,2643)	1:402:A:ILE:HD12	1:397:A:TYR:HD1	5	0.4
(1,2618)	1:375:A:LEU:HD22	1:378:A:ASN:HB2	1	0.4
(1,2618)	1:375:A:LEU:HD21	1:378:A:ASN:HB2	6	0.4
(1,2611)	1:393:A:ALA:HB3	1:397:A:TYR:HE1	11	0.4
(1,2600)	1:364:A:PHE:HA	1:365:A:ARG:HB3	12	0.4
(1,2597)	1:358:A:ASP:HB3	1:363:A:ILE:HG21	2	0.4
(1,2575)	1:344:A:LEU:H	1:354:A:ILE:HG21	12	0.4
(1,2556)	1:341:A:VAL:HG11	1:364:A:PHE:HZ	8	0.4
(1,2556)	1:341:A:VAL:HG12	1:364:A:PHE:HZ	10	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2551)	1:451:A:ALA:H	1:451:A:ALA:HB1	9	0.4
(1,2551)	1:451:A:ALA:H	1:451:A:ALA:HB1	11	0.4
(1,2551)	1:451:A:ALA:H	1:451:A:ALA:HB3	16	0.4
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG22	14	0.4
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD12	5	0.4
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD11	16	0.4
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD23	6	0.4
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD23	19	0.4
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG21	13	0.4
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD22	16	0.4
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD13	2	0.4
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD13	7	0.4
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD12	9	0.4
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD11	16	0.4
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD12	18	0.4
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD12	5	0.4
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD11	17	0.4
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	4	0.4
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	5	0.4
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	10	0.4
(1,2159)	1:389:A:LYS:H	1:388:A:GLU:HG2	3	0.4
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG22	7	0.4
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	10	0.4
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	14	0.4
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	17	0.4
(1,1921)	1:375:A:LEU:HD12	1:375:A:LEU:HD22	3	0.4
(1,1921)	1:375:A:LEU:HD11	1:375:A:LEU:HD21	15	0.4
(1,1919)	1:367:A:VAL:HG21	1:367:A:VAL:HG12	4	0.4
(1,1919)	1:367:A:VAL:HG21	1:367:A:VAL:HG12	13	0.4
(1,1906)	1:451:A:ALA:HB1	1:449:A:THR:HG21	6	0.4
(1,1906)	1:451:A:ALA:HB1	1:449:A:THR:HG23	7	0.4
(1,1899)	1:430:A:LEU:HD11	1:400:A:LEU:HD21	1	0.4
(1,1899)	1:430:A:LEU:HD12	1:400:A:LEU:HD23	10	0.4
(1,1897)	1:430:A:LEU:HD11	1:430:A:LEU:HD22	11	0.4
(1,1897)	1:430:A:LEU:HD12	1:430:A:LEU:HD23	18	0.4
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB1	18	0.4
(1,1861)	1:436:A:GLN:HG2	1:436:A:GLN:HA	19	0.4
(1,1778)	1:337:A:LEU:HD12	1:376:A:TRP:HB3	6	0.4
(1,1771)	1:341:A:VAL:HG13	1:337:A:LEU:HD11	16	0.4
(1,1761)	1:340:A:TYR:HB2	1:337:A:LEU:HA	11	0.4
(1,1726)	1:341:A:VAL:HG22	1:338:A:TRP:HA	4	0.4
(1,1726)	1:341:A:VAL:HG23	1:338:A:TRP:HA	19	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1686)	1:402:A:ILE:HG23	1:403:A:ILE:HG12	15	0.4
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG23	1	0.4
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG22	17	0.4
(1,1670)	1:403:A:ILE:HG22	1:397:A:TYR:HB2	19	0.4
(1,1644)	1:404:A:ARG:HD3	1:404:A:ARG:HB3	4	0.4
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	8	0.4
(1,1600)	1:412:A:LEU:HD23	1:412:A:LEU:H	1	0.4
(1,1600)	1:412:A:LEU:HD23	1:412:A:LEU:H	14	0.4
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD11	2	0.4
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD11	7	0.4
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	2	0.4
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	18	0.4
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	3	0.4
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	8	0.4
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	11	0.4
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	13	0.4
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	16	0.4
(1,1543)	1:420:A:ASP:HB3	1:420:A:ASP:HA	18	0.4
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG23	3	0.4
(1,1450)	1:442:A:THR:HG22	1:445:A:GLU:HB3	7	0.4
(1,1316)	1:433:A:LEU:HD22	1:396:A:HIS:HD2	14	0.4
(1,1316)	1:433:A:LEU:HD21	1:396:A:HIS:HD2	15	0.4
(1,1313)	1:375:A:LEU:HD12	1:376:A:TRP:H	4	0.4
(1,1313)	1:375:A:LEU:HD12	1:376:A:TRP:H	12	0.4
(1,1280)	1:379:A:HIS:HD2	1:380:A:LYS:HG2	19	0.4
(1,1266)	1:354:A:ILE:HD11	1:365:A:ARG:H	17	0.4
(1,1224)	1:363:A:ILE:HG21	1:357:A:GLU:HG2	13	0.4
(1,1193)	1:362:A:LYS:HE2	1:362:A:LYS:HA	9	0.4
(1,1172)	1:363:A:ILE:HG21	1:409:A:GLN:HE22	14	0.4
(1,1128)	1:355:A:ARG:HB3	1:367:A:VAL:HG22	5	0.4
(1,1060)	1:351:A:GLU:HB2	1:355:A:ARG:HD2	12	0.4
(1,1021)	1:437:A:VAL:HG13	1:396:A:HIS:HD2	9	0.4
(1,1021)	1:437:A:VAL:HG11	1:396:A:HIS:HD2	10	0.4
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	6	0.4
(1,876)	1:436:A:GLN:HB3	1:437:A:VAL:HG11	19	0.4
(1,834)	1:430:A:LEU:HD11	1:397:A:TYR:HD1	2	0.4
(1,834)	1:430:A:LEU:HD11	1:397:A:TYR:HD1	3	0.4
(1,834)	1:430:A:LEU:HD11	1:397:A:TYR:HD1	4	0.4
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	1	0.4
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	2	0.4
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	3	0.4
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	8	0.4
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	16	0.4
(1,690)	1:411:A:LEU:HD21	1:369:A:PRO:HB2	1	0.4
(1,627)	1:403:A:ILE:HG23	1:413:A:PHE:HB2	1	0.4
(1,627)	1:403:A:ILE:HG23	1:413:A:PHE:HB2	6	0.4
(1,627)	1:403:A:ILE:HG23	1:413:A:PHE:HB2	12	0.4
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD22	2	0.4
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD21	16	0.4
(1,577)	1:399:A:LYS:HA	1:399:A:LYS:HG3	6	0.4
(1,547)	1:395:A:ARG:HD2	1:395:A:ARG:H	17	0.4
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD21	1	0.4
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD13	18	0.4
(1,482)	1:389:A:LYS:HG2	1:389:A:LYS:HE2	13	0.4
(1,478)	1:389:A:LYS:HG3	1:389:A:LYS:HE2	8	0.4
(1,457)	1:386:A:THR:HG23	1:389:A:LYS:HB2	14	0.4
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	1	0.4
(1,403)	1:378:A:ASN:HA	1:378:A:ASN:HB3	2	0.4
(1,347)	1:373:A:ALA:HA	1:376:A:TRP:HB2	13	0.4
(1,306)	1:354:A:ILE:HD11	1:366:A:ILE:HG21	15	0.4
(1,300)	1:366:A:ILE:HG22	1:411:A:LEU:HB3	9	0.4
(1,300)	1:366:A:ILE:HG23	1:411:A:LEU:HB3	16	0.4
(1,300)	1:366:A:ILE:HG22	1:411:A:LEU:HB3	17	0.4
(1,297)	1:366:A:ILE:HG23	1:368:A:ASP:HA	16	0.4
(1,205)	1:357:A:GLU:HB3	1:363:A:ILE:HG21	16	0.4
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	13	0.4
(1,127)	1:349:A:ARG:HD2	1:350:A:TYR:HE1	17	0.4
(1,34)	1:341:A:VAL:HG13	1:337:A:LEU:HG	14	0.4
(1,34)	1:341:A:VAL:HG12	1:337:A:LEU:HG	19	0.4
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB1	14	0.39
(1,2972)	1:435:A:SER:H	1:436:A:GLN:HG3	13	0.39
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	11	0.39
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	1	0.39
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	5	0.39
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG23	13	0.39
(1,2872)	1:447:A:GLU:HG3	1:447:A:GLU:HB2	19	0.39
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	11	0.39
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD21	2	0.39
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD23	3	0.39
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD23	4	0.39
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD22	14	0.39
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD21	15	0.39
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	19	0.39
(1,2844)	1:402:A:ILE:HG21	1:397:A:TYR:HD2	3	0.39
(1,2844)	1:402:A:ILE:HG23	1:397:A:TYR:HD2	12	0.39
(1,2797)	1:433:A:LEU:HD12	1:434:A:GLU:HA	10	0.39
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	3	0.39
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	5	0.39
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	6	0.39
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	10	0.39
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	13	0.39
(1,2784)	1:407:A:PRO:HB3	1:407:A:PRO:HD2	16	0.39
(1,2749)	1:356:A:TRP:HZ2	1:342:A:TYR:HB2	14	0.39
(1,2725)	1:367:A:VAL:HG23	1:365:A:ARG:HB3	10	0.39
(1,2697)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	3	0.39
(1,2697)	1:447:A:GLU:HG3	1:447:A:GLU:HB2	17	0.39
(1,2696)	1:438:A:LEU:HD22	1:382:A:ARG:HD2	5	0.39
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG21	17	0.39
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG2	3	0.39
(1,2658)	1:366:A:ILE:HG22	1:411:A:LEU:HB2	3	0.39
(1,2658)	1:366:A:ILE:HG21	1:411:A:LEU:HB2	6	0.39
(1,2658)	1:366:A:ILE:HG22	1:411:A:LEU:HB2	9	0.39
(1,2645)	1:402:A:ILE:HD11	1:338:A:TRP:HB3	2	0.39
(1,2645)	1:402:A:ILE:HD11	1:338:A:TRP:HB3	17	0.39
(1,2643)	1:402:A:ILE:HD12	1:397:A:TYR:HD1	15	0.39
(1,2620)	1:382:A:ARG:H	1:378:A:ASN:HA	5	0.39
(1,2612)	1:393:A:ALA:HB1	1:376:A:TRP:HZ3	3	0.39
(1,2611)	1:393:A:ALA:HB2	1:397:A:TYR:HE1	9	0.39
(1,2611)	1:393:A:ALA:HB1	1:397:A:TYR:HE1	18	0.39
(1,2598)	1:363:A:ILE:HG22	1:357:A:GLU:HG3	17	0.39
(1,2597)	1:358:A:ASP:HB3	1:363:A:ILE:HG22	1	0.39
(1,2569)	1:349:A:ARG:HD3	1:350:A:TYR:HE1	18	0.39
(1,2557)	1:341:A:VAL:HG13	1:403:A:ILE:HD11	11	0.39
(1,2556)	1:341:A:VAL:HG13	1:364:A:PHE:HZ	2	0.39
(1,2556)	1:341:A:VAL:HG11	1:364:A:PHE:HZ	3	0.39
(1,2556)	1:341:A:VAL:HG11	1:364:A:PHE:HZ	5	0.39
(1,2556)	1:341:A:VAL:HG13	1:364:A:PHE:HZ	11	0.39
(1,2556)	1:341:A:VAL:HG12	1:364:A:PHE:HZ	17	0.39
(1,2555)	1:340:A:TYR:HA	1:339:A:ASP:HB3	5	0.39
(1,2555)	1:340:A:TYR:HA	1:339:A:ASP:HB3	14	0.39
(1,2555)	1:340:A:TYR:HA	1:339:A:ASP:HB3	15	0.39
(1,2550)	1:451:A:ALA:H	1:450:A:ILE:HG21	2	0.39
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG23	13	0.39
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD11	1	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD11	3	0.39
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD23	1	0.39
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD21	8	0.39
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD23	19	0.39
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD22	2	0.39
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD22	18	0.39
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD13	6	0.39
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD12	15	0.39
(1,2508)	1:434:A:GLU:H	1:434:A:GLU:HG2	9	0.39
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	4	0.39
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD13	4	0.39
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB3	6	0.39
(1,2322)	1:350:A:TYR:H	1:350:A:TYR:HE2	17	0.39
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	17	0.39
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB2	18	0.39
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD12	2	0.39
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG22	10	0.39
(1,2129)	1:447:A:GLU:H	1:447:A:GLU:HB3	10	0.39
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	7	0.39
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	8	0.39
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	9	0.39
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	11	0.39
(1,2067)	1:365:A:ARG:H	1:355:A:ARG:HG2	17	0.39
(1,2058)	1:363:A:ILE:H	1:358:A:ASP:HB2	14	0.39
(1,1969)	1:347:A:ASP:H	1:346:A:SER:HB2	4	0.39
(1,1919)	1:367:A:VAL:HG21	1:367:A:VAL:HG13	1	0.39
(1,1919)	1:367:A:VAL:HG22	1:367:A:VAL:HG12	19	0.39
(1,1904)	1:437:A:VAL:HG13	1:438:A:LEU:HD23	2	0.39
(1,1904)	1:437:A:VAL:HG12	1:438:A:LEU:HD22	6	0.39
(1,1904)	1:437:A:VAL:HG12	1:438:A:LEU:HD22	16	0.39
(1,1897)	1:430:A:LEU:HD13	1:430:A:LEU:HD21	16	0.39
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD21	11	0.39
(1,1804)	1:422:A:ILE:HD13	1:336:A:LEU:HD11	8	0.39
(1,1802)	1:336:A:LEU:HD13	1:431:A:GLU:HA	3	0.39
(1,1778)	1:337:A:LEU:HD11	1:376:A:TRP:HB3	5	0.39
(1,1778)	1:337:A:LEU:HD13	1:376:A:TRP:HB3	7	0.39
(1,1771)	1:341:A:VAL:HG13	1:337:A:LEU:HD11	8	0.39
(1,1771)	1:341:A:VAL:HG12	1:337:A:LEU:HD11	18	0.39
(1,1713)	1:343:A:GLN:HE21	1:343:A:GLN:HG2	9	0.39
(1,1686)	1:402:A:ILE:HG22	1:403:A:ILE:HG12	13	0.39
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG23	6	0.39
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG23	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1671)	1:403:A:ILE:HG21	1:405:A:LYS:HA	11	0.39
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	14	0.39
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	16	0.39
(1,1600)	1:412:A:LEU:HD22	1:412:A:LEU:H	15	0.39
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD11	16	0.39
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	7	0.39
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	12	0.39
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	19	0.39
(1,1484)	1:432:A:HIS:HB3	1:430:A:LEU:H	11	0.39
(1,1444)	1:442:A:THR:HG23	1:443:A:TYR:HA	12	0.39
(1,1442)	1:443:A:TYR:HE2	1:445:A:GLU:HG2	18	0.39
(1,1424)	1:450:A:ILE:HG23	1:452:A:SER:HB2	1	0.39
(1,1422)	1:451:A:ALA:HB2	1:450:A:ILE:HA	3	0.39
(1,1403)	1:383:A:THR:HG21	1:382:A:ARG:HD2	4	0.39
(1,1316)	1:433:A:LEU:HD22	1:396:A:HIS:HD2	13	0.39
(1,1316)	1:433:A:LEU:HD22	1:396:A:HIS:HD2	16	0.39
(1,1315)	1:375:A:LEU:HD21	1:376:A:TRP:H	3	0.39
(1,1313)	1:375:A:LEU:HD11	1:376:A:TRP:H	7	0.39
(1,1267)	1:354:A:ILE:HD11	1:367:A:VAL:H	12	0.39
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD3	12	0.39
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD2	13	0.39
(1,1142)	1:450:A:ILE:HD13	1:454:A:VAL:HA	4	0.39
(1,1135)	1:367:A:VAL:HG11	1:352:A:ASN:H	9	0.39
(1,1119)	1:367:A:VAL:HG21	1:355:A:ARG:HA	11	0.39
(1,1030)	1:348:A:SER:HB2	1:348:A:SER:HA	11	0.39
(1,1021)	1:437:A:VAL:HG11	1:396:A:HIS:HD2	6	0.39
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	14	0.39
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	10	0.39
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	4	0.39
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	9	0.39
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	10	0.39
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	13	0.39
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	14	0.39
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	17	0.39
(1,594)	1:400:A:LEU:HD21	1:426:A:ARG:HG3	1	0.39
(1,544)	1:395:A:ARG:HB3	1:395:A:ARG:HD2	4	0.39
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD22	19	0.39
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD11	1	0.39
(1,494)	1:360:A:GLU:HG2	1:360:A:GLU:HA	8	0.39
(1,482)	1:389:A:LYS:HG2	1:389:A:LYS:HE2	11	0.39
(1,478)	1:389:A:LYS:HG3	1:389:A:LYS:HE2	9	0.39
(1,454)	1:386:A:THR:HG21	1:370:A:ASN:HA	15	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,365)	1:374:A:ARG:H	1:374:A:ARG:HD2	8	0.39
(1,353)	1:373:A:ALA:HB1	1:385:A:MET:HG3	15	0.39
(1,306)	1:354:A:ILE:HD11	1:366:A:ILE:HG21	11	0.39
(1,300)	1:366:A:ILE:HG22	1:411:A:LEU:HB3	4	0.39
(1,300)	1:366:A:ILE:HG21	1:411:A:LEU:HB3	6	0.39
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	8	0.39
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	1	0.39
(1,34)	1:341:A:VAL:HG13	1:337:A:LEU:HG	3	0.39
(1,34)	1:341:A:VAL:HG13	1:337:A:LEU:HG	16	0.39
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB1	4	0.38
(1,2974)	1:433:A:LEU:H	1:431:A:GLU:HB2	14	0.38
(1,2972)	1:435:A:SER:H	1:436:A:GLN:HG3	12	0.38
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	18	0.38
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	2	0.38
(1,2947)	1:362:A:LYS:H	1:363:A:ILE:HB	17	0.38
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	6	0.38
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	17	0.38
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD23	12	0.38
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	4	0.38
(1,2837)	1:410:A:ARG:HB2	1:410:A:ARG:HD3	16	0.38
(1,2824)	1:413:A:PHE:HE2	1:411:A:LEU:HD22	3	0.38
(1,2775)	1:387:A:TYR:HD2	1:390:A:MET:HG2	19	0.38
(1,2768)	1:394:A:LEU:HD12	1:387:A:TYR:HD1	13	0.38
(1,2730)	1:366:A:ILE:HG21	1:370:A:ASN:H	1	0.38
(1,2730)	1:366:A:ILE:HG23	1:370:A:ASN:H	16	0.38
(1,2730)	1:366:A:ILE:HG23	1:370:A:ASN:H	18	0.38
(1,2716)	1:372:A:LEU:HG	1:341:A:VAL:HG22	10	0.38
(1,2693)	1:437:A:VAL:HG21	1:441:A:GLN:HE22	6	0.38
(1,2693)	1:437:A:VAL:HG22	1:441:A:GLN:HE22	12	0.38
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG22	4	0.38
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG3	15	0.38
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG2	6	0.38
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG3	12	0.38
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG3	13	0.38
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG2	14	0.38
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG3	19	0.38
(1,2658)	1:366:A:ILE:HG21	1:411:A:LEU:HB2	14	0.38
(1,2643)	1:402:A:ILE:HD13	1:397:A:TYR:HD1	9	0.38
(1,2587)	1:362:A:LYS:HA	1:415:A:PHE:HD2	6	0.38
(1,2579)	1:358:A:ASP:HB2	1:363:A:ILE:HG22	1	0.38
(1,2557)	1:341:A:VAL:HG11	1:403:A:ILE:HD12	8	0.38
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG21	15	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG21	16	0.38
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD23	15	0.38
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD22	16	0.38
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD23	18	0.38
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD21	1	0.38
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD22	4	0.38
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD22	13	0.38
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD22	14	0.38
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD21	15	0.38
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD11	8	0.38
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD12	17	0.38
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	14	0.38
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	18	0.38
(1,2472)	1:409:A:GLN:HE22	1:412:A:LEU:HD12	14	0.38
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	8	0.38
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	16	0.38
(1,2258)	1:450:A:ILE:H	1:450:A:ILE:HG13	12	0.38
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB2	2	0.38
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD12	7	0.38
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD13	13	0.38
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	16	0.38
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG22	8	0.38
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	1	0.38
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	13	0.38
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	15	0.38
(1,2054)	1:362:A:LYS:H	1:362:A:LYS:HG3	15	0.38
(1,1921)	1:375:A:LEU:HD11	1:375:A:LEU:HD22	8	0.38
(1,1921)	1:375:A:LEU:HD11	1:375:A:LEU:HD22	14	0.38
(1,1921)	1:375:A:LEU:HD13	1:375:A:LEU:HD21	18	0.38
(1,1909)	1:344:A:LEU:HD12	1:354:A:ILE:HG22	19	0.38
(1,1904)	1:437:A:VAL:HG11	1:438:A:LEU:HD21	1	0.38
(1,1899)	1:430:A:LEU:HD11	1:400:A:LEU:HD21	8	0.38
(1,1897)	1:430:A:LEU:HD11	1:430:A:LEU:HD22	1	0.38
(1,1895)	1:411:A:LEU:HD22	1:366:A:ILE:HD13	9	0.38
(1,1872)	1:426:A:ARG:HG2	1:426:A:ARG:HD2	6	0.38
(1,1872)	1:426:A:ARG:HG2	1:426:A:ARG:HD2	9	0.38
(1,1872)	1:426:A:ARG:HG2	1:426:A:ARG:HD2	10	0.38
(1,1872)	1:426:A:ARG:HG2	1:426:A:ARG:HD2	15	0.38
(1,1872)	1:426:A:ARG:HG2	1:426:A:ARG:HD2	16	0.38
(1,1872)	1:426:A:ARG:HG2	1:426:A:ARG:HD2	17	0.38
(1,1821)	1:386:A:THR:H	1:389:A:LYS:HD2	13	0.38
(1,1802)	1:336:A:LEU:HD13	1:431:A:GLU:HA	19	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1778)	1:337:A:LEU:HD13	1:376:A:TRP:HB3	4	0.38
(1,1778)	1:337:A:LEU:HD12	1:376:A:TRP:HB3	14	0.38
(1,1776)	1:337:A:LEU:HD11	1:390:A:MET:HG3	13	0.38
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD23	12	0.38
(1,1686)	1:402:A:ILE:HG22	1:403:A:ILE:HG12	7	0.38
(1,1686)	1:402:A:ILE:HG22	1:403:A:ILE:HG12	14	0.38
(1,1686)	1:402:A:ILE:HG22	1:403:A:ILE:HG12	17	0.38
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG21	5	0.38
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG22	18	0.38
(1,1671)	1:403:A:ILE:HG22	1:405:A:LYS:HA	7	0.38
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	15	0.38
(1,1607)	1:411:A:LEU:HD11	1:366:A:ILE:H	15	0.38
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	13	0.38
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	13	0.38
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG22	2	0.38
(1,1480)	1:412:A:LEU:HD21	1:357:A:GLU:HG2	1	0.38
(1,1467)	1:434:A:GLU:HB2	1:434:A:GLU:HA	17	0.38
(1,1432)	1:445:A:GLU:HG2	1:445:A:GLU:HA	11	0.38
(1,1432)	1:445:A:GLU:HG2	1:445:A:GLU:HA	13	0.38
(1,1430)	1:447:A:GLU:HB2	1:448:A:PRO:HD3	6	0.38
(1,1422)	1:451:A:ALA:HB3	1:450:A:ILE:HA	2	0.38
(1,1422)	1:451:A:ALA:HB3	1:450:A:ILE:HA	6	0.38
(1,1403)	1:383:A:THR:HG21	1:382:A:ARG:HD2	17	0.38
(1,1402)	1:383:A:THR:HG23	1:384:A:ASN:HD21	19	0.38
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	14	0.38
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD22	6	0.38
(1,1315)	1:375:A:LEU:HD23	1:376:A:TRP:H	7	0.38
(1,1315)	1:375:A:LEU:HD21	1:376:A:TRP:H	8	0.38
(1,1315)	1:375:A:LEU:HD22	1:376:A:TRP:H	17	0.38
(1,1315)	1:375:A:LEU:HD22	1:376:A:TRP:H	19	0.38
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	6	0.38
(1,1142)	1:450:A:ILE:HD13	1:454:A:VAL:HA	14	0.38
(1,1130)	1:365:A:ARG:HG2	1:367:A:VAL:HG23	4	0.38
(1,1130)	1:365:A:ARG:HG2	1:367:A:VAL:HG22	11	0.38
(1,1119)	1:367:A:VAL:HG23	1:355:A:ARG:HA	6	0.38
(1,1084)	1:372:A:LEU:HD13	1:344:A:LEU:HD13	3	0.38
(1,1021)	1:437:A:VAL:HG13	1:396:A:HIS:HD2	15	0.38
(1,978)	1:453:A:PRO:HA	1:450:A:ILE:HD13	15	0.38
(1,921)	1:441:A:GLN:HA	1:441:A:GLN:HB2	13	0.38
(1,921)	1:441:A:GLN:HA	1:441:A:GLN:HB2	19	0.38
(1,876)	1:436:A:GLN:HB3	1:437:A:VAL:HG11	4	0.38
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB3	18	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	11	0.38
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	12	0.38
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	18	0.38
(1,713)	1:414:A:ARG:HE	1:414:A:ARG:HB3	19	0.38
(1,690)	1:411:A:LEU:HD21	1:369:A:PRO:HB2	9	0.38
(1,627)	1:403:A:ILE:HG23	1:413:A:PHE:HB2	19	0.38
(1,620)	1:403:A:ILE:HG22	1:403:A:ILE:H	17	0.38
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD23	13	0.38
(1,577)	1:399:A:LYS:HA	1:399:A:LYS:HG3	12	0.38
(1,577)	1:399:A:LYS:HA	1:399:A:LYS:HG3	17	0.38
(1,544)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	19	0.38
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD22	9	0.38
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD23	15	0.38
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD11	8	0.38
(1,456)	1:386:A:THR:HG21	1:387:A:TYR:HB2	7	0.38
(1,347)	1:373:A:ALA:HA	1:376:A:TRP:HB2	1	0.38
(1,306)	1:354:A:ILE:HD13	1:366:A:ILE:HG21	13	0.38
(1,306)	1:354:A:ILE:HD13	1:366:A:ILE:HG22	16	0.38
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG22	18	0.38
(1,205)	1:357:A:GLU:HB3	1:363:A:ILE:HG21	13	0.38
(1,127)	1:349:A:ARG:HD2	1:350:A:TYR:HE1	9	0.38
(1,34)	1:341:A:VAL:HG11	1:337:A:LEU:HG	1	0.38
(1,34)	1:341:A:VAL:HG12	1:337:A:LEU:HG	2	0.38
(1,2974)	1:433:A:LEU:H	1:431:A:GLU:HB2	9	0.37
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	6	0.37
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	14	0.37
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	16	0.37
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	13	0.37
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG23	11	0.37
(1,2882)	1:402:A:ILE:HB	1:397:A:TYR:HD2	10	0.37
(1,2872)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	15	0.37
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD21	1	0.37
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD23	6	0.37
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD22	8	0.37
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD22	13	0.37
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD21	19	0.37
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	10	0.37
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	15	0.37
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	8	0.37
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	13	0.37
(1,2844)	1:402:A:ILE:HG22	1:397:A:TYR:HD2	8	0.37
(1,2813)	1:418:A:THR:HG22	1:362:A:LYS:HD2	13	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2799)	1:412:A:LEU:HD23	1:365:A:ARG:HD3	5	0.37
(1,2775)	1:387:A:TYR:HD2	1:390:A:MET:HG2	10	0.37
(1,2774)	1:443:A:TYR:HD2	1:445:A:GLU:HB2	10	0.37
(1,2752)	1:392:A:ARG:H	1:392:A:ARG:HD3	8	0.37
(1,2730)	1:366:A:ILE:HG22	1:370:A:ASN:H	9	0.37
(1,2697)	1:447:A:GLU:HG3	1:447:A:GLU:HB2	19	0.37
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG21	5	0.37
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG2	6	0.37
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG3	8	0.37
(1,2683)	1:429:A:ARG:HG2	1:429:A:ARG:H	7	0.37
(1,2675)	1:417:A:LYS:HD2	1:402:A:ILE:HG13	4	0.37
(1,2675)	1:417:A:LYS:HD2	1:402:A:ILE:HG13	10	0.37
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG3	1	0.37
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG2	2	0.37
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG2	5	0.37
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG2	7	0.37
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG3	8	0.37
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG3	10	0.37
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG2	18	0.37
(1,2658)	1:366:A:ILE:HG23	1:411:A:LEU:HB2	2	0.37
(1,2644)	1:402:A:ILE:HD12	1:397:A:TYR:HE1	18	0.37
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	15	0.37
(1,2618)	1:375:A:LEU:HD21	1:378:A:ASN:HB2	4	0.37
(1,2611)	1:393:A:ALA:HB1	1:397:A:TYR:HE1	2	0.37
(1,2611)	1:393:A:ALA:HB1	1:397:A:TYR:HE1	19	0.37
(1,2607)	1:367:A:VAL:HA	1:365:A:ARG:HD2	7	0.37
(1,2587)	1:362:A:LYS:HA	1:415:A:PHE:HD2	1	0.37
(1,2555)	1:340:A:TYR:HA	1:343:A:GLN:HG2	9	0.37
(1,2550)	1:451:A:ALA:H	1:450:A:ILE:HG22	8	0.37
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD12	8	0.37
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD12	11	0.37
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD12	18	0.37
(1,2532)	1:384:A:ASN:H	1:383:A:THR:HG23	11	0.37
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD21	2	0.37
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD21	7	0.37
(1,2527)	1:367:A:VAL:HG11	1:368:A:ASP:H	2	0.37
(1,2527)	1:367:A:VAL:HG11	1:368:A:ASP:H	13	0.37
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD22	12	0.37
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD21	17	0.37
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD21	6	0.37
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD21	7	0.37
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD21	11	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD22	16	0.37
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD21	17	0.37
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD13	3	0.37
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	11	0.37
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD11	1	0.37
(1,2158)	1:382:A:ARG:H	1:377:A:GLY:HA3	18	0.37
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	19	0.37
(1,1969)	1:347:A:ASP:H	1:346:A:SER:HB2	9	0.37
(1,1969)	1:347:A:ASP:H	1:346:A:SER:HB2	10	0.37
(1,1921)	1:375:A:LEU:HD12	1:375:A:LEU:HD23	1	0.37
(1,1921)	1:375:A:LEU:HD13	1:375:A:LEU:HD21	7	0.37
(1,1921)	1:375:A:LEU:HD13	1:375:A:LEU:HD22	16	0.37
(1,1904)	1:437:A:VAL:HG13	1:438:A:LEU:HD21	4	0.37
(1,1904)	1:437:A:VAL:HG11	1:438:A:LEU:HD22	18	0.37
(1,1897)	1:430:A:LEU:HD13	1:430:A:LEU:HD23	17	0.37
(1,1895)	1:411:A:LEU:HD23	1:366:A:ILE:HD13	6	0.37
(1,1887)	1:400:A:LEU:HD21	1:400:A:LEU:HD11	2	0.37
(1,1887)	1:400:A:LEU:HD23	1:400:A:LEU:HD13	19	0.37
(1,1872)	1:426:A:ARG:HG2	1:426:A:ARG:HD2	2	0.37
(1,1872)	1:426:A:ARG:HG2	1:426:A:ARG:HD2	4	0.37
(1,1872)	1:426:A:ARG:HG2	1:426:A:ARG:HD2	7	0.37
(1,1872)	1:426:A:ARG:HG2	1:426:A:ARG:HD2	8	0.37
(1,1872)	1:426:A:ARG:HG2	1:426:A:ARG:HD2	11	0.37
(1,1872)	1:426:A:ARG:HG2	1:426:A:ARG:HD2	12	0.37
(1,1872)	1:426:A:ARG:HG2	1:426:A:ARG:HD2	14	0.37
(1,1872)	1:426:A:ARG:HG2	1:426:A:ARG:HD2	18	0.37
(1,1872)	1:426:A:ARG:HG2	1:426:A:ARG:HD2	19	0.37
(1,1840)	1:374:A:ARG:HA	1:374:A:ARG:HD2	7	0.37
(1,1820)	1:392:A:ARG:HB3	1:392:A:ARG:HA	18	0.37
(1,1778)	1:337:A:LEU:HD13	1:376:A:TRP:HB3	9	0.37
(1,1771)	1:341:A:VAL:HG13	1:337:A:LEU:HD13	12	0.37
(1,1761)	1:340:A:TYR:HB2	1:337:A:LEU:HA	2	0.37
(1,1726)	1:341:A:VAL:HG21	1:338:A:TRP:HA	14	0.37
(1,1713)	1:343:A:GLN:HE21	1:343:A:GLN:HG2	2	0.37
(1,1713)	1:343:A:GLN:HE21	1:343:A:GLN:HG2	3	0.37
(1,1713)	1:343:A:GLN:HE21	1:343:A:GLN:HG2	10	0.37
(1,1713)	1:343:A:GLN:HE21	1:343:A:GLN:HG2	14	0.37
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG23	14	0.37
(1,1686)	1:402:A:ILE:HG22	1:403:A:ILE:HG12	12	0.37
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG21	8	0.37
(1,1679)	1:402:A:ILE:H	1:402:A:ILE:HG22	12	0.37
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD13	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD11	12	0.37
(1,1670)	1:403:A:ILE:HG22	1:397:A:TYR:HB2	12	0.37
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	3	0.37
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	10	0.37
(1,1607)	1:411:A:LEU:HD12	1:366:A:ILE:H	16	0.37
(1,1600)	1:412:A:LEU:HD23	1:412:A:LEU:H	13	0.37
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	15	0.37
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG21	9	0.37
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG23	16	0.37
(1,1523)	1:422:A:ILE:HG23	1:426:A:ARG:HG2	17	0.37
(1,1513)	1:424:A:SER:HB2	1:424:A:SER:H	10	0.37
(1,1427)	1:447:A:GLU:HA	1:448:A:PRO:HD3	19	0.37
(1,1422)	1:451:A:ALA:HB1	1:450:A:ILE:HA	1	0.37
(1,1422)	1:451:A:ALA:HB3	1:450:A:ILE:HA	5	0.37
(1,1422)	1:451:A:ALA:HB1	1:450:A:ILE:HA	12	0.37
(1,1422)	1:451:A:ALA:HB3	1:450:A:ILE:HA	19	0.37
(1,1315)	1:375:A:LEU:HD22	1:376:A:TRP:H	9	0.37
(1,1315)	1:375:A:LEU:HD21	1:376:A:TRP:H	11	0.37
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD2	5	0.37
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD3	15	0.37
(1,1182)	1:363:A:ILE:HD11	1:406:A:GLU:HG2	18	0.37
(1,1142)	1:450:A:ILE:HD11	1:454:A:VAL:HA	13	0.37
(1,1130)	1:365:A:ARG:HG2	1:367:A:VAL:HG21	9	0.37
(1,1128)	1:355:A:ARG:HB3	1:367:A:VAL:HG21	1	0.37
(1,1128)	1:355:A:ARG:HB3	1:367:A:VAL:HG21	13	0.37
(1,1084)	1:372:A:LEU:HD12	1:344:A:LEU:HD13	1	0.37
(1,1084)	1:372:A:LEU:HD11	1:344:A:LEU:HD13	11	0.37
(1,1084)	1:372:A:LEU:HD13	1:344:A:LEU:HD12	18	0.37
(1,1060)	1:351:A:GLU:HB2	1:355:A:ARG:HD3	11	0.37
(1,1021)	1:437:A:VAL:HG13	1:396:A:HIS:HD2	13	0.37
(1,973)	1:452:A:SER:H	1:452:A:SER:HB2	3	0.37
(1,924)	1:441:A:GLN:HE22	1:441:A:GLN:HG2	2	0.37
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	6	0.37
(1,731)	1:416:A:MET:H	1:415:A:PHE:HB2	19	0.37
(1,690)	1:411:A:LEU:HD23	1:369:A:PRO:HB2	19	0.37
(1,627)	1:403:A:ILE:HG21	1:413:A:PHE:HB2	17	0.37
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD21	7	0.37
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	1	0.37
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	3	0.37
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	6	0.37
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	8	0.37
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	10	0.37
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	11	0.37
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	15	0.37
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	16	0.37
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	18	0.37
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD23	3	0.37
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD23	8	0.37
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD23	16	0.37
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	1	0.37
(1,454)	1:386:A:THR:HG21	1:370:A:ASN:HA	17	0.37
(1,347)	1:373:A:ALA:HA	1:376:A:TRP:HB2	6	0.37
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG23	19	0.37
(1,300)	1:366:A:ILE:HG23	1:411:A:LEU:HB3	2	0.37
(1,300)	1:366:A:ILE:HG21	1:411:A:LEU:HB3	8	0.37
(1,246)	1:362:A:LYS:HA	1:362:A:LYS:HG3	13	0.37
(1,108)	1:345:A:LEU:HD23	1:345:A:LEU:HB2	13	0.37
(1,34)	1:341:A:VAL:HG11	1:337:A:LEU:HG	6	0.37
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB1	11	0.36
(1,2972)	1:435:A:SER:H	1:436:A:GLN:HG3	8	0.36
(1,2972)	1:435:A:SER:H	1:436:A:GLN:HG3	11	0.36
(1,2972)	1:435:A:SER:H	1:436:A:GLN:HG3	15	0.36
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	9	0.36
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	12	0.36
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	17	0.36
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	4	0.36
(1,2947)	1:362:A:LYS:H	1:362:A:LYS:HD2	6	0.36
(1,2940)	1:411:A:LEU:H	1:410:A:ARG:HG3	17	0.36
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD21	5	0.36
(1,2895)	1:353:A:PHE:H	1:367:A:VAL:HG21	4	0.36
(1,2882)	1:402:A:ILE:HB	1:397:A:TYR:HD2	8	0.36
(1,2872)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	7	0.36
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	16	0.36
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD22	5	0.36
(1,2861)	1:340:A:TYR:HE1	1:340:A:TYR:HB2	18	0.36
(1,2813)	1:418:A:THR:HG22	1:362:A:LYS:HD2	4	0.36
(1,2813)	1:418:A:THR:HG21	1:362:A:LYS:HD2	14	0.36
(1,2794)	1:433:A:LEU:HD23	1:429:A:ARG:HD3	12	0.36
(1,2745)	1:360:A:GLU:HA	1:359:A:LYS:HG2	6	0.36
(1,2730)	1:366:A:ILE:HG22	1:373:A:ALA:H	19	0.36
(1,2724)	1:367:A:VAL:HG23	1:352:A:ASN:HA	15	0.36
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG23	2	0.36
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG21	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2688)	1:431:A:GLU:HG2	1:431:A:GLU:HB3	1	0.36
(1,2688)	1:431:A:GLU:HG2	1:431:A:GLU:HB3	6	0.36
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG3	17	0.36
(1,2650)	1:403:A:ILE:HD11	1:338:A:TRP:HA	9	0.36
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	9	0.36
(1,2612)	1:393:A:ALA:HB3	1:376:A:TRP:HZ3	18	0.36
(1,2611)	1:393:A:ALA:HB1	1:397:A:TYR:HE1	10	0.36
(1,2598)	1:363:A:ILE:HG21	1:357:A:GLU:HG3	13	0.36
(1,2587)	1:362:A:LYS:HA	1:415:A:PHE:HD2	7	0.36
(1,2587)	1:361:A:SER:H	1:362:A:LYS:HA	12	0.36
(1,2567)	1:345:A:LEU:HD23	1:355:A:ARG:HA	19	0.36
(1,2556)	1:341:A:VAL:HG12	1:364:A:PHE:HZ	6	0.36
(1,2555)	1:340:A:TYR:HA	1:343:A:GLN:HG2	17	0.36
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD13	1	0.36
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG21	4	0.36
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD13	4	0.36
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD13	6	0.36
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD13	13	0.36
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD11	14	0.36
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD12	15	0.36
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD12	17	0.36
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD22	5	0.36
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD21	1	0.36
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD21	11	0.36
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD23	5	0.36
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD21	9	0.36
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD13	1	0.36
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD12	12	0.36
(1,2418)	1:444:A:GLN:H	1:441:A:GLN:HG2	18	0.36
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	11	0.36
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD11	10	0.36
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD11	12	0.36
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	11	0.36
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	3	0.36
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	5	0.36
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	6	0.36
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	16	0.36
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB2	5	0.36
(1,1921)	1:375:A:LEU:HD11	1:375:A:LEU:HD23	9	0.36
(1,1912)	1:354:A:ILE:HD12	1:372:A:LEU:HD13	18	0.36
(1,1904)	1:437:A:VAL:HG13	1:438:A:LEU:HD23	14	0.36
(1,1899)	1:430:A:LEU:HD13	1:400:A:LEU:HD21	13	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1899)	1:430:A:LEU:HD13	1:400:A:LEU:HD21	15	0.36
(1,1897)	1:430:A:LEU:HD11	1:430:A:LEU:HD23	5	0.36
(1,1897)	1:430:A:LEU:HD13	1:430:A:LEU:HD21	12	0.36
(1,1897)	1:430:A:LEU:HD11	1:430:A:LEU:HD22	15	0.36
(1,1885)	1:400:A:LEU:HD21	1:402:A:ILE:HD13	15	0.36
(1,1873)	1:383:A:THR:HG22	1:384:A:ASN:HD22	15	0.36
(1,1840)	1:374:A:ARG:HA	1:374:A:ARG:HD2	18	0.36
(1,1802)	1:336:A:LEU:HD12	1:431:A:GLU:HA	14	0.36
(1,1800)	1:336:A:LEU:HD13	1:338:A:TRP:HD1	12	0.36
(1,1780)	1:337:A:LEU:HD13	1:376:A:TRP:HA	6	0.36
(1,1778)	1:337:A:LEU:HD13	1:376:A:TRP:HB3	2	0.36
(1,1756)	1:402:A:ILE:HB	1:397:A:TYR:HB2	17	0.36
(1,1713)	1:343:A:GLN:HE21	1:343:A:GLN:HG2	1	0.36
(1,1713)	1:343:A:GLN:HE21	1:343:A:GLN:HG2	19	0.36
(1,1690)	1:402:A:ILE:HD13	1:400:A:LEU:HA	11	0.36
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG21	3	0.36
(1,1670)	1:403:A:ILE:HG21	1:397:A:TYR:HB2	2	0.36
(1,1670)	1:403:A:ILE:HG21	1:397:A:TYR:HB2	11	0.36
(1,1653)	1:404:A:ARG:HG2	1:414:A:ARG:HD3	1	0.36
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	6	0.36
(1,1607)	1:411:A:LEU:HD13	1:366:A:ILE:H	11	0.36
(1,1607)	1:411:A:LEU:HD12	1:366:A:ILE:H	12	0.36
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG22	17	0.36
(1,1507)	1:426:A:ARG:HG2	1:426:A:ARG:HA	19	0.36
(1,1486)	1:432:A:HIS:HD2	1:436:A:GLN:HB2	9	0.36
(1,1475)	1:433:A:LEU:HD23	1:434:A:GLU:H	9	0.36
(1,1448)	1:442:A:THR:HG22	1:456:A:TRP:HB3	1	0.36
(1,1444)	1:442:A:THR:HG21	1:443:A:TYR:HA	10	0.36
(1,1432)	1:445:A:GLU:HG2	1:445:A:GLU:HA	5	0.36
(1,1432)	1:445:A:GLU:HG2	1:445:A:GLU:HA	8	0.36
(1,1422)	1:451:A:ALA:HB3	1:450:A:ILE:HA	11	0.36
(1,1422)	1:451:A:ALA:HB3	1:450:A:ILE:HA	14	0.36
(1,1393)	1:386:A:THR:HG21	1:388:A:GLU:HB3	11	0.36
(1,1315)	1:375:A:LEU:HD22	1:376:A:TRP:H	1	0.36
(1,1315)	1:375:A:LEU:HD22	1:376:A:TRP:H	2	0.36
(1,1315)	1:375:A:LEU:HD21	1:376:A:TRP:H	14	0.36
(1,1278)	1:382:A:ARG:HG2	1:382:A:ARG:HA	10	0.36
(1,1250)	1:345:A:LEU:HD23	1:355:A:ARG:HA	19	0.36
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD3	7	0.36
(1,1155)	1:364:A:PHE:HA	1:345:A:LEU:HD12	19	0.36
(1,1142)	1:450:A:ILE:HD13	1:454:A:VAL:HA	17	0.36
(1,1133)	1:367:A:VAL:HG11	1:352:A:ASN:HB3	16	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	15	0.36
(1,1033)	1:348:A:SER:HB3	1:351:A:GLU:HB3	14	0.36
(1,1025)	1:336:A:LEU:HD21	1:430:A:LEU:H	15	0.36
(1,1021)	1:437:A:VAL:HG11	1:396:A:HIS:HD2	7	0.36
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB1	16	0.36
(1,834)	1:430:A:LEU:HD13	1:397:A:TYR:HD1	10	0.36
(1,790)	1:428:A:ASP:HA	1:428:A:ASP:HB2	19	0.36
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	2	0.36
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	3	0.36
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	5	0.36
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	6	0.36
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	9	0.36
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	11	0.36
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	12	0.36
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	13	0.36
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	16	0.36
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	17	0.36
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	18	0.36
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	19	0.36
(1,738)	1:417:A:LYS:HG3	1:416:A:MET:HB2	4	0.36
(1,690)	1:411:A:LEU:HD21	1:369:A:PRO:HB2	10	0.36
(1,627)	1:403:A:ILE:HG23	1:413:A:PHE:HB2	4	0.36
(1,627)	1:403:A:ILE:HG23	1:413:A:PHE:HB2	9	0.36
(1,590)	1:400:A:LEU:HD11	1:397:A:TYR:HE1	9	0.36
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	2	0.36
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	4	0.36
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	5	0.36
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	7	0.36
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	13	0.36
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	14	0.36
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	17	0.36
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	19	0.36
(1,577)	1:399:A:LYS:HA	1:399:A:LYS:HG3	1	0.36
(1,577)	1:399:A:LYS:HA	1:399:A:LYS:HG3	2	0.36
(1,577)	1:399:A:LYS:HA	1:399:A:LYS:HG3	11	0.36
(1,577)	1:399:A:LYS:HA	1:399:A:LYS:HG3	15	0.36
(1,577)	1:399:A:LYS:HA	1:399:A:LYS:HG3	18	0.36
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD21	11	0.36
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD11	16	0.36
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	13	0.36
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG21	3	0.36
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG22	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG21	9	0.36
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG22	16	0.36
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG21	17	0.36
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	5	0.36
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	9	0.36
(1,108)	1:345:A:LEU:HD23	1:345:A:LEU:HB2	2	0.36
(1,108)	1:345:A:LEU:HD23	1:345:A:LEU:HB2	10	0.36
(1,108)	1:345:A:LEU:HD21	1:345:A:LEU:HB2	19	0.36
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD23	8	0.36
(1,5)	1:337:A:LEU:HD23	1:390:A:MET:HG3	4	0.36
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB3	1	0.35
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB3	12	0.35
(1,2972)	1:435:A:SER:H	1:436:A:GLN:HG3	5	0.35
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	7	0.35
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	12	0.35
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	14	0.35
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	1	0.35
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	2	0.35
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	3	0.35
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	7	0.35
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	8	0.35
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	10	0.35
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	11	0.35
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	12	0.35
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	13	0.35
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	14	0.35
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	15	0.35
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	18	0.35
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	19	0.35
(1,2947)	1:362:A:LYS:H	1:363:A:ILE:HB	1	0.35
(1,2882)	1:402:A:ILE:HB	1:397:A:TYR:HD2	17	0.35
(1,2872)	1:447:A:GLU:HG3	1:447:A:GLU:HB2	1	0.35
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	2	0.35
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	12	0.35
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD23	7	0.35
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD23	9	0.35
(1,2866)	1:430:A:LEU:HB2	1:430:A:LEU:HD21	11	0.35
(1,2844)	1:402:A:ILE:HG22	1:397:A:TYR:HD2	5	0.35
(1,2730)	1:366:A:ILE:HG23	1:370:A:ASN:H	7	0.35
(1,2725)	1:367:A:VAL:HG22	1:365:A:ARG:HB3	13	0.35
(1,2724)	1:367:A:VAL:HG22	1:352:A:ASN:HA	6	0.35
(1,2724)	1:367:A:VAL:HG22	1:352:A:ASN:HA	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2697)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	15	0.35
(1,2689)	1:436:A:GLN:HB3	1:436:A:GLN:HG2	4	0.35
(1,2688)	1:431:A:GLU:HG2	1:431:A:GLU:HB3	3	0.35
(1,2688)	1:431:A:GLU:HG2	1:431:A:GLU:HB3	5	0.35
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG2	4	0.35
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG3	15	0.35
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG3	16	0.35
(1,2659)	1:366:A:ILE:HD11	1:411:A:LEU:HB3	19	0.35
(1,2658)	1:366:A:ILE:HG22	1:411:A:LEU:HB2	17	0.35
(1,2643)	1:402:A:ILE:HD13	1:397:A:TYR:HD1	4	0.35
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	4	0.35
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	14	0.35
(1,2611)	1:393:A:ALA:HB2	1:397:A:TYR:HE1	12	0.35
(1,2598)	1:363:A:ILE:HG22	1:357:A:GLU:HG3	12	0.35
(1,2587)	1:361:A:SER:H	1:362:A:LYS:HA	2	0.35
(1,2579)	1:358:A:ASP:HB2	1:363:A:ILE:HG22	2	0.35
(1,2579)	1:358:A:ASP:HB2	1:363:A:ILE:HG22	3	0.35
(1,2557)	1:341:A:VAL:HG13	1:403:A:ILE:HD11	9	0.35
(1,2556)	1:341:A:VAL:HG13	1:364:A:PHE:HZ	15	0.35
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG22	6	0.35
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD13	12	0.35
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD12	19	0.35
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG22	6	0.35
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG21	13	0.35
(1,2527)	1:367:A:VAL:HG11	1:368:A:ASP:H	6	0.35
(1,2527)	1:367:A:VAL:HG12	1:368:A:ASP:H	8	0.35
(1,2527)	1:367:A:VAL:HG13	1:368:A:ASP:H	9	0.35
(1,2527)	1:367:A:VAL:HG13	1:368:A:ASP:H	17	0.35
(1,2527)	1:367:A:VAL:HG13	1:368:A:ASP:H	19	0.35
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD22	11	0.35
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD22	17	0.35
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD21	19	0.35
(1,2518)	1:344:A:LEU:H	1:344:A:LEU:HD12	5	0.35
(1,2479)	1:401:A:ASN:HD21	1:399:A:LYS:HB3	13	0.35
(1,2472)	1:409:A:GLN:HE22	1:412:A:LEU:HD12	10	0.35
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB3	18	0.35
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	10	0.35
(1,2359)	1:382:A:ARG:H	1:382:A:ARG:HG3	3	0.35
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	10	0.35
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	2	0.35
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	4	0.35
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	12	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB3	18	0.35
(1,1921)	1:375:A:LEU:HD11	1:375:A:LEU:HD21	5	0.35
(1,1921)	1:375:A:LEU:HD13	1:375:A:LEU:HD22	6	0.35
(1,1921)	1:375:A:LEU:HD12	1:375:A:LEU:HD21	19	0.35
(1,1904)	1:437:A:VAL:HG12	1:438:A:LEU:HD23	3	0.35
(1,1904)	1:437:A:VAL:HG12	1:438:A:LEU:HD23	12	0.35
(1,1904)	1:437:A:VAL:HG11	1:438:A:LEU:HD23	13	0.35
(1,1904)	1:437:A:VAL:HG11	1:438:A:LEU:HD21	15	0.35
(1,1895)	1:411:A:LEU:HD22	1:366:A:ILE:HD12	3	0.35
(1,1887)	1:400:A:LEU:HD23	1:400:A:LEU:HD11	7	0.35
(1,1887)	1:400:A:LEU:HD21	1:400:A:LEU:HD13	10	0.35
(1,1887)	1:400:A:LEU:HD22	1:400:A:LEU:HD13	13	0.35
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD11	8	0.35
(1,1761)	1:340:A:TYR:HB2	1:337:A:LEU:HA	7	0.35
(1,1726)	1:341:A:VAL:HG21	1:338:A:TRP:HA	11	0.35
(1,1726)	1:341:A:VAL:HG22	1:338:A:TRP:HA	13	0.35
(1,1726)	1:341:A:VAL:HG22	1:338:A:TRP:HA	15	0.35
(1,1725)	1:341:A:VAL:HG21	1:342:A:TYR:HB2	4	0.35
(1,1725)	1:341:A:VAL:HG23	1:342:A:TYR:HB2	11	0.35
(1,1725)	1:341:A:VAL:HG23	1:342:A:TYR:HB2	12	0.35
(1,1725)	1:341:A:VAL:HG22	1:342:A:TYR:HB2	19	0.35
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG23	7	0.35
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG22	9	0.35
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG21	15	0.35
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG22	19	0.35
(1,1603)	1:357:A:GLU:HG2	1:412:A:LEU:HD11	11	0.35
(1,1600)	1:412:A:LEU:HD23	1:412:A:LEU:H	4	0.35
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD13	18	0.35
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	11	0.35
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG23	10	0.35
(1,1485)	1:432:A:HIS:HD2	1:433:A:LEU:HD22	2	0.35
(1,1478)	1:433:A:LEU:HD21	1:396:A:HIS:HE1	17	0.35
(1,1452)	1:361:A:SER:H	1:360:A:GLU:HG3	6	0.35
(1,1449)	1:442:A:THR:HG23	1:445:A:GLU:HB2	6	0.35
(1,1448)	1:442:A:THR:HG23	1:456:A:TRP:HB3	16	0.35
(1,1403)	1:383:A:THR:HG23	1:382:A:ARG:HD2	15	0.35
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	19	0.35
(1,1315)	1:375:A:LEU:HD22	1:376:A:TRP:H	10	0.35
(1,1286)	1:380:A:LYS:HD3	1:380:A:LYS:H	10	0.35
(1,1224)	1:363:A:ILE:HG21	1:357:A:GLU:HG2	3	0.35
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD2	10	0.35
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD3	19	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1142)	1:450:A:ILE:HD12	1:454:A:VAL:HA	10	0.35
(1,1130)	1:365:A:ARG:HG2	1:367:A:VAL:HG21	19	0.35
(1,1128)	1:355:A:ARG:HB3	1:367:A:VAL:HG23	8	0.35
(1,1084)	1:372:A:LEU:HD11	1:344:A:LEU:HD12	12	0.35
(1,1084)	1:372:A:LEU:HD12	1:344:A:LEU:HD12	15	0.35
(1,1026)	1:336:A:LEU:HD22	1:432:A:HIS:H	13	0.35
(1,978)	1:453:A:PRO:HA	1:450:A:ILE:HD11	9	0.35
(1,978)	1:453:A:PRO:HA	1:450:A:ILE:HD11	18	0.35
(1,888)	1:437:A:VAL:HG23	1:441:A:GLN:HE22	15	0.35
(1,888)	1:437:A:VAL:HG21	1:441:A:GLN:HE22	19	0.35
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD21	10	0.35
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD21	16	0.35
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD22	17	0.35
(1,822)	1:429:A:ARG:HA	1:429:A:ARG:HG2	10	0.35
(1,790)	1:428:A:ASP:HA	1:428:A:ASP:HB2	2	0.35
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	1	0.35
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	4	0.35
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	7	0.35
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	8	0.35
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	14	0.35
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	15	0.35
(1,715)	1:414:A:ARG:HD2	1:414:A:ARG:HH12	10	0.35
(1,713)	1:414:A:ARG:HE	1:414:A:ARG:HB2	9	0.35
(1,690)	1:411:A:LEU:HD21	1:369:A:PRO:HB2	3	0.35
(1,690)	1:411:A:LEU:HD23	1:369:A:PRO:HB2	16	0.35
(1,627)	1:403:A:ILE:HG23	1:413:A:PHE:HB2	14	0.35
(1,627)	1:403:A:ILE:HG22	1:413:A:PHE:HB2	16	0.35
(1,594)	1:400:A:LEU:HD23	1:426:A:ARG:HG3	11	0.35
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD22	5	0.35
(1,587)	1:400:A:LEU:HA	1:400:A:LEU:HB2	12	0.35
(1,577)	1:399:A:LYS:HA	1:399:A:LYS:HG3	10	0.35
(1,577)	1:399:A:LYS:HA	1:399:A:LYS:HG3	14	0.35
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD23	2	0.35
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	9	0.35
(1,454)	1:386:A:THR:HG22	1:370:A:ASN:HA	19	0.35
(1,453)	1:386:A:THR:HG21	1:386:A:THR:HB	6	0.35
(1,453)	1:386:A:THR:HG22	1:386:A:THR:HB	10	0.35
(1,453)	1:386:A:THR:HG23	1:386:A:THR:HB	14	0.35
(1,365)	1:374:A:ARG:H	1:374:A:ARG:HD2	19	0.35
(1,347)	1:373:A:ALA:HA	1:376:A:TRP:HB2	16	0.35
(1,306)	1:354:A:ILE:HD13	1:366:A:ILE:HG23	14	0.35
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG21	13	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,108)	1:345:A:LEU:HD22	1:345:A:LEU:HB2	1	0.35
(1,108)	1:345:A:LEU:HD23	1:345:A:LEU:HB2	4	0.35
(1,108)	1:345:A:LEU:HD22	1:345:A:LEU:HB2	15	0.35
(1,108)	1:345:A:LEU:HD22	1:345:A:LEU:HB2	17	0.35
(1,34)	1:341:A:VAL:HG13	1:337:A:LEU:HG	11	0.35
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB1	17	0.34
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	1	0.34
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	2	0.34
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	10	0.34
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	11	0.34
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	16	0.34
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	9	0.34
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	16	0.34
(1,2956)	1:398:A:TYR:H	1:395:A:ARG:HA	17	0.34
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG23	9	0.34
(1,2882)	1:402:A:ILE:HB	1:397:A:TYR:HD2	18	0.34
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	7	0.34
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	10	0.34
(1,2837)	1:404:A:ARG:HD3	1:404:A:ARG:HB3	11	0.34
(1,2786)	1:445:A:GLU:HG3	1:446:A:ASP:H	13	0.34
(1,2775)	1:387:A:TYR:HD1	1:390:A:MET:HG2	4	0.34
(1,2775)	1:387:A:TYR:HD2	1:390:A:MET:HG2	7	0.34
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB1	11	0.34
(1,2768)	1:394:A:LEU:HD12	1:387:A:TYR:HD1	12	0.34
(1,2724)	1:367:A:VAL:HG23	1:352:A:ASN:HA	3	0.34
(1,2724)	1:367:A:VAL:HG21	1:352:A:ASN:HA	18	0.34
(1,2708)	1:349:A:ARG:HD2	1:350:A:TYR:HE2	12	0.34
(1,2708)	1:349:A:ARG:HD2	1:350:A:TYR:HE1	17	0.34
(1,2697)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	7	0.34
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG22	3	0.34
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG2	10	0.34
(1,2689)	1:436:A:GLN:HB3	1:436:A:GLN:HG2	19	0.34
(1,2688)	1:431:A:GLU:HG2	1:431:A:GLU:HB3	16	0.34
(1,2684)	1:429:A:ARG:HG3	1:433:A:LEU:HD21	18	0.34
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG3	3	0.34
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG2	11	0.34
(1,2658)	1:366:A:ILE:HG23	1:411:A:LEU:HB2	5	0.34
(1,2649)	1:403:A:ILE:HG21	1:364:A:PHE:HZ	16	0.34
(1,2612)	1:393:A:ALA:HB3	1:376:A:TRP:HZ3	8	0.34
(1,2587)	1:362:A:LYS:HA	1:415:A:PHE:HD2	3	0.34
(1,2587)	1:362:A:LYS:HA	1:415:A:PHE:HD2	10	0.34
(1,2557)	1:341:A:VAL:HG11	1:403:A:ILE:HD11	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2557)	1:341:A:VAL:HG12	1:403:A:ILE:HD12	19	0.34
(1,2549)	1:450:A:ILE:H	1:449:A:THR:HG22	9	0.34
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD13	11	0.34
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG23	16	0.34
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD12	2	0.34
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG22	1	0.34
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG22	16	0.34
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD22	8	0.34
(1,2527)	1:367:A:VAL:HG12	1:368:A:ASP:H	1	0.34
(1,2527)	1:367:A:VAL:HG12	1:368:A:ASP:H	3	0.34
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD23	4	0.34
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD23	13	0.34
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD21	8	0.34
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD11	10	0.34
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB3	5	0.34
(1,2418)	1:444:A:GLN:H	1:441:A:GLN:HG2	13	0.34
(1,2415)	1:447:A:GLU:H	1:448:A:PRO:HD3	7	0.34
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	12	0.34
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	18	0.34
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	1	0.34
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	14	0.34
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	15	0.34
(1,2252)	1:442:A:THR:H	1:441:A:GLN:HB3	11	0.34
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD12	6	0.34
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD12	9	0.34
(1,2080)	1:370:A:ASN:H	1:369:A:PRO:HD3	18	0.34
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB3	19	0.34
(1,1921)	1:375:A:LEU:HD12	1:375:A:LEU:HD23	2	0.34
(1,1921)	1:375:A:LEU:HD11	1:375:A:LEU:HD22	12	0.34
(1,1912)	1:354:A:ILE:HD11	1:372:A:LEU:HD13	4	0.34
(1,1912)	1:354:A:ILE:HD11	1:372:A:LEU:HD12	7	0.34
(1,1912)	1:354:A:ILE:HD13	1:372:A:LEU:HD13	8	0.34
(1,1912)	1:354:A:ILE:HD11	1:372:A:LEU:HD11	11	0.34
(1,1912)	1:354:A:ILE:HD13	1:372:A:LEU:HD13	16	0.34
(1,1908)	1:341:A:VAL:HG22	1:345:A:LEU:HD13	3	0.34
(1,1897)	1:430:A:LEU:HD11	1:430:A:LEU:HD22	2	0.34
(1,1887)	1:400:A:LEU:HD23	1:400:A:LEU:HD11	14	0.34
(1,1887)	1:400:A:LEU:HD21	1:400:A:LEU:HD11	17	0.34
(1,1869)	1:338:A:TRP:HE1	1:430:A:LEU:HD12	18	0.34
(1,1800)	1:336:A:LEU:HD12	1:338:A:TRP:HD1	11	0.34
(1,1780)	1:337:A:LEU:HD11	1:376:A:TRP:HA	3	0.34
(1,1778)	1:337:A:LEU:HD12	1:376:A:TRP:HB3	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1778)	1:337:A:LEU:HD13	1:376:A:TRP:HB3	8	0.34
(1,1778)	1:337:A:LEU:HD12	1:376:A:TRP:HB3	11	0.34
(1,1778)	1:337:A:LEU:HD12	1:376:A:TRP:HB3	12	0.34
(1,1726)	1:341:A:VAL:HG22	1:338:A:TRP:HA	16	0.34
(1,1726)	1:341:A:VAL:HG23	1:338:A:TRP:HA	17	0.34
(1,1713)	1:343:A:GLN:HE21	1:343:A:GLN:HG2	13	0.34
(1,1690)	1:402:A:ILE:HD12	1:400:A:LEU:HA	16	0.34
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG21	1	0.34
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG21	16	0.34
(1,1686)	1:402:A:ILE:HG21	1:403:A:ILE:HG12	8	0.34
(1,1670)	1:403:A:ILE:HG22	1:397:A:TYR:HB2	6	0.34
(1,1670)	1:403:A:ILE:HG23	1:397:A:TYR:HB2	10	0.34
(1,1670)	1:403:A:ILE:HG21	1:397:A:TYR:HB2	13	0.34
(1,1670)	1:403:A:ILE:HG23	1:397:A:TYR:HB2	17	0.34
(1,1666)	1:403:A:ILE:HG13	1:364:A:PHE:HZ	19	0.34
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	5	0.34
(1,1607)	1:411:A:LEU:HD12	1:366:A:ILE:H	5	0.34
(1,1607)	1:411:A:LEU:HD12	1:366:A:ILE:H	14	0.34
(1,1600)	1:412:A:LEU:HD23	1:412:A:LEU:H	10	0.34
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG22	8	0.34
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG23	15	0.34
(1,1507)	1:426:A:ARG:HG2	1:426:A:ARG:HA	11	0.34
(1,1497)	1:429:A:ARG:HG2	1:429:A:ARG:HB3	8	0.34
(1,1497)	1:429:A:ARG:HG3	1:429:A:ARG:HB2	11	0.34
(1,1497)	1:429:A:ARG:HG2	1:429:A:ARG:HB3	13	0.34
(1,1497)	1:429:A:ARG:HG2	1:429:A:ARG:HB3	14	0.34
(1,1480)	1:412:A:LEU:HD22	1:357:A:GLU:HG2	19	0.34
(1,1475)	1:433:A:LEU:HD21	1:434:A:GLU:H	14	0.34
(1,1470)	1:433:A:LEU:HA	1:436:A:GLN:HB2	19	0.34
(1,1453)	1:438:A:LEU:HD11	1:435:A:SER:H	10	0.34
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	11	0.34
(1,1427)	1:447:A:GLU:HA	1:448:A:PRO:HD3	10	0.34
(1,1422)	1:451:A:ALA:HB3	1:450:A:ILE:HA	4	0.34
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	18	0.34
(1,1344)	1:398:A:TYR:HD1	1:398:A:TYR:H	16	0.34
(1,1315)	1:375:A:LEU:HD21	1:376:A:TRP:H	12	0.34
(1,1315)	1:375:A:LEU:HD21	1:376:A:TRP:H	16	0.34
(1,1313)	1:375:A:LEU:HD12	1:376:A:TRP:H	10	0.34
(1,1313)	1:375:A:LEU:HD12	1:376:A:TRP:H	14	0.34
(1,1277)	1:382:A:ARG:HG3	1:382:A:ARG:HB2	10	0.34
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD21	12	0.34
(1,1224)	1:363:A:ILE:HG23	1:357:A:GLU:HG2	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	1:363:A:ILE:HG22	1:357:A:GLU:HG2	19	0.34
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD3	16	0.34
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD3	18	0.34
(1,1130)	1:365:A:ARG:HG2	1:367:A:VAL:HG23	10	0.34
(1,1128)	1:355:A:ARG:HB3	1:367:A:VAL:HG22	17	0.34
(1,1123)	1:354:A:ILE:H	1:367:A:VAL:HG22	18	0.34
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	13	0.34
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG23	17	0.34
(1,876)	1:436:A:GLN:HB2	1:437:A:VAL:HG12	9	0.34
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB1	13	0.34
(1,836)	1:430:A:LEU:HD11	1:427:A:THR:HB	12	0.34
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD21	2	0.34
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD23	3	0.34
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD23	4	0.34
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD22	14	0.34
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD21	15	0.34
(1,690)	1:411:A:LEU:HD22	1:369:A:PRO:HB2	5	0.34
(1,627)	1:403:A:ILE:HG21	1:413:A:PHE:HB2	5	0.34
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD22	14	0.34
(1,577)	1:399:A:LYS:HA	1:399:A:LYS:HG3	13	0.34
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD22	10	0.34
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD22	13	0.34
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD13	12	0.34
(1,453)	1:386:A:THR:HG21	1:386:A:THR:HB	5	0.34
(1,306)	1:354:A:ILE:HD13	1:366:A:ILE:HG21	17	0.34
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG22	2	0.34
(1,300)	1:366:A:ILE:HG21	1:411:A:LEU:HB3	14	0.34
(1,203)	1:357:A:GLU:HB2	1:412:A:LEU:HD21	10	0.34
(1,168)	1:354:A:ILE:HG21	1:354:A:ILE:HG13	14	0.34
(1,108)	1:345:A:LEU:HD22	1:345:A:LEU:HB2	9	0.34
(1,108)	1:345:A:LEU:HD22	1:345:A:LEU:HB2	11	0.34
(1,85)	1:344:A:LEU:HD22	1:350:A:TYR:HD1	11	0.34
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD22	4	0.34
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB2	10	0.33
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB3	13	0.33
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	3	0.33
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	8	0.33
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	15	0.33
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	17	0.33
(1,2956)	1:398:A:TYR:H	1:398:A:TYR:HB3	5	0.33
(1,2956)	1:398:A:TYR:H	1:395:A:ARG:HA	6	0.33
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	12	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2941)	1:434:A:GLU:H	1:430:A:LEU:HD22	3	0.33
(1,2931)	1:420:A:ASP:H	1:421:A:GLU:HG3	16	0.33
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	1	0.33
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	5	0.33
(1,2872)	1:447:A:GLU:HG3	1:447:A:GLU:HB2	5	0.33
(1,2872)	1:444:A:GLN:HG2	1:444:A:GLN:HB3	17	0.33
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	13	0.33
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	9	0.33
(1,2850)	1:344:A:LEU:HD13	1:350:A:TYR:HD1	8	0.33
(1,2844)	1:402:A:ILE:HG21	1:397:A:TYR:HD2	15	0.33
(1,2791)	1:380:A:LYS:HE3	1:438:A:LEU:HD22	11	0.33
(1,2730)	1:366:A:ILE:HG23	1:373:A:ALA:H	13	0.33
(1,2725)	1:367:A:VAL:HG21	1:365:A:ARG:HB3	11	0.33
(1,2697)	1:447:A:GLU:HG3	1:447:A:GLU:HB2	1	0.33
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG23	9	0.33
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG22	15	0.33
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG2	2	0.33
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG2	7	0.33
(1,2684)	1:429:A:ARG:HG2	1:433:A:LEU:HD22	19	0.33
(1,2658)	1:366:A:ILE:HG22	1:411:A:LEU:HB2	15	0.33
(1,2658)	1:366:A:ILE:HG23	1:411:A:LEU:HB2	16	0.33
(1,2658)	1:366:A:ILE:HG21	1:411:A:LEU:HB2	19	0.33
(1,2643)	1:402:A:ILE:HD13	1:397:A:TYR:HD1	12	0.33
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	19	0.33
(1,2611)	1:393:A:ALA:HB1	1:397:A:TYR:HE1	15	0.33
(1,2587)	1:362:A:LYS:HA	1:415:A:PHE:HD2	4	0.33
(1,2586)	1:446:A:ASP:H	1:445:A:GLU:HG2	3	0.33
(1,2569)	1:349:A:ARG:HD3	1:350:A:TYR:HE1	8	0.33
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG21	19	0.33
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD11	10	0.33
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD21	4	0.33
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD22	15	0.33
(1,2519)	1:345:A:LEU:H	1:345:A:LEU:HD22	10	0.33
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	8	0.33
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	16	0.33
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD12	17	0.33
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD12	18	0.33
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB3	4	0.33
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB3	9	0.33
(1,2058)	1:363:A:ILE:H	1:358:A:ASP:HB2	3	0.33
(1,1921)	1:375:A:LEU:HD11	1:375:A:LEU:HD23	17	0.33
(1,1916)	1:366:A:ILE:HG22	1:411:A:LEU:HD11	15	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1912)	1:354:A:ILE:HD13	1:372:A:LEU:HD12	17	0.33
(1,1908)	1:341:A:VAL:HG21	1:345:A:LEU:HD12	7	0.33
(1,1904)	1:437:A:VAL:HG12	1:438:A:LEU:HD22	7	0.33
(1,1897)	1:430:A:LEU:HD11	1:430:A:LEU:HD21	4	0.33
(1,1897)	1:430:A:LEU:HD11	1:430:A:LEU:HD21	7	0.33
(1,1895)	1:411:A:LEU:HD22	1:366:A:ILE:HD12	14	0.33
(1,1892)	1:403:A:ILE:HD13	1:402:A:ILE:HG21	2	0.33
(1,1892)	1:403:A:ILE:HD12	1:402:A:ILE:HG23	3	0.33
(1,1887)	1:400:A:LEU:HD22	1:400:A:LEU:HD11	15	0.33
(1,1842)	1:433:A:LEU:H	1:433:A:LEU:HD22	2	0.33
(1,1840)	1:374:A:ARG:HA	1:374:A:ARG:HD2	4	0.33
(1,1761)	1:340:A:TYR:HB2	1:337:A:LEU:HA	10	0.33
(1,1726)	1:341:A:VAL:HG21	1:338:A:TRP:HA	2	0.33
(1,1726)	1:341:A:VAL:HG22	1:338:A:TRP:HA	6	0.33
(1,1726)	1:341:A:VAL:HG22	1:338:A:TRP:HA	7	0.33
(1,1726)	1:341:A:VAL:HG22	1:338:A:TRP:HA	9	0.33
(1,1726)	1:341:A:VAL:HG21	1:338:A:TRP:HA	10	0.33
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG23	4	0.33
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG21	6	0.33
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG23	17	0.33
(1,1670)	1:403:A:ILE:HG22	1:397:A:TYR:HB2	1	0.33
(1,1616)	1:406:A:GLU:HA	1:406:A:GLU:HG3	19	0.33
(1,1604)	1:365:A:ARG:HB2	1:412:A:LEU:HD12	4	0.33
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG21	1	0.33
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG21	4	0.33
(1,1523)	1:422:A:ILE:HG23	1:426:A:ARG:HG2	1	0.33
(1,1523)	1:422:A:ILE:HG21	1:426:A:ARG:HG2	6	0.33
(1,1507)	1:426:A:ARG:HG2	1:426:A:ARG:HA	18	0.33
(1,1497)	1:429:A:ARG:HG3	1:429:A:ARG:HB2	3	0.33
(1,1497)	1:429:A:ARG:HG2	1:429:A:ARG:HB3	7	0.33
(1,1497)	1:429:A:ARG:HG2	1:429:A:ARG:HB3	10	0.33
(1,1497)	1:429:A:ARG:HG2	1:429:A:ARG:HB3	12	0.33
(1,1497)	1:429:A:ARG:HG2	1:429:A:ARG:HB3	15	0.33
(1,1497)	1:429:A:ARG:HG2	1:429:A:ARG:HB3	16	0.33
(1,1480)	1:412:A:LEU:HD22	1:357:A:GLU:HG2	7	0.33
(1,1480)	1:412:A:LEU:HD21	1:357:A:GLU:HG2	11	0.33
(1,1480)	1:412:A:LEU:HD23	1:357:A:GLU:HG2	15	0.33
(1,1475)	1:433:A:LEU:HD22	1:434:A:GLU:H	11	0.33
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	9	0.33
(1,1357)	1:394:A:LEU:HD21	1:390:A:MET:HG3	13	0.33
(1,1344)	1:398:A:TYR:HD1	1:398:A:TYR:H	3	0.33
(1,1315)	1:375:A:LEU:HD23	1:376:A:TRP:H	18	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	1:363:A:ILE:HG22	1:357:A:GLU:HG2	17	0.33
(1,1182)	1:363:A:ILE:HD11	1:406:A:GLU:HG2	2	0.33
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG21	8	0.33
(1,1142)	1:450:A:ILE:HD12	1:454:A:VAL:HA	5	0.33
(1,1130)	1:365:A:ARG:HG2	1:367:A:VAL:HG21	15	0.33
(1,1121)	1:367:A:VAL:HG21	1:365:A:ARG:HA	2	0.33
(1,1060)	1:351:A:GLU:HB2	1:355:A:ARG:HD3	2	0.33
(1,1060)	1:351:A:GLU:HB2	1:355:A:ARG:HD3	10	0.33
(1,1033)	1:348:A:SER:HB3	1:351:A:GLU:HB3	1	0.33
(1,1026)	1:336:A:LEU:HD21	1:432:A:HIS:H	3	0.33
(1,1026)	1:336:A:LEU:HD22	1:432:A:HIS:H	18	0.33
(1,1021)	1:437:A:VAL:HG12	1:396:A:HIS:HD2	4	0.33
(1,890)	1:439:A:ASP:H	1:438:A:LEU:HB2	8	0.33
(1,884)	1:437:A:VAL:HG23	1:392:A:ARG:HG3	6	0.33
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD23	12	0.33
(1,822)	1:429:A:ARG:HA	1:429:A:ARG:HG2	7	0.33
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	2	0.33
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	12	0.33
(1,746)	1:417:A:LYS:HE2	1:417:A:LYS:HD3	10	0.33
(1,627)	1:403:A:ILE:HG22	1:413:A:PHE:HB2	3	0.33
(1,627)	1:403:A:ILE:HG23	1:413:A:PHE:HB2	11	0.33
(1,627)	1:403:A:ILE:HG21	1:413:A:PHE:HB2	15	0.33
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD22	8	0.33
(1,577)	1:399:A:LYS:HA	1:399:A:LYS:HG3	5	0.33
(1,530)	1:394:A:LEU:HD22	1:397:A:TYR:HB3	12	0.33
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD13	9	0.33
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD13	13	0.33
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	16	0.33
(1,455)	1:386:A:THR:HG22	1:389:A:LYS:HE3	6	0.33
(1,453)	1:386:A:THR:HG22	1:386:A:THR:HB	7	0.33
(1,453)	1:386:A:THR:HG22	1:386:A:THR:HB	8	0.33
(1,367)	1:374:A:ARG:HB3	1:374:A:ARG:HD2	15	0.33
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG21	12	0.33
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG23	14	0.33
(1,300)	1:366:A:ILE:HG21	1:411:A:LEU:HB3	1	0.33
(1,300)	1:366:A:ILE:HG22	1:411:A:LEU:HB3	11	0.33
(1,300)	1:366:A:ILE:HG22	1:411:A:LEU:HB3	15	0.33
(1,237)	1:361:A:SER:HB3	1:363:A:ILE:HG12	2	0.33
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	14	0.33
(1,168)	1:354:A:ILE:HG22	1:354:A:ILE:HG13	1	0.33
(1,168)	1:354:A:ILE:HG22	1:354:A:ILE:HG13	7	0.33
(1,168)	1:354:A:ILE:HG23	1:354:A:ILE:HG13	8	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,168)	1:354:A:ILE:HG21	1:354:A:ILE:HG13	11	0.33
(1,168)	1:354:A:ILE:HG22	1:354:A:ILE:HG13	12	0.33
(1,108)	1:345:A:LEU:HD22	1:345:A:LEU:HB2	6	0.33
(1,108)	1:345:A:LEU:HD22	1:345:A:LEU:HB2	8	0.33
(1,108)	1:345:A:LEU:HD23	1:345:A:LEU:HB2	14	0.33
(1,108)	1:345:A:LEU:HD23	1:345:A:LEU:HB2	16	0.33
(1,108)	1:345:A:LEU:HD23	1:345:A:LEU:HB2	18	0.33
(1,34)	1:341:A:VAL:HG13	1:337:A:LEU:HG	5	0.33
(1,34)	1:341:A:VAL:HG13	1:337:A:LEU:HG	18	0.33
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB2	15	0.32
(1,2974)	1:433:A:LEU:H	1:431:A:GLU:HB2	5	0.32
(1,2974)	1:433:A:LEU:H	1:431:A:GLU:HB2	15	0.32
(1,2972)	1:435:A:SER:H	1:436:A:GLN:HG3	9	0.32
(1,2972)	1:435:A:SER:H	1:436:A:GLN:HG3	14	0.32
(1,2972)	1:435:A:SER:H	1:436:A:GLN:HG3	16	0.32
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	5	0.32
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	13	0.32
(1,2940)	1:411:A:LEU:H	1:410:A:ARG:HG3	8	0.32
(1,2895)	1:353:A:PHE:H	1:367:A:VAL:HG21	13	0.32
(1,2882)	1:402:A:ILE:HB	1:397:A:TYR:HD2	12	0.32
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	19	0.32
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	1	0.32
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	2	0.32
(1,2850)	1:344:A:LEU:HD13	1:350:A:TYR:HD1	16	0.32
(1,2837)	1:404:A:ARG:HD3	1:404:A:ARG:HB3	2	0.32
(1,2824)	1:413:A:PHE:HE1	1:411:A:LEU:HD23	11	0.32
(1,2824)	1:413:A:PHE:HE2	1:411:A:LEU:HD21	19	0.32
(1,2798)	1:412:A:LEU:HD23	1:410:A:ARG:HD2	5	0.32
(1,2730)	1:366:A:ILE:HG23	1:370:A:ASN:H	2	0.32
(1,2730)	1:366:A:ILE:HG23	1:370:A:ASN:H	10	0.32
(1,2730)	1:366:A:ILE:HG21	1:370:A:ASN:H	14	0.32
(1,2706)	1:349:A:ARG:HB3	1:350:A:TYR:HE2	13	0.32
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG23	16	0.32
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG2	5	0.32
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG3	17	0.32
(1,2659)	1:366:A:ILE:HG21	1:411:A:LEU:HB3	14	0.32
(1,2643)	1:402:A:ILE:HD12	1:397:A:TYR:HD1	11	0.32
(1,2611)	1:393:A:ALA:HB3	1:397:A:TYR:HE1	4	0.32
(1,2598)	1:363:A:ILE:HG21	1:357:A:GLU:HG3	1	0.32
(1,2587)	1:362:A:LYS:HA	1:415:A:PHE:HD2	16	0.32
(1,2587)	1:362:A:LYS:HA	1:415:A:PHE:HD2	17	0.32
(1,2579)	1:358:A:ASP:HB2	1:363:A:ILE:HG21	14	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2557)	1:341:A:VAL:HG12	1:403:A:ILE:HD12	6	0.32
(1,2555)	1:340:A:TYR:HA	1:339:A:ASP:HB3	7	0.32
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG13	12	0.32
(1,2539)	1:404:A:ARG:H	1:403:A:ILE:HG23	12	0.32
(1,2538)	1:402:A:ILE:H	1:402:A:ILE:HD13	7	0.32
(1,2527)	1:367:A:VAL:HG11	1:368:A:ASP:H	4	0.32
(1,2527)	1:367:A:VAL:HG11	1:368:A:ASP:H	7	0.32
(1,2527)	1:367:A:VAL:HG12	1:368:A:ASP:H	14	0.32
(1,2527)	1:367:A:VAL:HG13	1:368:A:ASP:H	16	0.32
(1,2527)	1:367:A:VAL:HG13	1:368:A:ASP:H	18	0.32
(1,2510)	1:412:A:LEU:H	1:410:A:ARG:HB2	9	0.32
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB2	13	0.32
(1,2418)	1:444:A:GLN:H	1:441:A:GLN:HG2	7	0.32
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	4	0.32
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	6	0.32
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	15	0.32
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	17	0.32
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	4	0.32
(1,2359)	1:382:A:ARG:H	1:382:A:ARG:HG3	19	0.32
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD12	3	0.32
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD12	16	0.32
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD12	19	0.32
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	12	0.32
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	14	0.32
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	18	0.32
(1,2131)	1:380:A:LYS:H	1:380:A:LYS:HG2	19	0.32
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB3	11	0.32
(1,2067)	1:365:A:ARG:H	1:355:A:ARG:HG2	9	0.32
(1,1974)	1:349:A:ARG:H	1:349:A:ARG:HB2	19	0.32
(1,1921)	1:375:A:LEU:HD11	1:375:A:LEU:HD23	10	0.32
(1,1921)	1:375:A:LEU:HD11	1:375:A:LEU:HD21	13	0.32
(1,1920)	1:372:A:LEU:HD13	1:366:A:ILE:HD13	10	0.32
(1,1912)	1:354:A:ILE:HD12	1:372:A:LEU:HD11	2	0.32
(1,1912)	1:354:A:ILE:HD12	1:372:A:LEU:HD13	3	0.32
(1,1912)	1:354:A:ILE:HD11	1:372:A:LEU:HD12	6	0.32
(1,1912)	1:354:A:ILE:HD13	1:372:A:LEU:HD11	9	0.32
(1,1912)	1:354:A:ILE:HD11	1:372:A:LEU:HD12	15	0.32
(1,1897)	1:430:A:LEU:HD13	1:430:A:LEU:HD22	10	0.32
(1,1894)	1:411:A:LEU:HD23	1:411:A:LEU:HD13	1	0.32
(1,1894)	1:411:A:LEU:HD23	1:411:A:LEU:HD11	2	0.32
(1,1894)	1:411:A:LEU:HD23	1:411:A:LEU:HD11	15	0.32
(1,1894)	1:411:A:LEU:HD21	1:411:A:LEU:HD11	17	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1887)	1:400:A:LEU:HD22	1:400:A:LEU:HD13	1	0.32
(1,1887)	1:400:A:LEU:HD23	1:400:A:LEU:HD11	12	0.32
(1,1885)	1:400:A:LEU:HD23	1:402:A:ILE:HD13	8	0.32
(1,1884)	1:394:A:LEU:HD11	1:394:A:LEU:HD23	1	0.32
(1,1867)	1:380:A:LYS:HE2	1:438:A:LEU:HD13	18	0.32
(1,1821)	1:386:A:THR:H	1:389:A:LYS:HD2	12	0.32
(1,1800)	1:336:A:LEU:HD11	1:338:A:TRP:HD1	18	0.32
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD11	7	0.32
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD11	10	0.32
(1,1726)	1:341:A:VAL:HG21	1:338:A:TRP:HA	12	0.32
(1,1725)	1:341:A:VAL:HG21	1:342:A:TYR:HB2	9	0.32
(1,1725)	1:341:A:VAL:HG23	1:342:A:TYR:HB2	18	0.32
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG22	5	0.32
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG21	10	0.32
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG23	11	0.32
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG23	18	0.32
(1,1671)	1:403:A:ILE:HG21	1:405:A:LYS:HA	9	0.32
(1,1671)	1:403:A:ILE:HG21	1:405:A:LYS:HA	12	0.32
(1,1670)	1:403:A:ILE:HG22	1:397:A:TYR:HB2	14	0.32
(1,1670)	1:403:A:ILE:HG23	1:397:A:TYR:HB2	15	0.32
(1,1607)	1:411:A:LEU:HD13	1:366:A:ILE:H	1	0.32
(1,1607)	1:411:A:LEU:HD12	1:366:A:ILE:H	17	0.32
(1,1600)	1:412:A:LEU:HD21	1:412:A:LEU:H	7	0.32
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG21	7	0.32
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG23	18	0.32
(1,1497)	1:429:A:ARG:HG2	1:429:A:ARG:HB3	6	0.32
(1,1497)	1:429:A:ARG:HG2	1:429:A:ARG:HB3	17	0.32
(1,1493)	1:430:A:LEU:HA	1:430:A:LEU:HG	18	0.32
(1,1480)	1:412:A:LEU:HD23	1:357:A:GLU:HG2	16	0.32
(1,1474)	1:433:A:LEU:HB2	1:433:A:LEU:HD21	4	0.32
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	14	0.32
(1,1403)	1:383:A:THR:HG23	1:382:A:ARG:HD2	5	0.32
(1,1393)	1:386:A:THR:HG21	1:388:A:GLU:HB3	4	0.32
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	1	0.32
(1,1355)	1:395:A:ARG:HB3	1:395:A:ARG:HG2	3	0.32
(1,1355)	1:395:A:ARG:HB3	1:395:A:ARG:HG2	6	0.32
(1,1355)	1:395:A:ARG:HB3	1:395:A:ARG:HG2	9	0.32
(1,1355)	1:395:A:ARG:HB3	1:395:A:ARG:HG2	14	0.32
(1,1355)	1:395:A:ARG:HB2	1:395:A:ARG:HG3	17	0.32
(1,1344)	1:398:A:TYR:HD1	1:398:A:TYR:H	9	0.32
(1,1340)	1:399:A:LYS:HD3	1:396:A:HIS:HA	10	0.32
(1,1340)	1:399:A:LYS:HD3	1:396:A:HIS:HA	13	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1313)	1:375:A:LEU:HD12	1:376:A:TRP:H	5	0.32
(1,1313)	1:375:A:LEU:HD12	1:376:A:TRP:H	9	0.32
(1,1297)	1:379:A:HIS:HB2	1:380:A:LYS:HG3	18	0.32
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD3	8	0.32
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD3	11	0.32
(1,1121)	1:367:A:VAL:HG22	1:365:A:ARG:HA	1	0.32
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD13	3	0.32
(1,1033)	1:348:A:SER:HB3	1:351:A:GLU:HB3	18	0.32
(1,1026)	1:336:A:LEU:HD22	1:432:A:HIS:H	2	0.32
(1,1021)	1:437:A:VAL:HG12	1:396:A:HIS:HD2	14	0.32
(1,1021)	1:437:A:VAL:HG12	1:396:A:HIS:HD2	19	0.32
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	14	0.32
(1,924)	1:441:A:GLN:HE22	1:441:A:GLN:HG2	11	0.32
(1,866)	1:434:A:GLU:HA	1:434:A:GLU:HG3	10	0.32
(1,836)	1:430:A:LEU:HD12	1:427:A:THR:HB	13	0.32
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD21	1	0.32
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD23	6	0.32
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD22	8	0.32
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD22	13	0.32
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD21	19	0.32
(1,803)	1:426:A:ARG:H	1:426:A:ARG:HG2	18	0.32
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	1	0.32
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	3	0.32
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	4	0.32
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	5	0.32
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	6	0.32
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	7	0.32
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	9	0.32
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	10	0.32
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	11	0.32
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	14	0.32
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	15	0.32
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	16	0.32
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	17	0.32
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	18	0.32
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	19	0.32
(1,790)	1:428:A:ASP:HA	1:428:A:ASP:HB2	3	0.32
(1,742)	1:349:A:ARG:HB2	1:350:A:TYR:HA	13	0.32
(1,690)	1:411:A:LEU:HD22	1:369:A:PRO:HB2	8	0.32
(1,690)	1:411:A:LEU:HD21	1:369:A:PRO:HB2	15	0.32
(1,627)	1:403:A:ILE:HG22	1:413:A:PHE:HB2	2	0.32
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD23	17	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:399:A:LYS:HA	1:399:A:LYS:HG3	7	0.32
(1,544)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	8	0.32
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	4	0.32
(1,478)	1:389:A:LYS:HG3	1:389:A:LYS:HE2	19	0.32
(1,457)	1:386:A:THR:HG21	1:389:A:LYS:HB2	5	0.32
(1,456)	1:386:A:THR:HG22	1:387:A:TYR:HB2	3	0.32
(1,453)	1:386:A:THR:HG22	1:386:A:THR:HB	3	0.32
(1,453)	1:386:A:THR:HG23	1:386:A:THR:HB	18	0.32
(1,445)	1:384:A:ASN:HD22	1:384:A:ASN:HB2	5	0.32
(1,432)	1:381:A:ASN:H	1:381:A:ASN:HB2	4	0.32
(1,432)	1:381:A:ASN:H	1:381:A:ASN:HB2	15	0.32
(1,347)	1:373:A:ALA:HA	1:376:A:TRP:HB2	14	0.32
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG23	6	0.32
(1,168)	1:354:A:ILE:HG22	1:354:A:ILE:HG13	2	0.32
(1,168)	1:354:A:ILE:HG21	1:354:A:ILE:HG13	3	0.32
(1,168)	1:354:A:ILE:HG23	1:354:A:ILE:HG13	4	0.32
(1,168)	1:354:A:ILE:HG23	1:354:A:ILE:HG13	5	0.32
(1,168)	1:354:A:ILE:HG21	1:354:A:ILE:HG13	6	0.32
(1,168)	1:354:A:ILE:HG22	1:354:A:ILE:HG13	9	0.32
(1,168)	1:354:A:ILE:HG21	1:354:A:ILE:HG13	16	0.32
(1,168)	1:354:A:ILE:HG22	1:354:A:ILE:HG13	17	0.32
(1,168)	1:354:A:ILE:HG23	1:354:A:ILE:HG13	19	0.32
(1,166)	1:354:A:ILE:HG23	1:372:A:LEU:HD22	11	0.32
(1,140)	1:352:A:ASN:H	1:352:A:ASN:HB2	5	0.32
(1,108)	1:345:A:LEU:HD22	1:345:A:LEU:HB2	7	0.32
(1,57)	1:343:A:GLN:HG2	1:344:A:LEU:HD23	3	0.32
(1,34)	1:341:A:VAL:HG11	1:337:A:LEU:HG	7	0.32
(1,34)	1:341:A:VAL:HG11	1:337:A:LEU:HG	12	0.32
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB3	16	0.31
(1,2974)	1:433:A:LEU:H	1:436:A:GLN:HB2	6	0.31
(1,2964)	1:446:A:ASP:H	1:445:A:GLU:HB3	7	0.31
(1,2942)	1:372:A:LEU:H	1:368:A:ASP:HB2	4	0.31
(1,2931)	1:420:A:ASP:H	1:421:A:GLU:HG3	3	0.31
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	6	0.31
(1,2918)	1:374:A:ARG:H	1:376:A:TRP:H	16	0.31
(1,2906)	1:361:A:SER:H	1:360:A:GLU:HA	14	0.31
(1,2895)	1:353:A:PHE:H	1:367:A:VAL:HG23	19	0.31
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	9	0.31
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	14	0.31
(1,2862)	1:379:A:HIS:HB3	1:340:A:TYR:HE1	4	0.31
(1,2852)	1:343:A:GLN:HB3	1:340:A:TYR:HD1	15	0.31
(1,2844)	1:402:A:ILE:HG22	1:397:A:TYR:HD2	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2825)	1:413:A:PHE:HE2	1:366:A:ILE:HB	3	0.31
(1,2794)	1:433:A:LEU:HD23	1:429:A:ARG:HD3	3	0.31
(1,2791)	1:438:A:LEU:HD21	1:385:A:MET:HG2	6	0.31
(1,2752)	1:392:A:ARG:H	1:392:A:ARG:HD2	18	0.31
(1,2730)	1:366:A:ILE:HG23	1:370:A:ASN:H	5	0.31
(1,2697)	1:447:A:GLU:HG3	1:447:A:GLU:HB2	5	0.31
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG23	19	0.31
(1,2683)	1:429:A:ARG:HG2	1:429:A:ARG:H	10	0.31
(1,2659)	1:366:A:ILE:HD11	1:411:A:LEU:HB3	2	0.31
(1,2659)	1:366:A:ILE:HD13	1:411:A:LEU:HB3	6	0.31
(1,2655)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	11	0.31
(1,2650)	1:403:A:ILE:HD13	1:338:A:TRP:HA	17	0.31
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	5	0.31
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	11	0.31
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	16	0.31
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	17	0.31
(1,2611)	1:393:A:ALA:HB2	1:397:A:TYR:HE1	3	0.31
(1,2611)	1:393:A:ALA:HB3	1:397:A:TYR:HE1	6	0.31
(1,2611)	1:393:A:ALA:HB3	1:397:A:TYR:HE1	14	0.31
(1,2569)	1:349:A:ARG:HD3	1:350:A:TYR:HE1	10	0.31
(1,2555)	1:340:A:TYR:HA	1:343:A:GLN:HG2	8	0.31
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	9	0.31
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG12	13	0.31
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG12	15	0.31
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD11	17	0.31
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG22	5	0.31
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD21	3	0.31
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD21	6	0.31
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD22	6	0.31
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD22	7	0.31
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD23	16	0.31
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD21	9	0.31
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB3	4	0.31
(1,2433)	1:411:A:LEU:H	1:410:A:ARG:HG2	9	0.31
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	2	0.31
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	14	0.31
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	19	0.31
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	2	0.31
(1,2359)	1:382:A:ARG:H	1:382:A:ARG:HG3	2	0.31
(1,2252)	1:442:A:THR:H	1:441:A:GLN:HB3	7	0.31
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	1	0.31
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	18	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2227)	1:415:A:PHE:H	1:414:A:ARG:HB3	10	0.31
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD11	8	0.31
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	19	0.31
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	8	0.31
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB2	2	0.31
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	2	0.31
(1,1921)	1:375:A:LEU:HD11	1:375:A:LEU:HD22	4	0.31
(1,1916)	1:366:A:ILE:HG23	1:411:A:LEU:HD11	2	0.31
(1,1912)	1:354:A:ILE:HD13	1:372:A:LEU:HD12	13	0.31
(1,1912)	1:354:A:ILE:HD11	1:372:A:LEU:HD11	19	0.31
(1,1909)	1:344:A:LEU:HD13	1:354:A:ILE:HG23	6	0.31
(1,1908)	1:341:A:VAL:HG21	1:345:A:LEU:HD13	15	0.31
(1,1908)	1:341:A:VAL:HG22	1:345:A:LEU:HD11	19	0.31
(1,1899)	1:430:A:LEU:HD13	1:400:A:LEU:HD23	5	0.31
(1,1897)	1:430:A:LEU:HD12	1:430:A:LEU:HD23	8	0.31
(1,1897)	1:430:A:LEU:HD12	1:430:A:LEU:HD22	19	0.31
(1,1895)	1:411:A:LEU:HD23	1:366:A:ILE:HD11	8	0.31
(1,1895)	1:411:A:LEU:HD22	1:366:A:ILE:HD11	10	0.31
(1,1894)	1:411:A:LEU:HD21	1:411:A:LEU:HD13	7	0.31
(1,1894)	1:411:A:LEU:HD21	1:411:A:LEU:HD13	9	0.31
(1,1894)	1:411:A:LEU:HD23	1:411:A:LEU:HD11	12	0.31
(1,1887)	1:400:A:LEU:HD23	1:400:A:LEU:HD13	4	0.31
(1,1887)	1:400:A:LEU:HD23	1:400:A:LEU:HD11	5	0.31
(1,1884)	1:394:A:LEU:HD11	1:394:A:LEU:HD21	2	0.31
(1,1884)	1:394:A:LEU:HD12	1:394:A:LEU:HD22	6	0.31
(1,1884)	1:394:A:LEU:HD13	1:394:A:LEU:HD21	9	0.31
(1,1884)	1:394:A:LEU:HD12	1:394:A:LEU:HD23	11	0.31
(1,1802)	1:336:A:LEU:HD13	1:431:A:GLU:HA	1	0.31
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD11	2	0.31
(1,1761)	1:340:A:TYR:HB2	1:337:A:LEU:HA	1	0.31
(1,1726)	1:341:A:VAL:HG22	1:338:A:TRP:HA	5	0.31
(1,1726)	1:341:A:VAL:HG22	1:338:A:TRP:HA	8	0.31
(1,1725)	1:341:A:VAL:HG23	1:342:A:TYR:HB2	2	0.31
(1,1725)	1:341:A:VAL:HG21	1:342:A:TYR:HB2	15	0.31
(1,1690)	1:402:A:ILE:HD13	1:400:A:LEU:HA	18	0.31
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG22	2	0.31
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG23	13	0.31
(1,1670)	1:403:A:ILE:HG23	1:397:A:TYR:HB2	7	0.31
(1,1670)	1:403:A:ILE:HG22	1:397:A:TYR:HB2	8	0.31
(1,1653)	1:404:A:ARG:HG2	1:414:A:ARG:HD3	16	0.31
(1,1604)	1:365:A:ARG:HB2	1:412:A:LEU:HD11	9	0.31
(1,1600)	1:412:A:LEU:HD23	1:412:A:LEU:H	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1600)	1:412:A:LEU:HD22	1:412:A:LEU:H	16	0.31
(1,1497)	1:429:A:ARG:HG3	1:429:A:ARG:HB2	1	0.31
(1,1497)	1:429:A:ARG:HG2	1:429:A:ARG:HB3	4	0.31
(1,1488)	1:431:A:GLU:HB2	1:336:A:LEU:HD21	3	0.31
(1,1484)	1:432:A:HIS:HB3	1:430:A:LEU:H	17	0.31
(1,1448)	1:442:A:THR:HG21	1:456:A:TRP:HB3	3	0.31
(1,1448)	1:442:A:THR:HG21	1:456:A:TRP:HB3	13	0.31
(1,1427)	1:447:A:GLU:HA	1:448:A:PRO:HD3	12	0.31
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	7	0.31
(1,1397)	1:385:A:MET:HB2	1:374:A:ARG:HA	9	0.31
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	2	0.31
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	8	0.31
(1,1355)	1:395:A:ARG:HB3	1:395:A:ARG:HG2	7	0.31
(1,1355)	1:395:A:ARG:HB3	1:395:A:ARG:HG2	11	0.31
(1,1315)	1:375:A:LEU:HD21	1:376:A:TRP:H	6	0.31
(1,1267)	1:354:A:ILE:HD13	1:367:A:VAL:H	13	0.31
(1,1259)	1:354:A:ILE:HA	1:345:A:LEU:HD23	5	0.31
(1,1224)	1:363:A:ILE:HG23	1:357:A:GLU:HG2	8	0.31
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	9	0.31
(1,1121)	1:367:A:VAL:HG22	1:365:A:ARG:HA	4	0.31
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	15	0.31
(1,1077)	1:372:A:LEU:HD11	1:340:A:TYR:HD2	16	0.31
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD12	15	0.31
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	10	0.31
(1,1033)	1:348:A:SER:HB3	1:351:A:GLU:HB3	9	0.31
(1,1021)	1:437:A:VAL:HG13	1:396:A:HIS:HD2	18	0.31
(1,934)	1:444:A:GLN:H	1:444:A:GLN:HB3	6	0.31
(1,876)	1:436:A:GLN:HB2	1:437:A:VAL:HG12	11	0.31
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD22	5	0.31
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD21	11	0.31
(1,813)	1:427:A:THR:HG23	1:425:A:GLY:H	2	0.31
(1,803)	1:426:A:ARG:H	1:426:A:ARG:HG2	3	0.31
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	8	0.31
(1,797)	1:423:A:MET:HG3	1:423:A:MET:HB3	13	0.31
(1,594)	1:400:A:LEU:HD22	1:426:A:ARG:HG3	4	0.31
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD22	4	0.31
(1,544)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	14	0.31
(1,530)	1:394:A:LEU:HD22	1:397:A:TYR:HB3	9	0.31
(1,523)	1:394:A:LEU:HD11	1:390:A:MET:HG2	17	0.31
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD13	2	0.31
(1,456)	1:386:A:THR:HG22	1:387:A:TYR:HB2	19	0.31
(1,453)	1:386:A:THR:HG22	1:386:A:THR:HB	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:386:A:THR:HG22	1:386:A:THR:HB	9	0.31
(1,453)	1:386:A:THR:HG21	1:386:A:THR:HB	13	0.31
(1,443)	1:384:A:ASN:H	1:384:A:ASN:HB2	15	0.31
(1,432)	1:381:A:ASN:H	1:381:A:ASN:HB2	7	0.31
(1,432)	1:381:A:ASN:H	1:381:A:ASN:HB2	11	0.31
(1,432)	1:381:A:ASN:H	1:381:A:ASN:HB2	13	0.31
(1,432)	1:381:A:ASN:H	1:381:A:ASN:HB2	14	0.31
(1,365)	1:374:A:ARG:H	1:374:A:ARG:HD2	12	0.31
(1,365)	1:374:A:ARG:H	1:374:A:ARG:HD2	17	0.31
(1,359)	1:374:A:ARG:HA	1:374:A:ARG:HB2	18	0.31
(1,347)	1:373:A:ALA:HA	1:376:A:TRP:HB2	18	0.31
(1,306)	1:354:A:ILE:HD11	1:366:A:ILE:HG23	19	0.31
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG21	4	0.31
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG21	11	0.31
(1,300)	1:366:A:ILE:HG22	1:411:A:LEU:HB3	12	0.31
(1,228)	1:359:A:LYS:HA	1:359:A:LYS:HD2	14	0.31
(1,168)	1:354:A:ILE:HG22	1:354:A:ILE:HG13	10	0.31
(1,168)	1:354:A:ILE:HG22	1:354:A:ILE:HG13	13	0.31
(1,168)	1:354:A:ILE:HG22	1:354:A:ILE:HG13	18	0.31
(1,108)	1:345:A:LEU:HD23	1:345:A:LEU:HB2	3	0.31
(1,108)	1:345:A:LEU:HD21	1:345:A:LEU:HB2	5	0.31
(1,34)	1:341:A:VAL:HG11	1:337:A:LEU:HG	13	0.31
(1,5)	1:337:A:LEU:HD21	1:390:A:MET:HG3	9	0.31
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB2	19	0.3
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	4	0.3
(1,2964)	1:446:A:ASP:H	1:445:A:GLU:HB3	15	0.3
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	4	0.3
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	6	0.3
(1,2960)	1:392:A:ARG:H	1:393:A:ALA:HA	19	0.3
(1,2940)	1:434:A:GLU:H	1:433:A:LEU:HB2	16	0.3
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD12	4	0.3
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	14	0.3
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	17	0.3
(1,2906)	1:361:A:SER:H	1:360:A:GLU:HA	15	0.3
(1,2872)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	2	0.3
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	3	0.3
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	5	0.3
(1,2850)	1:344:A:LEU:HD13	1:350:A:TYR:HD1	10	0.3
(1,2844)	1:402:A:ILE:HG23	1:397:A:TYR:HD2	14	0.3
(1,2798)	1:412:A:LEU:HD22	1:410:A:ARG:HD2	15	0.3
(1,2762)	1:394:A:LEU:HD22	1:398:A:TYR:HE1	1	0.3
(1,2752)	1:392:A:ARG:H	1:392:A:ARG:HD3	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2730)	1:366:A:ILE:HG23	1:373:A:ALA:H	3	0.3
(1,2730)	1:366:A:ILE:HG23	1:373:A:ALA:H	17	0.3
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	5	0.3
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	11	0.3
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	16	0.3
(1,2712)	1:349:A:ARG:HB2	1:350:A:TYR:HE1	13	0.3
(1,2693)	1:437:A:VAL:HG21	1:441:A:GLN:HE22	9	0.3
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG23	1	0.3
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG23	6	0.3
(1,2689)	1:388:A:GLU:HB2	1:388:A:GLU:HG2	1	0.3
(1,2659)	1:366:A:ILE:HG22	1:411:A:LEU:HB3	11	0.3
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD3	8	0.3
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD2	9	0.3
(1,2655)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	9	0.3
(1,2655)	1:395:A:ARG:HB3	1:395:A:ARG:HD2	10	0.3
(1,2655)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	16	0.3
(1,2649)	1:403:A:ILE:HG22	1:364:A:PHE:HZ	19	0.3
(1,2643)	1:402:A:ILE:HD12	1:397:A:TYR:HD1	8	0.3
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	10	0.3
(1,2611)	1:393:A:ALA:HB2	1:397:A:TYR:HE1	1	0.3
(1,2611)	1:393:A:ALA:HB2	1:397:A:TYR:HE1	16	0.3
(1,2597)	1:358:A:ASP:HB2	1:363:A:ILE:HG23	10	0.3
(1,2597)	1:358:A:ASP:HB2	1:363:A:ILE:HG22	13	0.3
(1,2577)	1:356:A:TRP:HB3	1:359:A:LYS:HB3	14	0.3
(1,2555)	1:340:A:TYR:HA	1:339:A:ASP:HB3	12	0.3
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG11	4	0.3
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG23	3	0.3
(1,2537)	1:394:A:LEU:H	1:394:A:LEU:HD11	17	0.3
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD21	11	0.3
(1,2527)	1:367:A:VAL:HG13	1:368:A:ASP:H	12	0.3
(1,2527)	1:367:A:VAL:HG12	1:368:A:ASP:H	15	0.3
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB2	14	0.3
(1,2418)	1:444:A:GLN:H	1:441:A:GLN:HG2	19	0.3
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	3	0.3
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	7	0.3
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	9	0.3
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG3	12	0.3
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	7	0.3
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	13	0.3
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	9	0.3
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	15	0.3
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB2	1	0.3
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB2	3	0.3
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB2	10	0.3
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB2	13	0.3
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB3	14	0.3
(1,2048)	1:361:A:SER:H	1:358:A:ASP:HB2	7	0.3
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	5	0.3
(1,1921)	1:375:A:LEU:HD12	1:375:A:LEU:HD22	11	0.3
(1,1912)	1:354:A:ILE:HD11	1:372:A:LEU:HD12	1	0.3
(1,1909)	1:344:A:LEU:HD13	1:354:A:ILE:HG23	3	0.3
(1,1909)	1:344:A:LEU:HD11	1:354:A:ILE:HG21	17	0.3
(1,1908)	1:341:A:VAL:HG22	1:345:A:LEU:HD12	1	0.3
(1,1908)	1:341:A:VAL:HG21	1:345:A:LEU:HD11	9	0.3
(1,1908)	1:341:A:VAL:HG23	1:345:A:LEU:HD13	11	0.3
(1,1908)	1:341:A:VAL:HG21	1:345:A:LEU:HD11	13	0.3
(1,1908)	1:341:A:VAL:HG22	1:345:A:LEU:HD11	17	0.3
(1,1903)	1:438:A:LEU:HD21	1:438:A:LEU:HD12	19	0.3
(1,1897)	1:430:A:LEU:HD11	1:430:A:LEU:HD23	13	0.3
(1,1897)	1:430:A:LEU:HD13	1:430:A:LEU:HD23	14	0.3
(1,1894)	1:411:A:LEU:HD21	1:411:A:LEU:HD13	4	0.3
(1,1894)	1:411:A:LEU:HD22	1:411:A:LEU:HD11	13	0.3
(1,1894)	1:411:A:LEU:HD23	1:411:A:LEU:HD12	14	0.3
(1,1887)	1:400:A:LEU:HD21	1:400:A:LEU:HD13	8	0.3
(1,1887)	1:400:A:LEU:HD22	1:400:A:LEU:HD13	18	0.3
(1,1884)	1:394:A:LEU:HD11	1:394:A:LEU:HD22	16	0.3
(1,1873)	1:383:A:THR:HG22	1:384:A:ASN:HD22	14	0.3
(1,1867)	1:380:A:LYS:HE2	1:438:A:LEU:HD11	12	0.3
(1,1800)	1:336:A:LEU:HD12	1:338:A:TRP:HD1	13	0.3
(1,1761)	1:340:A:TYR:HB2	1:337:A:LEU:HA	9	0.3
(1,1761)	1:340:A:TYR:HB2	1:337:A:LEU:HA	13	0.3
(1,1757)	1:337:A:LEU:HA	1:337:A:LEU:HD23	18	0.3
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	1	0.3
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	6	0.3
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	9	0.3
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	13	0.3
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	16	0.3
(1,1726)	1:341:A:VAL:HG23	1:338:A:TRP:HA	1	0.3
(1,1725)	1:341:A:VAL:HG22	1:342:A:TYR:HB2	1	0.3
(1,1725)	1:341:A:VAL:HG21	1:342:A:TYR:HB2	6	0.3
(1,1725)	1:341:A:VAL:HG21	1:342:A:TYR:HB2	7	0.3
(1,1725)	1:341:A:VAL:HG21	1:342:A:TYR:HB2	13	0.3
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD22	19	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1607)	1:411:A:LEU:HD12	1:366:A:ILE:H	13	0.3
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	9	0.3
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	16	0.3
(1,1554)	1:417:A:LYS:HE3	1:402:A:ILE:HG13	9	0.3
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG22	11	0.3
(1,1507)	1:426:A:ARG:HG2	1:426:A:ARG:HA	3	0.3
(1,1497)	1:429:A:ARG:HG2	1:429:A:ARG:HB3	5	0.3
(1,1484)	1:432:A:HIS:HB3	1:430:A:LEU:H	8	0.3
(1,1475)	1:433:A:LEU:HD23	1:434:A:GLU:H	1	0.3
(1,1453)	1:438:A:LEU:HD12	1:435:A:SER:H	5	0.3
(1,1452)	1:361:A:SER:H	1:360:A:GLU:HG3	13	0.3
(1,1403)	1:383:A:THR:HG23	1:382:A:ARG:HD2	8	0.3
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	7	0.3
(1,1355)	1:395:A:ARG:HB3	1:395:A:ARG:HG2	2	0.3
(1,1355)	1:395:A:ARG:HB3	1:395:A:ARG:HG2	8	0.3
(1,1355)	1:395:A:ARG:HB2	1:395:A:ARG:HG3	12	0.3
(1,1355)	1:395:A:ARG:HB3	1:395:A:ARG:HG2	13	0.3
(1,1355)	1:395:A:ARG:HB3	1:395:A:ARG:HG2	15	0.3
(1,1316)	1:433:A:LEU:HD23	1:396:A:HIS:HD2	8	0.3
(1,1304)	1:376:A:TRP:HZ2	1:380:A:LYS:HE3	2	0.3
(1,1224)	1:363:A:ILE:HG21	1:357:A:GLU:HG2	11	0.3
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD3	9	0.3
(1,1217)	1:359:A:LYS:HD2	1:356:A:TRP:HZ2	3	0.3
(1,1193)	1:362:A:LYS:HE2	1:362:A:LYS:HA	1	0.3
(1,1193)	1:362:A:LYS:HE2	1:362:A:LYS:HA	17	0.3
(1,1182)	1:363:A:ILE:HD13	1:406:A:GLU:HG2	15	0.3
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG22	13	0.3
(1,1060)	1:351:A:GLU:HB2	1:355:A:ARG:HD3	6	0.3
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	2	0.3
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	6	0.3
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	8	0.3
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	13	0.3
(1,999)	1:409:A:GLN:HE22	1:409:A:GLN:HG2	4	0.3
(1,958)	1:449:A:THR:H	1:449:A:THR:HG22	5	0.3
(1,942)	1:446:A:ASP:H	1:446:A:ASP:HB2	15	0.3
(1,941)	1:447:A:GLU:H	1:446:A:ASP:HB2	16	0.3
(1,926)	1:442:A:THR:H	1:441:A:GLN:HG2	19	0.3
(1,902)	1:438:A:LEU:HD11	1:376:A:TRP:HZ2	17	0.3
(1,890)	1:439:A:ASP:H	1:438:A:LEU:HB2	19	0.3
(1,884)	1:437:A:VAL:HG23	1:392:A:ARG:HG3	19	0.3
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB3	2	0.3
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD23	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,832)	1:430:A:LEU:HB2	1:430:A:LEU:HD23	9	0.3
(1,627)	1:403:A:ILE:HG23	1:413:A:PHE:HB2	8	0.3
(1,530)	1:394:A:LEU:HD23	1:397:A:TYR:HB3	6	0.3
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD23	17	0.3
(1,478)	1:389:A:LYS:HG3	1:389:A:LYS:HE2	6	0.3
(1,455)	1:386:A:THR:HG21	1:389:A:LYS:HE2	18	0.3
(1,453)	1:386:A:THR:HG21	1:386:A:THR:HB	11	0.3
(1,453)	1:386:A:THR:HG22	1:386:A:THR:HB	17	0.3
(1,445)	1:384:A:ASN:HD22	1:384:A:ASN:HB2	9	0.3
(1,432)	1:381:A:ASN:H	1:381:A:ASN:HB2	1	0.3
(1,400)	1:377:A:GLY:HA3	1:382:A:ARG:HB3	2	0.3
(1,400)	1:377:A:GLY:HA3	1:382:A:ARG:HB3	14	0.3
(1,360)	1:374:A:ARG:HA	1:374:A:ARG:HG2	3	0.3
(1,306)	1:354:A:ILE:HD12	1:366:A:ILE:HG22	2	0.3
(1,306)	1:354:A:ILE:HD11	1:366:A:ILE:HG23	6	0.3
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG21	15	0.3
(1,174)	1:354:A:ILE:HD13	1:341:A:VAL:HA	1	0.3
(1,174)	1:354:A:ILE:HD13	1:341:A:VAL:HA	12	0.3
(1,108)	1:345:A:LEU:HD22	1:345:A:LEU:HB2	12	0.3
(1,57)	1:343:A:GLN:HG2	1:344:A:LEU:HD23	14	0.3
(1,35)	1:341:A:VAL:HG11	1:345:A:LEU:HD11	18	0.3
(1,34)	1:341:A:VAL:HG13	1:337:A:LEU:HG	4	0.3
(1,5)	1:337:A:LEU:HD21	1:390:A:MET:HG3	13	0.3
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG22	18	0.29
(1,2974)	1:433:A:LEU:H	1:431:A:GLU:HB2	8	0.29
(1,2974)	1:433:A:LEU:H	1:431:A:GLU:HB2	16	0.29
(1,2972)	1:435:A:SER:H	1:436:A:GLN:HG3	1	0.29
(1,2972)	1:435:A:SER:H	1:436:A:GLN:HG3	7	0.29
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD22	6	0.29
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD21	8	0.29
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD22	15	0.29
(1,2906)	1:361:A:SER:H	1:360:A:GLU:HA	2	0.29
(1,2906)	1:361:A:SER:H	1:360:A:GLU:HA	6	0.29
(1,2906)	1:361:A:SER:H	1:360:A:GLU:HA	12	0.29
(1,2895)	1:353:A:PHE:H	1:367:A:VAL:HG23	3	0.29
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	8	0.29
(1,2825)	1:413:A:PHE:HE2	1:366:A:ILE:HB	16	0.29
(1,2789)	1:438:A:LEU:HD13	1:381:A:ASN:HD22	7	0.29
(1,2774)	1:443:A:TYR:HD1	1:445:A:GLU:HB2	12	0.29
(1,2774)	1:443:A:TYR:HD1	1:445:A:GLU:HB2	15	0.29
(1,2762)	1:394:A:LEU:HD23	1:398:A:TYR:HE1	19	0.29
(1,2730)	1:366:A:ILE:HG22	1:370:A:ASN:H	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2724)	1:367:A:VAL:HG23	1:352:A:ASN:HA	19	0.29
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	17	0.29
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG21	12	0.29
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG21	14	0.29
(1,2684)	1:429:A:ARG:HG2	1:433:A:LEU:HD23	12	0.29
(1,2669)	1:414:A:ARG:HB2	1:414:A:ARG:HD3	5	0.29
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD2	1	0.29
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD2	10	0.29
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD3	11	0.29
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD3	12	0.29
(1,2655)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	6	0.29
(1,2645)	1:402:A:ILE:HD11	1:338:A:TRP:HB3	19	0.29
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	2	0.29
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	13	0.29
(1,2618)	1:375:A:LEU:HD23	1:378:A:ASN:HB2	5	0.29
(1,2612)	1:393:A:ALA:HB2	1:376:A:TRP:HZ3	14	0.29
(1,2596)	1:363:A:ILE:HG23	1:364:A:PHE:HA	8	0.29
(1,2557)	1:341:A:VAL:HG11	1:403:A:ILE:HD12	16	0.29
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	6	0.29
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	13	0.29
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG13	6	0.29
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG13	7	0.29
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG11	14	0.29
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG13	17	0.29
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG12	18	0.29
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG21	9	0.29
(1,2539)	1:404:A:ARG:H	1:403:A:ILE:HG22	2	0.29
(1,2539)	1:404:A:ARG:H	1:403:A:ILE:HG23	8	0.29
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG22	6	0.29
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD22	1	0.29
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD22	8	0.29
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD22	9	0.29
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD22	4	0.29
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD22	14	0.29
(1,2418)	1:444:A:GLN:H	1:441:A:GLN:HG3	17	0.29
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	1	0.29
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	12	0.29
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD13	15	0.29
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	8	0.29
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	14	0.29
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	17	0.29
(1,2146)	1:386:A:THR:H	1:386:A:THR:HG21	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB2	8	0.29
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB2	12	0.29
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB2	16	0.29
(1,2067)	1:365:A:ARG:H	1:355:A:ARG:HG2	4	0.29
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	3	0.29
(1,1916)	1:366:A:ILE:HG21	1:411:A:LEU:HD12	14	0.29
(1,1916)	1:366:A:ILE:HG23	1:411:A:LEU:HD12	16	0.29
(1,1916)	1:366:A:ILE:HG22	1:411:A:LEU:HD12	17	0.29
(1,1912)	1:354:A:ILE:HD11	1:372:A:LEU:HD11	10	0.29
(1,1908)	1:341:A:VAL:HG23	1:345:A:LEU:HD12	2	0.29
(1,1908)	1:341:A:VAL:HG21	1:345:A:LEU:HD11	6	0.29
(1,1908)	1:341:A:VAL:HG21	1:345:A:LEU:HD13	8	0.29
(1,1908)	1:341:A:VAL:HG23	1:345:A:LEU:HD12	18	0.29
(1,1903)	1:438:A:LEU:HD23	1:438:A:LEU:HD12	1	0.29
(1,1901)	1:433:A:LEU:HD21	1:433:A:LEU:HD12	3	0.29
(1,1901)	1:433:A:LEU:HD21	1:433:A:LEU:HD11	4	0.29
(1,1901)	1:433:A:LEU:HD22	1:433:A:LEU:HD11	8	0.29
(1,1901)	1:433:A:LEU:HD21	1:433:A:LEU:HD13	16	0.29
(1,1895)	1:411:A:LEU:HD21	1:366:A:ILE:HD12	16	0.29
(1,1894)	1:411:A:LEU:HD21	1:411:A:LEU:HD13	8	0.29
(1,1894)	1:411:A:LEU:HD21	1:411:A:LEU:HD13	11	0.29
(1,1884)	1:394:A:LEU:HD13	1:394:A:LEU:HD22	3	0.29
(1,1884)	1:394:A:LEU:HD11	1:394:A:LEU:HD21	5	0.29
(1,1884)	1:394:A:LEU:HD13	1:394:A:LEU:HD22	7	0.29
(1,1884)	1:394:A:LEU:HD11	1:394:A:LEU:HD22	14	0.29
(1,1884)	1:394:A:LEU:HD12	1:394:A:LEU:HD21	19	0.29
(1,1883)	1:393:A:ALA:HB2	1:437:A:VAL:HG21	4	0.29
(1,1883)	1:393:A:ALA:HB3	1:437:A:VAL:HG22	19	0.29
(1,1840)	1:374:A:ARG:HA	1:374:A:ARG:HD2	5	0.29
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD13	11	0.29
(1,1761)	1:340:A:TYR:HB2	1:337:A:LEU:HA	16	0.29
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	2	0.29
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	3	0.29
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	5	0.29
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	11	0.29
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	14	0.29
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	17	0.29
(1,1725)	1:341:A:VAL:HG22	1:342:A:TYR:HB2	3	0.29
(1,1725)	1:341:A:VAL:HG21	1:342:A:TYR:HB2	5	0.29
(1,1725)	1:341:A:VAL:HG21	1:342:A:TYR:HB2	8	0.29
(1,1725)	1:341:A:VAL:HG23	1:342:A:TYR:HB2	10	0.29
(1,1725)	1:341:A:VAL:HG21	1:342:A:TYR:HB2	16	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1725)	1:341:A:VAL:HG22	1:342:A:TYR:HB2	17	0.29
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD21	3	0.29
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG22	8	0.29
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD11	4	0.29
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD11	13	0.29
(1,1670)	1:403:A:ILE:HG22	1:397:A:TYR:HB2	4	0.29
(1,1670)	1:403:A:ILE:HG22	1:397:A:TYR:HB2	9	0.29
(1,1644)	1:404:A:ARG:HD3	1:404:A:ARG:HB3	10	0.29
(1,1604)	1:365:A:ARG:HB2	1:412:A:LEU:HD12	15	0.29
(1,1604)	1:365:A:ARG:HB2	1:412:A:LEU:HD11	18	0.29
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG21	14	0.29
(1,1498)	1:429:A:ARG:HD2	1:429:A:ARG:HB2	17	0.29
(1,1497)	1:429:A:ARG:HG2	1:429:A:ARG:HB3	9	0.29
(1,1475)	1:433:A:LEU:HD21	1:434:A:GLU:H	7	0.29
(1,1462)	1:435:A:SER:H	1:434:A:GLU:HB3	18	0.29
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	15	0.29
(1,1355)	1:395:A:ARG:HB2	1:395:A:ARG:HG3	4	0.29
(1,1355)	1:395:A:ARG:HB2	1:395:A:ARG:HG3	10	0.29
(1,1340)	1:399:A:LYS:HD3	1:396:A:HIS:HA	14	0.29
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	13	0.29
(1,1328)	1:399:A:LYS:H	1:400:A:LEU:HD11	19	0.29
(1,1315)	1:375:A:LEU:HD23	1:376:A:TRP:H	5	0.29
(1,1313)	1:375:A:LEU:HD11	1:376:A:TRP:H	6	0.29
(1,1304)	1:376:A:TRP:HZ2	1:380:A:LYS:HE3	1	0.29
(1,1304)	1:376:A:TRP:HZ2	1:380:A:LYS:HE3	7	0.29
(1,1225)	1:357:A:GLU:HG3	1:412:A:LEU:HD21	14	0.29
(1,1217)	1:359:A:LYS:HD3	1:356:A:TRP:HZ2	14	0.29
(1,1193)	1:362:A:LYS:HE2	1:362:A:LYS:HA	16	0.29
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG21	5	0.29
(1,1142)	1:450:A:ILE:HD12	1:454:A:VAL:HA	12	0.29
(1,1133)	1:367:A:VAL:HG13	1:352:A:ASN:HB3	14	0.29
(1,1077)	1:372:A:LEU:HD13	1:340:A:TYR:HD2	13	0.29
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	1	0.29
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	5	0.29
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	7	0.29
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	9	0.29
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	14	0.29
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	18	0.29
(1,1042)	1:349:A:ARG:HD3	1:349:A:ARG:HB3	19	0.29
(1,999)	1:409:A:GLN:HE22	1:409:A:GLN:HG2	5	0.29
(1,999)	1:409:A:GLN:HE22	1:409:A:GLN:HG2	9	0.29
(1,999)	1:409:A:GLN:HE22	1:409:A:GLN:HG2	19	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,929)	1:443:A:TYR:H	1:442:A:THR:HB	5	0.29
(1,921)	1:441:A:GLN:HA	1:441:A:GLN:HB2	2	0.29
(1,902)	1:438:A:LEU:HD11	1:376:A:TRP:HZ2	12	0.29
(1,890)	1:439:A:ASP:H	1:438:A:LEU:HB2	4	0.29
(1,888)	1:437:A:VAL:HG21	1:441:A:GLN:HE22	6	0.29
(1,888)	1:437:A:VAL:HG22	1:441:A:GLN:HE22	12	0.29
(1,865)	1:438:A:LEU:HD12	1:380:A:LYS:HE3	3	0.29
(1,713)	1:414:A:ARG:HE	1:414:A:ARG:HB3	8	0.29
(1,556)	1:397:A:TYR:HA	1:400:A:LEU:HB3	2	0.29
(1,556)	1:397:A:TYR:HA	1:400:A:LEU:HB3	17	0.29
(1,528)	1:394:A:LEU:HD21	1:364:A:PHE:HZ	18	0.29
(1,456)	1:386:A:THR:HG23	1:387:A:TYR:HB2	11	0.29
(1,454)	1:386:A:THR:HG23	1:370:A:ASN:HA	13	0.29
(1,454)	1:386:A:THR:HG23	1:370:A:ASN:HA	16	0.29
(1,453)	1:386:A:THR:HG21	1:386:A:THR:HB	4	0.29
(1,432)	1:381:A:ASN:H	1:381:A:ASN:HB2	9	0.29
(1,432)	1:381:A:ASN:H	1:381:A:ASN:HB2	12	0.29
(1,309)	1:366:A:ILE:HD12	1:364:A:PHE:HZ	17	0.29
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG23	8	0.29
(1,300)	1:366:A:ILE:HG22	1:411:A:LEU:HB3	13	0.29
(1,268)	1:364:A:PHE:HA	1:345:A:LEU:HD22	8	0.29
(1,237)	1:361:A:SER:HB3	1:363:A:ILE:HG12	6	0.29
(1,237)	1:361:A:SER:HB3	1:363:A:ILE:HG12	12	0.29
(1,174)	1:354:A:ILE:HD13	1:341:A:VAL:HA	7	0.29
(1,168)	1:354:A:ILE:HG22	1:354:A:ILE:HG13	15	0.29
(1,124)	1:349:A:ARG:H	1:349:A:ARG:HG2	13	0.29
(1,34)	1:341:A:VAL:HG12	1:337:A:LEU:HG	15	0.29
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB1	7	0.28
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG22	3	0.28
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG21	13	0.28
(1,2974)	1:433:A:LEU:H	1:436:A:GLN:HB2	2	0.28
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	8	0.28
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD23	13	0.28
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	12	0.28
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	19	0.28
(1,2872)	1:445:A:GLU:HB2	1:445:A:GLU:HG2	16	0.28
(1,2872)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	18	0.28
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	1	0.28
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	4	0.28
(1,2844)	1:402:A:ILE:HG21	1:397:A:TYR:HD2	16	0.28
(1,2824)	1:413:A:PHE:HE2	1:411:A:LEU:HD22	17	0.28
(1,2791)	1:438:A:LEU:HD23	1:385:A:MET:HG2	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2791)	1:438:A:LEU:HD21	1:385:A:MET:HG2	13	0.28
(1,2789)	1:438:A:LEU:HD13	1:444:A:GLN:HE22	19	0.28
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB1	18	0.28
(1,2730)	1:366:A:ILE:HG22	1:373:A:ALA:H	8	0.28
(1,2730)	1:366:A:ILE:HG23	1:373:A:ALA:H	15	0.28
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	6	0.28
(1,2697)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	2	0.28
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG21	11	0.28
(1,2686)	1:430:A:LEU:HD13	1:430:A:LEU:HD21	3	0.28
(1,2686)	1:430:A:LEU:HD13	1:430:A:LEU:HD23	9	0.28
(1,2673)	1:417:A:LYS:HA	1:417:A:LYS:HG3	9	0.28
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD2	2	0.28
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD2	13	0.28
(1,2655)	1:395:A:ARG:HB3	1:395:A:ARG:HD2	17	0.28
(1,2612)	1:393:A:ALA:HB3	1:376:A:TRP:HZ3	19	0.28
(1,2611)	1:393:A:ALA:HB1	1:397:A:TYR:HE1	5	0.28
(1,2611)	1:393:A:ALA:HB3	1:397:A:TYR:HE1	7	0.28
(1,2611)	1:393:A:ALA:HB2	1:397:A:TYR:HE1	13	0.28
(1,2555)	1:340:A:TYR:HA	1:343:A:GLN:HG2	13	0.28
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	3	0.28
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	12	0.28
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	14	0.28
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	16	0.28
(1,2552)	1:452:A:SER:H	1:451:A:ALA:HB3	10	0.28
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG12	1	0.28
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG22	8	0.28
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG21	10	0.28
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG23	11	0.28
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG23	11	0.28
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD22	13	0.28
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD23	18	0.28
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG22	8	0.28
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD23	2	0.28
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD23	10	0.28
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD21	7	0.28
(1,2508)	1:434:A:GLU:H	1:434:A:GLU:HG2	2	0.28
(1,2508)	1:434:A:GLU:H	1:434:A:GLU:HG2	8	0.28
(1,2508)	1:434:A:GLU:H	1:434:A:GLU:HG2	16	0.28
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	5	0.28
(1,2359)	1:382:A:ARG:H	1:382:A:ARG:HG3	5	0.28
(1,2359)	1:382:A:ARG:H	1:382:A:ARG:HG3	13	0.28
(1,2359)	1:382:A:ARG:H	1:382:A:ARG:HG3	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD12	14	0.28
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	7	0.28
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	9	0.28
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	13	0.28
(1,2129)	1:447:A:GLU:H	1:447:A:GLU:HB3	18	0.28
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB2	7	0.28
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB3	15	0.28
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG23	1	0.28
(1,1986)	1:351:A:GLU:H	1:351:A:GLU:HG2	17	0.28
(1,1920)	1:372:A:LEU:HD13	1:366:A:ILE:HD11	14	0.28
(1,1916)	1:366:A:ILE:HG23	1:411:A:LEU:HD12	5	0.28
(1,1916)	1:366:A:ILE:HG21	1:411:A:LEU:HD13	19	0.28
(1,1912)	1:354:A:ILE:HD13	1:372:A:LEU:HD11	14	0.28
(1,1909)	1:344:A:LEU:HD12	1:354:A:ILE:HG21	12	0.28
(1,1908)	1:341:A:VAL:HG21	1:345:A:LEU:HD12	4	0.28
(1,1908)	1:341:A:VAL:HG21	1:345:A:LEU:HD11	5	0.28
(1,1908)	1:341:A:VAL:HG23	1:345:A:LEU:HD12	12	0.28
(1,1903)	1:438:A:LEU:HD22	1:438:A:LEU:HD13	14	0.28
(1,1903)	1:438:A:LEU:HD22	1:438:A:LEU:HD12	15	0.28
(1,1901)	1:433:A:LEU:HD21	1:433:A:LEU:HD11	6	0.28
(1,1899)	1:430:A:LEU:HD11	1:400:A:LEU:HD23	11	0.28
(1,1899)	1:430:A:LEU:HD12	1:400:A:LEU:HD23	12	0.28
(1,1895)	1:411:A:LEU:HD22	1:366:A:ILE:HD11	2	0.28
(1,1895)	1:411:A:LEU:HD22	1:366:A:ILE:HD13	15	0.28
(1,1894)	1:411:A:LEU:HD22	1:411:A:LEU:HD11	6	0.28
(1,1894)	1:411:A:LEU:HD21	1:411:A:LEU:HD11	10	0.28
(1,1894)	1:411:A:LEU:HD23	1:411:A:LEU:HD11	16	0.28
(1,1894)	1:411:A:LEU:HD23	1:411:A:LEU:HD12	19	0.28
(1,1887)	1:400:A:LEU:HD23	1:400:A:LEU:HD13	6	0.28
(1,1884)	1:394:A:LEU:HD11	1:394:A:LEU:HD22	8	0.28
(1,1884)	1:394:A:LEU:HD13	1:394:A:LEU:HD21	13	0.28
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD13	9	0.28
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD11	17	0.28
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD11	18	0.28
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	8	0.28
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	12	0.28
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	19	0.28
(1,1689)	1:338:A:TRP:HE1	1:402:A:ILE:HG23	12	0.28
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD12	2	0.28
(1,1607)	1:411:A:LEU:HD12	1:366:A:ILE:H	6	0.28
(1,1603)	1:357:A:GLU:HG2	1:412:A:LEU:HD13	18	0.28
(1,1558)	1:418:A:THR:H	1:417:A:LYS:HG2	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1502)	1:422:A:ILE:HA	1:427:A:THR:HG21	6	0.28
(1,1488)	1:431:A:GLU:HB2	1:336:A:LEU:HD22	9	0.28
(1,1488)	1:431:A:GLU:HB2	1:336:A:LEU:HD22	18	0.28
(1,1475)	1:433:A:LEU:HD22	1:434:A:GLU:H	18	0.28
(1,1444)	1:442:A:THR:HG21	1:443:A:TYR:HA	19	0.28
(1,1442)	1:443:A:TYR:HE2	1:445:A:GLU:HG2	6	0.28
(1,1427)	1:447:A:GLU:HA	1:448:A:PRO:HD3	8	0.28
(1,1422)	1:451:A:ALA:HB1	1:450:A:ILE:HA	8	0.28
(1,1422)	1:451:A:ALA:HB1	1:450:A:ILE:HA	15	0.28
(1,1412)	1:454:A:VAL:HB	1:450:A:ILE:HA	7	0.28
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	2	0.28
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	6	0.28
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	19	0.28
(1,1403)	1:383:A:THR:HG23	1:382:A:ARG:HD2	2	0.28
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	7	0.28
(1,1355)	1:395:A:ARG:HB3	1:395:A:ARG:HG2	5	0.28
(1,1355)	1:395:A:ARG:HB3	1:395:A:ARG:HG2	16	0.28
(1,1315)	1:375:A:LEU:HD21	1:376:A:TRP:H	4	0.28
(1,1315)	1:375:A:LEU:HD22	1:376:A:TRP:H	13	0.28
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD2	3	0.28
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD3	4	0.28
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	18	0.28
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG11	15	0.28
(1,1121)	1:367:A:VAL:HG21	1:365:A:ARG:HA	3	0.28
(1,1084)	1:372:A:LEU:HD11	1:344:A:LEU:HD12	5	0.28
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	4	0.28
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	11	0.28
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	11	0.28
(1,999)	1:409:A:GLN:HE22	1:409:A:GLN:HG2	3	0.28
(1,941)	1:447:A:GLU:H	1:446:A:ASP:HB2	19	0.28
(1,902)	1:438:A:LEU:HD11	1:376:A:TRP:HZ2	8	0.28
(1,865)	1:438:A:LEU:HD13	1:380:A:LYS:HE3	18	0.28
(1,836)	1:430:A:LEU:HD12	1:427:A:THR:HB	15	0.28
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD3	6	0.28
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD3	17	0.28
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD11	14	0.28
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	14	0.28
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	15	0.28
(1,454)	1:386:A:THR:HG21	1:370:A:ASN:HA	1	0.28
(1,454)	1:386:A:THR:HG22	1:370:A:ASN:HA	12	0.28
(1,453)	1:386:A:THR:HG23	1:386:A:THR:HB	12	0.28
(1,453)	1:386:A:THR:HG22	1:386:A:THR:HB	15	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:386:A:THR:HG21	1:386:A:THR:HB	16	0.28
(1,309)	1:366:A:ILE:HD12	1:364:A:PHE:HZ	11	0.28
(1,309)	1:366:A:ILE:HD11	1:364:A:PHE:HZ	15	0.28
(1,309)	1:366:A:ILE:HD13	1:364:A:PHE:HZ	16	0.28
(1,306)	1:354:A:ILE:HD11	1:366:A:ILE:HG23	1	0.28
(1,306)	1:354:A:ILE:HD11	1:366:A:ILE:HG22	7	0.28
(1,301)	1:366:A:ILE:HG22	1:372:A:LEU:HB3	10	0.28
(1,301)	1:366:A:ILE:HG23	1:372:A:LEU:HB3	14	0.28
(1,237)	1:361:A:SER:HB3	1:363:A:ILE:HG12	15	0.28
(1,174)	1:354:A:ILE:HD13	1:341:A:VAL:HA	6	0.28
(1,104)	1:345:A:LEU:HD22	1:356:A:TRP:HE3	15	0.28
(1,85)	1:344:A:LEU:HD23	1:350:A:TYR:HD1	17	0.28
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	4	0.28
(1,52)	1:443:A:TYR:HE2	1:456:A:TRP:HD1	17	0.28
(1,34)	1:341:A:VAL:HG11	1:337:A:LEU:HG	8	0.28
(1,34)	1:341:A:VAL:HG12	1:337:A:LEU:HG	9	0.28
(1,16)	1:340:A:TYR:HA	1:343:A:GLN:HB2	9	0.28
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB2	2	0.27
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB3	3	0.27
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB3	9	0.27
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG21	14	0.27
(1,2951)	1:382:A:ARG:H	1:377:A:GLY:HA3	18	0.27
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD23	7	0.27
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	18	0.27
(1,2906)	1:361:A:SER:H	1:360:A:GLU:HA	4	0.27
(1,2893)	1:344:A:LEU:H	1:341:A:VAL:HG22	19	0.27
(1,2882)	1:402:A:ILE:HB	1:397:A:TYR:HD2	2	0.27
(1,2850)	1:344:A:LEU:HD11	1:350:A:TYR:HD1	14	0.27
(1,2837)	1:404:A:ARG:HD3	1:404:A:ARG:HB3	6	0.27
(1,2824)	1:413:A:PHE:HE2	1:411:A:LEU:HD22	10	0.27
(1,2824)	1:413:A:PHE:HE2	1:411:A:LEU:HD21	16	0.27
(1,2794)	1:433:A:LEU:HD22	1:429:A:ARG:HD3	6	0.27
(1,2762)	1:394:A:LEU:HD23	1:398:A:TYR:HE1	10	0.27
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	9	0.27
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	12	0.27
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	13	0.27
(1,2705)	1:394:A:LEU:HA	1:397:A:TYR:HD2	13	0.27
(1,2705)	1:394:A:LEU:HA	1:397:A:TYR:HD2	19	0.27
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG23	7	0.27
(1,2686)	1:430:A:LEU:HD13	1:430:A:LEU:HD23	6	0.27
(1,2669)	1:365:A:ARG:HB3	1:365:A:ARG:HD3	11	0.27
(1,2667)	1:414:A:ARG:HA	1:414:A:ARG:HD2	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2659)	1:366:A:ILE:HD11	1:411:A:LEU:HB3	12	0.27
(1,2659)	1:366:A:ILE:HD11	1:411:A:LEU:HB3	17	0.27
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD2	3	0.27
(1,2645)	1:402:A:ILE:HD11	1:338:A:TRP:HB3	15	0.27
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	1	0.27
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	18	0.27
(1,2618)	1:433:A:LEU:HD21	1:396:A:HIS:HB3	17	0.27
(1,2612)	1:393:A:ALA:HB2	1:376:A:TRP:HZ3	6	0.27
(1,2587)	1:362:A:LYS:HA	1:415:A:PHE:HD2	8	0.27
(1,2557)	1:341:A:VAL:HG12	1:403:A:ILE:HD13	1	0.27
(1,2557)	1:341:A:VAL:HG11	1:403:A:ILE:HD12	12	0.27
(1,2556)	1:341:A:VAL:HG12	1:364:A:PHE:HZ	13	0.27
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	5	0.27
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	7	0.27
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	8	0.27
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	19	0.27
(1,2552)	1:452:A:SER:H	1:451:A:ALA:HB3	5	0.27
(1,2549)	1:450:A:ILE:H	1:449:A:THR:HG23	1	0.27
(1,2549)	1:450:A:ILE:H	1:449:A:THR:HG21	12	0.27
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG12	9	0.27
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG13	16	0.27
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD13	19	0.27
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG23	1	0.27
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG23	10	0.27
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD21	12	0.27
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD22	19	0.27
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD22	9	0.27
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD21	10	0.27
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG21	19	0.27
(1,2508)	1:434:A:GLU:H	1:434:A:GLU:HG2	13	0.27
(1,2359)	1:382:A:ARG:H	1:382:A:ARG:HG3	1	0.27
(1,2359)	1:382:A:ARG:H	1:382:A:ARG:HG3	12	0.27
(1,2324)	1:352:A:ASN:HD21	1:367:A:VAL:HG22	6	0.27
(1,2258)	1:450:A:ILE:H	1:450:A:ILE:HG13	19	0.27
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	2	0.27
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	3	0.27
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	15	0.27
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	18	0.27
(1,2133)	1:383:A:THR:H	1:384:A:ASN:H	3	0.27
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG23	9	0.27
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG23	10	0.27
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	14	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1920)	1:372:A:LEU:HD13	1:366:A:ILE:HD12	9	0.27
(1,1916)	1:366:A:ILE:HG21	1:411:A:LEU:HD13	8	0.27
(1,1916)	1:366:A:ILE:HG22	1:411:A:LEU:HD11	9	0.27
(1,1912)	1:354:A:ILE:HD11	1:372:A:LEU:HD11	12	0.27
(1,1908)	1:341:A:VAL:HG23	1:345:A:LEU:HD12	14	0.27
(1,1908)	1:341:A:VAL:HG21	1:345:A:LEU:HD13	16	0.27
(1,1903)	1:438:A:LEU:HD22	1:438:A:LEU:HD12	2	0.27
(1,1903)	1:438:A:LEU:HD21	1:438:A:LEU:HD11	6	0.27
(1,1903)	1:438:A:LEU:HD23	1:438:A:LEU:HD13	7	0.27
(1,1901)	1:433:A:LEU:HD23	1:433:A:LEU:HD11	1	0.27
(1,1901)	1:433:A:LEU:HD22	1:433:A:LEU:HD11	10	0.27
(1,1901)	1:433:A:LEU:HD22	1:433:A:LEU:HD11	12	0.27
(1,1901)	1:433:A:LEU:HD23	1:433:A:LEU:HD11	18	0.27
(1,1895)	1:411:A:LEU:HD23	1:366:A:ILE:HD13	7	0.27
(1,1894)	1:411:A:LEU:HD21	1:411:A:LEU:HD12	3	0.27
(1,1894)	1:411:A:LEU:HD21	1:411:A:LEU:HD12	5	0.27
(1,1887)	1:400:A:LEU:HD23	1:400:A:LEU:HD12	3	0.27
(1,1887)	1:400:A:LEU:HD23	1:400:A:LEU:HD11	16	0.27
(1,1884)	1:394:A:LEU:HD11	1:394:A:LEU:HD21	4	0.27
(1,1840)	1:374:A:ARG:HA	1:374:A:ARG:HD2	13	0.27
(1,1821)	1:386:A:THR:H	1:389:A:LYS:HD2	8	0.27
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	2	0.27
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	3	0.27
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	4	0.27
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	6	0.27
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	8	0.27
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	9	0.27
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	10	0.27
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	11	0.27
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	12	0.27
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	13	0.27
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	14	0.27
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	16	0.27
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	17	0.27
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	18	0.27
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	19	0.27
(1,1800)	1:336:A:LEU:HD12	1:338:A:TRP:HD1	9	0.27
(1,1787)	1:376:A:TRP:HZ2	1:337:A:LEU:HD22	17	0.27
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD12	1	0.27
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD12	11	0.27
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD13	12	0.27
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	7	0.27
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	10	0.27
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD23	7	0.27
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD23	17	0.27
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD21	18	0.27
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD12	10	0.27
(1,1672)	1:403:A:ILE:HG21	1:405:A:LYS:H	8	0.27
(1,1670)	1:403:A:ILE:HG21	1:397:A:TYR:HB2	3	0.27
(1,1670)	1:403:A:ILE:HG23	1:397:A:TYR:HB2	5	0.27
(1,1670)	1:403:A:ILE:HG21	1:397:A:TYR:HB2	16	0.27
(1,1497)	1:429:A:ARG:HG2	1:429:A:ARG:HB3	2	0.27
(1,1485)	1:432:A:HIS:HD2	1:433:A:LEU:HD23	1	0.27
(1,1462)	1:435:A:SER:H	1:434:A:GLU:HB3	3	0.27
(1,1452)	1:361:A:SER:H	1:360:A:GLU:HG2	17	0.27
(1,1444)	1:442:A:THR:HG22	1:443:A:TYR:HA	3	0.27
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	12	0.27
(1,1355)	1:395:A:ARG:HB3	1:395:A:ARG:HG2	19	0.27
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	10	0.27
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	15	0.27
(1,1316)	1:433:A:LEU:HD21	1:396:A:HIS:HD2	1	0.27
(1,1313)	1:375:A:LEU:HD13	1:376:A:TRP:H	3	0.27
(1,1313)	1:375:A:LEU:HD11	1:376:A:TRP:H	16	0.27
(1,1217)	1:359:A:LYS:HD2	1:356:A:TRP:HZ2	13	0.27
(1,1192)	1:362:A:LYS:H	1:362:A:LYS:HD2	14	0.27
(1,1121)	1:367:A:VAL:HG22	1:365:A:ARG:HA	13	0.27
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	2	0.27
(1,1084)	1:372:A:LEU:HD13	1:344:A:LEU:HD11	8	0.27
(1,1084)	1:372:A:LEU:HD12	1:344:A:LEU:HD12	13	0.27
(1,1078)	1:372:A:LEU:HD12	1:340:A:TYR:HE2	12	0.27
(1,1077)	1:372:A:LEU:HD13	1:340:A:TYR:HD2	1	0.27
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD13	1	0.27
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD11	8	0.27
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	2	0.27
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	6	0.27
(1,1033)	1:348:A:SER:HB3	1:351:A:GLU:HB3	4	0.27
(1,1016)	1:338:A:TRP:HH2	1:422:A:ILE:HG21	14	0.27
(1,999)	1:409:A:GLN:HE22	1:409:A:GLN:HG2	17	0.27
(1,902)	1:438:A:LEU:HD13	1:376:A:TRP:HZ2	9	0.27
(1,898)	1:438:A:LEU:HD13	1:382:A:ARG:HG2	10	0.27
(1,890)	1:439:A:ASP:H	1:438:A:LEU:HB2	5	0.27
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB2	4	0.27
(1,836)	1:430:A:LEU:HD12	1:427:A:THR:HB	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,836)	1:430:A:LEU:HD11	1:427:A:THR:HB	10	0.27
(1,836)	1:430:A:LEU:HD13	1:427:A:THR:HB	19	0.27
(1,803)	1:426:A:ARG:H	1:426:A:ARG:HG2	11	0.27
(1,713)	1:414:A:ARG:HE	1:414:A:ARG:HB3	13	0.27
(1,713)	1:414:A:ARG:HE	1:414:A:ARG:HB3	15	0.27
(1,690)	1:411:A:LEU:HD21	1:369:A:PRO:HB2	17	0.27
(1,627)	1:403:A:ILE:HG22	1:413:A:PHE:HB2	18	0.27
(1,594)	1:400:A:LEU:HD22	1:426:A:ARG:HG3	6	0.27
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD2	4	0.27
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	19	0.27
(1,486)	1:391:A:SER:H	1:391:A:SER:HB3	8	0.27
(1,454)	1:386:A:THR:HG21	1:370:A:ASN:HA	3	0.27
(1,454)	1:386:A:THR:HG23	1:370:A:ASN:HA	11	0.27
(1,453)	1:386:A:THR:HG22	1:386:A:THR:HB	1	0.27
(1,453)	1:386:A:THR:HG23	1:386:A:THR:HB	19	0.27
(1,400)	1:377:A:GLY:HA3	1:382:A:ARG:HB3	4	0.27
(1,309)	1:366:A:ILE:HD11	1:364:A:PHE:HZ	1	0.27
(1,309)	1:366:A:ILE:HD12	1:364:A:PHE:HZ	2	0.27
(1,309)	1:366:A:ILE:HD12	1:364:A:PHE:HZ	8	0.27
(1,309)	1:366:A:ILE:HD11	1:364:A:PHE:HZ	9	0.27
(1,309)	1:366:A:ILE:HD12	1:364:A:PHE:HZ	10	0.27
(1,303)	1:368:A:ASP:H	1:366:A:ILE:HG23	1	0.27
(1,205)	1:357:A:GLU:HB3	1:363:A:ILE:HG22	19	0.27
(1,204)	1:357:A:GLU:HB3	1:412:A:LEU:HD11	15	0.27
(1,204)	1:357:A:GLU:HB3	1:412:A:LEU:HD13	16	0.27
(1,203)	1:357:A:GLU:HB2	1:412:A:LEU:HD23	3	0.27
(1,203)	1:357:A:GLU:HB2	1:412:A:LEU:HD21	5	0.27
(1,203)	1:357:A:GLU:HB2	1:412:A:LEU:HD23	18	0.27
(1,174)	1:354:A:ILE:HD13	1:341:A:VAL:HA	4	0.27
(1,174)	1:354:A:ILE:HD12	1:341:A:VAL:HA	14	0.27
(1,166)	1:354:A:ILE:HG21	1:372:A:LEU:HD22	17	0.27
(1,104)	1:345:A:LEU:HD21	1:356:A:TRP:HE3	5	0.27
(1,104)	1:345:A:LEU:HD23	1:356:A:TRP:HE3	14	0.27
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG22	2	0.26
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	5	0.26
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	16	0.26
(1,2964)	1:446:A:ASP:H	1:445:A:GLU:HB3	12	0.26
(1,2940)	1:434:A:GLU:H	1:433:A:LEU:HB2	6	0.26
(1,2940)	1:411:A:LEU:H	1:410:A:ARG:HG3	12	0.26
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD21	10	0.26
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD23	12	0.26
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD23	14	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD23	16	0.26
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD21	18	0.26
(1,2931)	1:420:A:ASP:H	1:421:A:GLU:HG3	12	0.26
(1,2872)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	6	0.26
(1,2871)	1:445:A:GLU:HB3	1:445:A:GLU:HG2	17	0.26
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	15	0.26
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	3	0.26
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	6	0.26
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	17	0.26
(1,2836)	1:404:A:ARG:HG3	1:405:A:LYS:H	3	0.26
(1,2799)	1:433:A:LEU:HD11	1:396:A:HIS:HB3	17	0.26
(1,2791)	1:380:A:LYS:HE3	1:438:A:LEU:HD23	4	0.26
(1,2730)	1:366:A:ILE:HG22	1:373:A:ALA:H	6	0.26
(1,2728)	1:366:A:ILE:HB	1:413:A:PHE:HZ	8	0.26
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	1	0.26
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	2	0.26
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	10	0.26
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	15	0.26
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	19	0.26
(1,2697)	1:445:A:GLU:HB2	1:445:A:GLU:HG2	16	0.26
(1,2697)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	18	0.26
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG22	13	0.26
(1,2686)	1:430:A:LEU:HD11	1:430:A:LEU:HD22	11	0.26
(1,2686)	1:430:A:LEU:HD13	1:430:A:LEU:HD21	16	0.26
(1,2686)	1:430:A:LEU:HD12	1:430:A:LEU:HD23	18	0.26
(1,2669)	1:365:A:ARG:HB3	1:365:A:ARG:HD3	1	0.26
(1,2659)	1:366:A:ILE:HD13	1:411:A:LEU:HB3	4	0.26
(1,2659)	1:366:A:ILE:HG22	1:411:A:LEU:HB3	13	0.26
(1,2649)	1:403:A:ILE:HG22	1:364:A:PHE:HZ	8	0.26
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	6	0.26
(1,2618)	1:375:A:LEU:HD23	1:378:A:ASN:HB2	7	0.26
(1,2597)	1:358:A:ASP:HB2	1:363:A:ILE:HG21	6	0.26
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	2	0.26
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	15	0.26
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	17	0.26
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG13	5	0.26
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD12	3	0.26
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD12	7	0.26
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG23	2	0.26
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG23	7	0.26
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG21	12	0.26
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG23	12	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG23	3	0.26
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG23	16	0.26
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD23	14	0.26
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB2	11	0.26
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB3	17	0.26
(1,2400)	1:387:A:TYR:H	1:387:A:TYR:HD1	13	0.26
(1,2390)	1:392:A:ARG:H	1:390:A:MET:HG3	18	0.26
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	5	0.26
(1,2322)	1:350:A:TYR:H	1:350:A:TYR:HE2	3	0.26
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	6	0.26
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	13	0.26
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD13	4	0.26
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	6	0.26
(1,2133)	1:383:A:THR:H	1:384:A:ASN:H	16	0.26
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB2	6	0.26
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD11	9	0.26
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG21	5	0.26
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG23	17	0.26
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	1	0.26
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	11	0.26
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	16	0.26
(1,1920)	1:372:A:LEU:HD13	1:366:A:ILE:HD13	2	0.26
(1,1916)	1:366:A:ILE:HG21	1:411:A:LEU:HD13	1	0.26
(1,1916)	1:366:A:ILE:HG23	1:411:A:LEU:HD13	7	0.26
(1,1916)	1:366:A:ILE:HG22	1:411:A:LEU:HD12	13	0.26
(1,1912)	1:354:A:ILE:HD11	1:372:A:LEU:HD11	5	0.26
(1,1903)	1:438:A:LEU:HD22	1:438:A:LEU:HD12	3	0.26
(1,1903)	1:438:A:LEU:HD23	1:438:A:LEU:HD11	8	0.26
(1,1903)	1:438:A:LEU:HD22	1:438:A:LEU:HD13	11	0.26
(1,1901)	1:433:A:LEU:HD21	1:433:A:LEU:HD11	7	0.26
(1,1901)	1:433:A:LEU:HD21	1:433:A:LEU:HD11	13	0.26
(1,1887)	1:400:A:LEU:HD21	1:400:A:LEU:HD11	11	0.26
(1,1884)	1:394:A:LEU:HD11	1:394:A:LEU:HD21	10	0.26
(1,1884)	1:394:A:LEU:HD11	1:394:A:LEU:HD22	15	0.26
(1,1821)	1:386:A:THR:H	1:389:A:LYS:HD2	2	0.26
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	1	0.26
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	5	0.26
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	7	0.26
(1,1815)	1:419:A:PRO:HB2	1:419:A:PRO:HG3	15	0.26
(1,1800)	1:336:A:LEU:HD12	1:338:A:TRP:HD1	4	0.26
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD13	10	0.26
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD11	13	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1776)	1:337:A:LEU:HD12	1:390:A:MET:HG3	19	0.26
(1,1756)	1:402:A:ILE:HB	1:397:A:TYR:HB2	18	0.26
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	15	0.26
(1,1725)	1:341:A:VAL:HG23	1:342:A:TYR:HB2	14	0.26
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD23	9	0.26
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD12	1	0.26
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD13	5	0.26
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD12	15	0.26
(1,1607)	1:411:A:LEU:HD11	1:366:A:ILE:H	9	0.26
(1,1603)	1:357:A:GLU:HG2	1:412:A:LEU:HD12	1	0.26
(1,1600)	1:412:A:LEU:HD21	1:412:A:LEU:H	17	0.26
(1,1523)	1:422:A:ILE:HG21	1:426:A:ARG:HG2	16	0.26
(1,1488)	1:431:A:GLU:HB2	1:336:A:LEU:HD21	5	0.26
(1,1488)	1:431:A:GLU:HB2	1:336:A:LEU:HD22	7	0.26
(1,1475)	1:433:A:LEU:HD22	1:434:A:GLU:H	8	0.26
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG21	1	0.26
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG21	2	0.26
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG21	3	0.26
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG21	4	0.26
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG22	17	0.26
(1,1432)	1:445:A:GLU:HG2	1:445:A:GLU:HA	10	0.26
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	16	0.26
(1,1422)	1:451:A:ALA:HB3	1:450:A:ILE:HA	9	0.26
(1,1402)	1:383:A:THR:HG23	1:384:A:ASN:HD21	10	0.26
(1,1393)	1:386:A:THR:HG21	1:388:A:GLU:HB3	16	0.26
(1,1365)	1:391:A:SER:HB3	1:387:A:TYR:HE2	12	0.26
(1,1344)	1:398:A:TYR:HD1	1:398:A:TYR:H	10	0.26
(1,1313)	1:375:A:LEU:HD13	1:376:A:TRP:H	15	0.26
(1,1304)	1:376:A:TRP:HZ2	1:380:A:LYS:HE3	13	0.26
(1,1208)	1:360:A:GLU:HA	1:360:A:GLU:HB2	4	0.26
(1,1208)	1:360:A:GLU:HA	1:360:A:GLU:HB2	13	0.26
(1,1207)	1:360:A:GLU:HB2	1:360:A:GLU:HG3	7	0.26
(1,1207)	1:360:A:GLU:HB2	1:360:A:GLU:HG3	8	0.26
(1,1207)	1:360:A:GLU:HB3	1:360:A:GLU:HG2	11	0.26
(1,1175)	1:363:A:ILE:HG21	1:363:A:ILE:HG13	17	0.26
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	4	0.26
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	15	0.26
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG21	2	0.26
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG23	6	0.26
(1,1121)	1:367:A:VAL:HG23	1:365:A:ARG:HA	14	0.26
(1,1121)	1:367:A:VAL:HG21	1:365:A:ARG:HA	19	0.26
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	19	0.26
(1,1084)	1:372:A:LEU:HD11	1:344:A:LEU:HD13	2	0.26
(1,1078)	1:372:A:LEU:HD13	1:340:A:TYR:HE2	7	0.26
(1,1078)	1:372:A:LEU:HD13	1:340:A:TYR:HE2	15	0.26
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD13	6	0.26
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD12	17	0.26
(1,1052)	1:347:A:ASP:HB2	1:350:A:TYR:HD1	3	0.26
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	16	0.26
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	19	0.26
(1,1011)	1:356:A:TRP:HH2	1:418:A:THR:HG22	19	0.26
(1,929)	1:443:A:TYR:H	1:442:A:THR:HB	11	0.26
(1,929)	1:443:A:TYR:H	1:442:A:THR:HB	13	0.26
(1,902)	1:438:A:LEU:HD12	1:376:A:TRP:HZ2	4	0.26
(1,890)	1:439:A:ASP:H	1:438:A:LEU:HB2	11	0.26
(1,864)	1:433:A:LEU:HA	1:433:A:LEU:HD12	15	0.26
(1,850)	1:431:A:GLU:HG3	1:431:A:GLU:HB2	16	0.26
(1,836)	1:430:A:LEU:HD12	1:427:A:THR:HB	2	0.26
(1,834)	1:430:A:LEU:HD13	1:397:A:TYR:HD1	17	0.26
(1,822)	1:429:A:ARG:HA	1:429:A:ARG:HG2	13	0.26
(1,627)	1:403:A:ILE:HG21	1:413:A:PHE:HB2	7	0.26
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD3	3	0.26
(1,528)	1:394:A:LEU:HD23	1:364:A:PHE:HZ	13	0.26
(1,486)	1:391:A:SER:H	1:391:A:SER:HB3	13	0.26
(1,456)	1:386:A:THR:HG21	1:387:A:TYR:HB2	8	0.26
(1,400)	1:377:A:GLY:HA3	1:382:A:ARG:HB3	12	0.26
(1,381)	1:375:A:LEU:HD12	1:350:A:TYR:HE2	3	0.26
(1,381)	1:375:A:LEU:HD11	1:350:A:TYR:HE2	17	0.26
(1,367)	1:374:A:ARG:HB3	1:374:A:ARG:HD2	11	0.26
(1,365)	1:374:A:ARG:H	1:374:A:ARG:HD2	9	0.26
(1,359)	1:374:A:ARG:HA	1:374:A:ARG:HB3	4	0.26
(1,309)	1:366:A:ILE:HD13	1:364:A:PHE:HZ	5	0.26
(1,309)	1:366:A:ILE:HD12	1:364:A:PHE:HZ	12	0.26
(1,309)	1:366:A:ILE:HD13	1:364:A:PHE:HZ	14	0.26
(1,309)	1:366:A:ILE:HD12	1:364:A:PHE:HZ	19	0.26
(1,306)	1:354:A:ILE:HD13	1:366:A:ILE:HG21	9	0.26
(1,237)	1:361:A:SER:HB3	1:363:A:ILE:HG12	4	0.26
(1,237)	1:361:A:SER:HB3	1:363:A:ILE:HG12	14	0.26
(1,231)	1:359:A:LYS:HG3	1:359:A:LYS:HE2	8	0.26
(1,187)	1:356:A:TRP:HB2	1:359:A:LYS:HD3	17	0.26
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	18	0.26
(1,174)	1:354:A:ILE:HD12	1:341:A:VAL:HA	8	0.26
(1,174)	1:354:A:ILE:HD12	1:341:A:VAL:HA	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,174)	1:354:A:ILE:HD13	1:341:A:VAL:HA	11	0.26
(1,141)	1:352:A:ASN:HD22	1:352:A:ASN:HB3	8	0.26
(1,141)	1:352:A:ASN:HD22	1:352:A:ASN:HB3	9	0.26
(1,141)	1:352:A:ASN:HD22	1:352:A:ASN:HB3	13	0.26
(1,141)	1:352:A:ASN:HD22	1:352:A:ASN:HB3	19	0.26
(1,104)	1:345:A:LEU:HD22	1:356:A:TRP:HE3	1	0.26
(1,104)	1:345:A:LEU:HD22	1:356:A:TRP:HE3	6	0.26
(1,104)	1:345:A:LEU:HD22	1:356:A:TRP:HE3	8	0.26
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	1	0.25
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	3	0.25
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	5	0.25
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	6	0.25
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	7	0.25
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	8	0.25
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	9	0.25
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	10	0.25
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	14	0.25
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	15	0.25
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	16	0.25
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	17	0.25
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	18	0.25
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	12	0.25
(1,2964)	1:446:A:ASP:H	1:445:A:GLU:HB3	4	0.25
(1,2940)	1:434:A:GLU:H	1:433:A:LEU:HB2	7	0.25
(1,2940)	1:434:A:GLU:H	1:433:A:LEU:HB2	13	0.25
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD23	3	0.25
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD22	19	0.25
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	15	0.25
(1,2871)	1:447:A:GLU:HG2	1:447:A:GLU:HB3	12	0.25
(1,2844)	1:402:A:ILE:HG23	1:397:A:TYR:HD2	13	0.25
(1,2824)	1:413:A:PHE:HE2	1:411:A:LEU:HD22	9	0.25
(1,2800)	1:432:A:HIS:HB3	1:433:A:LEU:HD12	4	0.25
(1,2752)	1:392:A:ARG:H	1:392:A:ARG:HD2	14	0.25
(1,2725)	1:367:A:VAL:HG21	1:365:A:ARG:HB3	3	0.25
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	3	0.25
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	7	0.25
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	14	0.25
(1,2705)	1:394:A:LEU:HA	1:397:A:TYR:HD1	1	0.25
(1,2705)	1:394:A:LEU:HA	1:397:A:TYR:HD2	4	0.25
(1,2705)	1:394:A:LEU:HA	1:397:A:TYR:HD1	6	0.25
(1,2697)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	6	0.25
(1,2690)	1:437:A:VAL:HA	1:437:A:VAL:HG21	18	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2684)	1:429:A:ARG:HG2	1:433:A:LEU:HD21	11	0.25
(1,2669)	1:414:A:ARG:HB3	1:414:A:ARG:HD3	3	0.25
(1,2669)	1:365:A:ARG:HB3	1:365:A:ARG:HD3	10	0.25
(1,2659)	1:366:A:ILE:HD13	1:411:A:LEU:HB3	1	0.25
(1,2655)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	2	0.25
(1,2643)	1:402:A:ILE:HD12	1:397:A:TYR:HD1	17	0.25
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	3	0.25
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	12	0.25
(1,2612)	1:393:A:ALA:HB2	1:376:A:TRP:HZ3	7	0.25
(1,2596)	1:363:A:ILE:HG22	1:364:A:PHE:HA	12	0.25
(1,2587)	1:362:A:LYS:HA	1:415:A:PHE:HD2	18	0.25
(1,2557)	1:341:A:VAL:HG11	1:403:A:ILE:HD12	3	0.25
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	1	0.25
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	11	0.25
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	18	0.25
(1,2551)	1:451:A:ALA:H	1:451:A:ALA:HB2	18	0.25
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG13	3	0.25
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG13	10	0.25
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD12	5	0.25
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD11	6	0.25
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD12	13	0.25
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD11	16	0.25
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG21	17	0.25
(1,2540)	1:413:A:PHE:H	1:363:A:ILE:HG23	18	0.25
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD22	2	0.25
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD22	15	0.25
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD22	18	0.25
(1,2508)	1:434:A:GLU:H	1:434:A:GLU:HG2	14	0.25
(1,2499)	1:421:A:GLU:H	1:420:A:ASP:HB2	18	0.25
(1,2447)	1:385:A:MET:H	1:444:A:GLN:HE21	2	0.25
(1,2425)	1:440:A:GLU:H	1:440:A:GLU:HG2	15	0.25
(1,2406)	1:383:A:THR:H	1:382:A:ARG:HG2	5	0.25
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD23	14	0.25
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	5	0.25
(1,2129)	1:447:A:GLU:H	1:447:A:GLU:HB3	15	0.25
(1,2129)	1:447:A:GLU:H	1:447:A:GLU:HB3	16	0.25
(1,2073)	1:366:A:ILE:H	1:365:A:ARG:HB2	17	0.25
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG21	8	0.25
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG23	13	0.25
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	4	0.25
(1,1920)	1:372:A:LEU:HD13	1:366:A:ILE:HD13	11	0.25
(1,1916)	1:366:A:ILE:HG23	1:411:A:LEU:HD12	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1916)	1:366:A:ILE:HG22	1:411:A:LEU:HD12	12	0.25
(1,1908)	1:341:A:VAL:HG23	1:345:A:LEU:HD12	10	0.25
(1,1903)	1:438:A:LEU:HD22	1:438:A:LEU:HD11	13	0.25
(1,1903)	1:438:A:LEU:HD21	1:438:A:LEU:HD11	16	0.25
(1,1901)	1:433:A:LEU:HD23	1:433:A:LEU:HD13	5	0.25
(1,1898)	1:427:A:THR:HG23	1:430:A:LEU:HD12	5	0.25
(1,1895)	1:411:A:LEU:HD21	1:366:A:ILE:HD11	18	0.25
(1,1892)	1:403:A:ILE:HD11	1:402:A:ILE:HG21	9	0.25
(1,1892)	1:403:A:ILE:HD12	1:402:A:ILE:HG22	13	0.25
(1,1884)	1:394:A:LEU:HD12	1:394:A:LEU:HD22	17	0.25
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB3	13	0.25
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD11	3	0.25
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD13	15	0.25
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD13	16	0.25
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD11	4	0.25
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD12	5	0.25
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD12	17	0.25
(1,1770)	1:394:A:LEU:HD22	1:337:A:LEU:HD13	17	0.25
(1,1761)	1:340:A:TYR:HB2	1:337:A:LEU:HA	5	0.25
(1,1730)	1:340:A:TYR:HB3	1:340:A:TYR:HD1	18	0.25
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD21	4	0.25
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD23	6	0.25
(1,1607)	1:411:A:LEU:HD13	1:366:A:ILE:H	7	0.25
(1,1607)	1:411:A:LEU:HD13	1:366:A:ILE:H	8	0.25
(1,1600)	1:412:A:LEU:HD22	1:412:A:LEU:H	18	0.25
(1,1523)	1:422:A:ILE:HG21	1:426:A:ARG:HG2	2	0.25
(1,1523)	1:422:A:ILE:HG23	1:426:A:ARG:HG2	8	0.25
(1,1488)	1:431:A:GLU:HB2	1:336:A:LEU:HD23	4	0.25
(1,1475)	1:433:A:LEU:HD21	1:434:A:GLU:H	16	0.25
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG22	9	0.25
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG23	15	0.25
(1,1432)	1:445:A:GLU:HG2	1:445:A:GLU:HA	3	0.25
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	18	0.25
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	11	0.25
(1,1355)	1:395:A:ARG:HB3	1:395:A:ARG:HG2	18	0.25
(1,1344)	1:398:A:TYR:HD1	1:398:A:TYR:H	17	0.25
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	4	0.25
(1,1328)	1:399:A:LYS:H	1:400:A:LEU:HD11	4	0.25
(1,1217)	1:359:A:LYS:HD2	1:356:A:TRP:HZ2	19	0.25
(1,1207)	1:360:A:GLU:HB3	1:360:A:GLU:HG2	19	0.25
(1,1175)	1:363:A:ILE:HG22	1:363:A:ILE:HG13	2	0.25
(1,1175)	1:363:A:ILE:HG23	1:363:A:ILE:HG13	18	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	14	0.25
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG12	19	0.25
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG23	3	0.25
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG21	11	0.25
(1,1121)	1:367:A:VAL:HG21	1:365:A:ARG:HA	8	0.25
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	1	0.25
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	2	0.25
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	3	0.25
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	6	0.25
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	8	0.25
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	9	0.25
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	12	0.25
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	13	0.25
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	15	0.25
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	16	0.25
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	17	0.25
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	18	0.25
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	19	0.25
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	13	0.25
(1,1078)	1:372:A:LEU:HD11	1:340:A:TYR:HE2	18	0.25
(1,1077)	1:372:A:LEU:HD12	1:340:A:TYR:HD2	5	0.25
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD11	16	0.25
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	2	0.25
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	8	0.25
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	15	0.25
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	18	0.25
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	19	0.25
(1,1005)	1:382:A:ARG:HD2	1:382:A:ARG:HA	18	0.25
(1,970)	1:450:A:ILE:HG22	1:450:A:ILE:HG12	3	0.25
(1,957)	1:449:A:THR:H	1:449:A:THR:HB	18	0.25
(1,956)	1:450:A:ILE:H	1:449:A:THR:HB	6	0.25
(1,954)	1:450:A:ILE:H	1:449:A:THR:HA	17	0.25
(1,923)	1:441:A:GLN:HB2	1:441:A:GLN:HG2	13	0.25
(1,907)	1:438:A:LEU:HD21	1:376:A:TRP:HZ2	19	0.25
(1,902)	1:438:A:LEU:HD13	1:376:A:TRP:HZ2	5	0.25
(1,902)	1:438:A:LEU:HD13	1:376:A:TRP:HZ2	18	0.25
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB1	12	0.25
(1,836)	1:430:A:LEU:HD12	1:427:A:THR:HB	3	0.25
(1,834)	1:430:A:LEU:HD11	1:397:A:TYR:HD1	11	0.25
(1,822)	1:429:A:ARG:HA	1:429:A:ARG:HG2	2	0.25
(1,813)	1:427:A:THR:HG21	1:425:A:GLY:H	9	0.25
(1,699)	1:413:A:PHE:HB2	1:364:A:PHE:HE2	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,699)	1:413:A:PHE:HB2	1:364:A:PHE:HE2	11	0.25
(1,629)	1:403:A:ILE:HD12	1:415:A:PHE:HD1	13	0.25
(1,627)	1:403:A:ILE:HG21	1:413:A:PHE:HB2	10	0.25
(1,602)	1:401:A:ASN:HD22	1:401:A:ASN:HB3	4	0.25
(1,556)	1:397:A:TYR:HA	1:400:A:LEU:HB3	13	0.25
(1,530)	1:394:A:LEU:HD21	1:397:A:TYR:HB3	1	0.25
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD22	12	0.25
(1,468)	1:388:A:GLU:HA	1:391:A:SER:HB3	8	0.25
(1,454)	1:386:A:THR:HG21	1:370:A:ASN:HA	9	0.25
(1,454)	1:386:A:THR:HG22	1:370:A:ASN:HA	18	0.25
(1,347)	1:373:A:ALA:HA	1:376:A:TRP:HB2	3	0.25
(1,309)	1:366:A:ILE:HD13	1:364:A:PHE:HZ	3	0.25
(1,309)	1:366:A:ILE:HD11	1:364:A:PHE:HZ	4	0.25
(1,309)	1:366:A:ILE:HD11	1:364:A:PHE:HZ	6	0.25
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	7	0.25
(1,174)	1:354:A:ILE:HD11	1:341:A:VAL:HA	2	0.25
(1,174)	1:354:A:ILE:HD11	1:341:A:VAL:HA	3	0.25
(1,174)	1:354:A:ILE:HD11	1:341:A:VAL:HA	18	0.25
(1,166)	1:354:A:ILE:HG23	1:372:A:LEU:HD21	3	0.25
(1,141)	1:352:A:ASN:HD22	1:352:A:ASN:HB3	2	0.25
(1,141)	1:352:A:ASN:HD22	1:352:A:ASN:HB3	15	0.25
(1,141)	1:352:A:ASN:HD22	1:352:A:ASN:HB3	18	0.25
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD21	10	0.25
(1,104)	1:345:A:LEU:HD23	1:356:A:TRP:HE3	16	0.25
(1,85)	1:344:A:LEU:HD21	1:350:A:TYR:HD1	4	0.25
(1,85)	1:344:A:LEU:HD23	1:350:A:TYR:HD1	9	0.25
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	1	0.25
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	7	0.25
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	8	0.25
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB1	6	0.24
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	2	0.24
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	4	0.24
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	11	0.24
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	13	0.24
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	19	0.24
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG22	16	0.24
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	14	0.24
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	15	0.24
(1,2972)	1:435:A:SER:H	1:436:A:GLN:HG3	3	0.24
(1,2940)	1:411:A:LEU:H	1:410:A:ARG:HG3	14	0.24
(1,2931)	1:420:A:ASP:H	1:421:A:GLU:HG3	17	0.24
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	8	0.24
(1,2882)	1:402:A:ILE:HB	1:397:A:TYR:HD2	15	0.24
(1,2872)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	4	0.24
(1,2852)	1:343:A:GLN:HB3	1:340:A:TYR:HD1	19	0.24
(1,2825)	1:413:A:PHE:HE2	1:366:A:ILE:HB	1	0.24
(1,2825)	1:413:A:PHE:HE2	1:366:A:ILE:HB	4	0.24
(1,2824)	1:413:A:PHE:HE2	1:411:A:LEU:HD21	18	0.24
(1,2775)	1:443:A:TYR:HD2	1:445:A:GLU:HB2	3	0.24
(1,2775)	1:387:A:TYR:HD1	1:390:A:MET:HG2	15	0.24
(1,2769)	1:386:A:THR:H	1:373:A:ALA:HB2	4	0.24
(1,2724)	1:367:A:VAL:HG21	1:352:A:ASN:HA	4	0.24
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	4	0.24
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	8	0.24
(1,2723)	1:369:A:PRO:HA	1:368:A:ASP:H	18	0.24
(1,2705)	1:394:A:LEU:HA	1:397:A:TYR:HD1	7	0.24
(1,2693)	1:437:A:VAL:HG21	1:441:A:GLN:HE22	5	0.24
(1,2686)	1:430:A:LEU:HD11	1:430:A:LEU:HD22	1	0.24
(1,2669)	1:365:A:ARG:HB3	1:365:A:ARG:HD3	14	0.24
(1,2659)	1:366:A:ILE:HD13	1:411:A:LEU:HB3	9	0.24
(1,2659)	1:366:A:ILE:HD13	1:411:A:LEU:HB3	15	0.24
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD2	16	0.24
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD2	17	0.24
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	8	0.24
(1,2612)	1:393:A:ALA:HB1	1:376:A:TRP:HZ3	1	0.24
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	5	0.24
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	10	0.24
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	11	0.24
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	18	0.24
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	19	0.24
(1,2567)	1:345:A:LEU:HD21	1:355:A:ARG:HA	11	0.24
(1,2567)	1:345:A:LEU:HD22	1:355:A:ARG:HA	13	0.24
(1,2567)	1:345:A:LEU:HD22	1:355:A:ARG:HA	16	0.24
(1,2567)	1:345:A:LEU:HD22	1:355:A:ARG:HA	18	0.24
(1,2556)	1:341:A:VAL:HG11	1:364:A:PHE:HZ	4	0.24
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	4	0.24
(1,2552)	1:452:A:SER:H	1:451:A:ALA:HB3	19	0.24
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG11	2	0.24
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG11	8	0.24
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG12	11	0.24
(1,2537)	1:394:A:LEU:H	1:394:A:LEU:HD12	18	0.24
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD21	8	0.24
(1,2528)	1:372:A:LEU:H	1:372:A:LEU:HD23	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG21	4	0.24
(1,2522)	1:356:A:TRP:H	1:345:A:LEU:HD21	5	0.24
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD21	6	0.24
(1,2508)	1:434:A:GLU:H	1:434:A:GLU:HG2	6	0.24
(1,2191)	1:403:A:ILE:H	1:397:A:TYR:HB2	17	0.24
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	1	0.24
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	10	0.24
(1,2126)	1:410:A:ARG:H	1:410:A:ARG:HB2	3	0.24
(1,2067)	1:365:A:ARG:H	1:355:A:ARG:HG2	5	0.24
(1,2048)	1:361:A:SER:H	1:358:A:ASP:HB2	9	0.24
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD12	5	0.24
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG22	14	0.24
(1,1986)	1:351:A:GLU:H	1:351:A:GLU:HG3	10	0.24
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	8	0.24
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	12	0.24
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	13	0.24
(1,1920)	1:372:A:LEU:HD11	1:366:A:ILE:HD12	7	0.24
(1,1916)	1:366:A:ILE:HG22	1:411:A:LEU:HD13	3	0.24
(1,1916)	1:366:A:ILE:HG21	1:411:A:LEU:HD12	6	0.24
(1,1903)	1:438:A:LEU:HD22	1:438:A:LEU:HD11	5	0.24
(1,1903)	1:438:A:LEU:HD21	1:438:A:LEU:HD11	9	0.24
(1,1903)	1:438:A:LEU:HD22	1:438:A:LEU:HD11	12	0.24
(1,1903)	1:438:A:LEU:HD21	1:438:A:LEU:HD11	17	0.24
(1,1901)	1:433:A:LEU:HD23	1:433:A:LEU:HD11	19	0.24
(1,1899)	1:430:A:LEU:HD13	1:400:A:LEU:HD23	4	0.24
(1,1895)	1:411:A:LEU:HD22	1:366:A:ILE:HD13	1	0.24
(1,1895)	1:411:A:LEU:HD23	1:366:A:ILE:HD13	4	0.24
(1,1892)	1:403:A:ILE:HD11	1:402:A:ILE:HG21	5	0.24
(1,1892)	1:403:A:ILE:HD13	1:402:A:ILE:HG22	7	0.24
(1,1892)	1:403:A:ILE:HD12	1:402:A:ILE:HG21	8	0.24
(1,1887)	1:400:A:LEU:HD21	1:400:A:LEU:HD12	9	0.24
(1,1884)	1:394:A:LEU:HD13	1:394:A:LEU:HD21	12	0.24
(1,1821)	1:386:A:THR:H	1:389:A:LYS:HD2	16	0.24
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD11	5	0.24
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD12	14	0.24
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD11	15	0.24
(1,1761)	1:340:A:TYR:HB2	1:337:A:LEU:HA	15	0.24
(1,1709)	1:344:A:LEU:HD23	1:345:A:LEU:H	4	0.24
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD11	8	0.24
(1,1666)	1:403:A:ILE:HG13	1:364:A:PHE:HZ	11	0.24
(1,1604)	1:365:A:ARG:HB2	1:412:A:LEU:HD11	19	0.24
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD11	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	19	0.24
(1,1505)	1:385:A:MET:HA	1:389:A:LYS:HB2	12	0.24
(1,1505)	1:385:A:MET:HA	1:389:A:LYS:HB2	16	0.24
(1,1502)	1:422:A:ILE:HA	1:427:A:THR:HG23	11	0.24
(1,1502)	1:422:A:ILE:HA	1:427:A:THR:HG22	17	0.24
(1,1498)	1:429:A:ARG:HD2	1:429:A:ARG:HB2	4	0.24
(1,1475)	1:433:A:LEU:HD21	1:434:A:GLU:H	3	0.24
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG21	7	0.24
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG23	8	0.24
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG21	12	0.24
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG23	13	0.24
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG21	16	0.24
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG21	18	0.24
(1,1444)	1:442:A:THR:HG22	1:443:A:TYR:HA	4	0.24
(1,1427)	1:447:A:GLU:HA	1:448:A:PRO:HD3	4	0.24
(1,1427)	1:447:A:GLU:HA	1:448:A:PRO:HD3	7	0.24
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	16	0.24
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD23	12	0.24
(1,1357)	1:394:A:LEU:HD22	1:390:A:MET:HG3	8	0.24
(1,1344)	1:398:A:TYR:HD1	1:398:A:TYR:H	2	0.24
(1,1267)	1:354:A:ILE:HD13	1:367:A:VAL:H	16	0.24
(1,1250)	1:345:A:LEU:HD22	1:355:A:ARG:HA	13	0.24
(1,1250)	1:345:A:LEU:HD22	1:355:A:ARG:HA	16	0.24
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD3	1	0.24
(1,1217)	1:359:A:LYS:HD2	1:356:A:TRP:HZ2	8	0.24
(1,1217)	1:359:A:LYS:HD2	1:356:A:TRP:HZ2	11	0.24
(1,1207)	1:360:A:GLU:HB2	1:360:A:GLU:HG3	2	0.24
(1,1207)	1:360:A:GLU:HB2	1:360:A:GLU:HG3	12	0.24
(1,1207)	1:360:A:GLU:HB2	1:360:A:GLU:HG3	18	0.24
(1,1180)	1:363:A:ILE:HD13	1:414:A:ARG:HD2	3	0.24
(1,1179)	1:361:A:SER:HB3	1:363:A:ILE:HD13	4	0.24
(1,1179)	1:361:A:SER:HB3	1:363:A:ILE:HD12	14	0.24
(1,1175)	1:363:A:ILE:HG21	1:363:A:ILE:HG13	9	0.24
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG12	18	0.24
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG23	5	0.24
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG21	7	0.24
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG23	9	0.24
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG22	10	0.24
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG22	12	0.24
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG22	13	0.24
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG23	14	0.24
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG23	16	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG23	19	0.24
(1,1123)	1:354:A:ILE:H	1:367:A:VAL:HG21	8	0.24
(1,1121)	1:367:A:VAL:HG23	1:365:A:ARG:HA	9	0.24
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	4	0.24
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	11	0.24
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	14	0.24
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	6	0.24
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	8	0.24
(1,1084)	1:372:A:LEU:HD13	1:344:A:LEU:HD11	16	0.24
(1,1078)	1:372:A:LEU:HD13	1:340:A:TYR:HE2	1	0.24
(1,1078)	1:372:A:LEU:HD12	1:340:A:TYR:HE2	2	0.24
(1,1078)	1:372:A:LEU:HD12	1:340:A:TYR:HE2	5	0.24
(1,1078)	1:372:A:LEU:HD12	1:340:A:TYR:HE2	10	0.24
(1,1078)	1:372:A:LEU:HD13	1:340:A:TYR:HE2	13	0.24
(1,1078)	1:372:A:LEU:HD12	1:340:A:TYR:HE2	14	0.24
(1,1077)	1:372:A:LEU:HD13	1:340:A:TYR:HD2	7	0.24
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD12	5	0.24
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD12	18	0.24
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	9	0.24
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	13	0.24
(1,1033)	1:348:A:SER:HB3	1:351:A:GLU:HB3	8	0.24
(1,1033)	1:348:A:SER:HB3	1:351:A:GLU:HB3	13	0.24
(1,1025)	1:336:A:LEU:HD22	1:430:A:LEU:H	12	0.24
(1,1016)	1:338:A:TRP:HH2	1:422:A:ILE:HG22	4	0.24
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	3	0.24
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	10	0.24
(1,978)	1:453:A:PRO:HA	1:450:A:ILE:HD12	19	0.24
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG22	7	0.24
(1,903)	1:438:A:LEU:HD22	1:438:A:LEU:HB3	15	0.24
(1,902)	1:438:A:LEU:HD12	1:376:A:TRP:HZ2	3	0.24
(1,890)	1:439:A:ASP:H	1:438:A:LEU:HB2	3	0.24
(1,890)	1:439:A:ASP:H	1:438:A:LEU:HB2	18	0.24
(1,871)	1:435:A:SER:HB2	1:435:A:SER:HA	1	0.24
(1,871)	1:435:A:SER:HB2	1:435:A:SER:HA	3	0.24
(1,871)	1:435:A:SER:HB2	1:435:A:SER:HA	12	0.24
(1,850)	1:431:A:GLU:HG3	1:431:A:GLU:HB2	1	0.24
(1,850)	1:431:A:GLU:HG3	1:431:A:GLU:HB2	5	0.24
(1,836)	1:430:A:LEU:HD11	1:427:A:THR:HB	16	0.24
(1,760)	1:338:A:TRP:HZ2	1:419:A:PRO:HA	9	0.24
(1,627)	1:403:A:ILE:HG22	1:413:A:PHE:HB2	13	0.24
(1,602)	1:401:A:ASN:HD22	1:401:A:ASN:HB3	2	0.24
(1,602)	1:401:A:ASN:HD22	1:401:A:ASN:HB3	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,602)	1:401:A:ASN:HD22	1:401:A:ASN:HB3	9	0.24
(1,602)	1:401:A:ASN:HD22	1:401:A:ASN:HB3	10	0.24
(1,602)	1:401:A:ASN:HD22	1:401:A:ASN:HB3	13	0.24
(1,602)	1:401:A:ASN:HD22	1:401:A:ASN:HB3	15	0.24
(1,594)	1:400:A:LEU:HD22	1:426:A:ARG:HG3	7	0.24
(1,556)	1:397:A:TYR:HA	1:400:A:LEU:HB3	19	0.24
(1,538)	1:395:A:ARG:HA	1:395:A:ARG:HB2	7	0.24
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	7	0.24
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	11	0.24
(1,495)	1:392:A:ARG:HA	1:392:A:ARG:HG2	18	0.24
(1,429)	1:381:A:ASN:HA	1:381:A:ASN:HB2	2	0.24
(1,387)	1:375:A:LEU:HD21	1:353:A:PHE:HE1	17	0.24
(1,383)	1:375:A:LEU:HD13	1:353:A:PHE:HE1	17	0.24
(1,309)	1:366:A:ILE:HD11	1:364:A:PHE:HZ	7	0.24
(1,174)	1:354:A:ILE:HD13	1:341:A:VAL:HA	5	0.24
(1,174)	1:354:A:ILE:HD13	1:341:A:VAL:HA	15	0.24
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD23	15	0.24
(1,104)	1:345:A:LEU:HD23	1:356:A:TRP:HE3	2	0.24
(1,104)	1:345:A:LEU:HD22	1:356:A:TRP:HE3	7	0.24
(1,104)	1:345:A:LEU:HD22	1:356:A:TRP:HE3	11	0.24
(1,42)	1:341:A:VAL:HG21	1:415:A:PHE:HE2	6	0.24
(1,2988)	1:344:A:LEU:H	1:344:A:LEU:HB3	12	0.23
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG22	5	0.23
(1,2940)	1:434:A:GLU:H	1:433:A:LEU:HB2	2	0.23
(1,2940)	1:411:A:LEU:H	1:410:A:ARG:HG3	4	0.23
(1,2940)	1:434:A:GLU:H	1:433:A:LEU:HB2	19	0.23
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD22	9	0.23
(1,2931)	1:420:A:ASP:H	1:421:A:GLU:HG3	6	0.23
(1,2852)	1:343:A:GLN:HB2	1:340:A:TYR:HD1	4	0.23
(1,2852)	1:343:A:GLN:HB3	1:340:A:TYR:HD1	18	0.23
(1,2844)	1:402:A:ILE:HG23	1:397:A:TYR:HD2	7	0.23
(1,2825)	1:413:A:PHE:HE2	1:366:A:ILE:HB	10	0.23
(1,2825)	1:413:A:PHE:HE2	1:366:A:ILE:HB	17	0.23
(1,2824)	1:413:A:PHE:HE2	1:411:A:LEU:HD23	4	0.23
(1,2792)	1:375:A:LEU:H	1:375:A:LEU:HD21	4	0.23
(1,2774)	1:443:A:TYR:HD1	1:445:A:GLU:HB2	3	0.23
(1,2762)	1:394:A:LEU:HD21	1:398:A:TYR:HE1	15	0.23
(1,2697)	1:445:A:GLU:HG3	1:445:A:GLU:HB2	4	0.23
(1,2686)	1:430:A:LEU:HD13	1:430:A:LEU:HD21	12	0.23
(1,2686)	1:430:A:LEU:HD13	1:430:A:LEU:HD23	17	0.23
(1,2669)	1:365:A:ARG:HB3	1:365:A:ARG:HD3	4	0.23
(1,2659)	1:366:A:ILE:HD12	1:411:A:LEU:HB3	16	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD2	6	0.23
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD2	7	0.23
(1,2645)	1:402:A:ILE:HD12	1:338:A:TRP:HB3	4	0.23
(1,2625)	1:387:A:TYR:HA	1:387:A:TYR:HD2	7	0.23
(1,2612)	1:393:A:ALA:HB3	1:376:A:TRP:HZ3	2	0.23
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	1	0.23
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	2	0.23
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	3	0.23
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	4	0.23
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	7	0.23
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	8	0.23
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	9	0.23
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	12	0.23
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	13	0.23
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	15	0.23
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	16	0.23
(1,2567)	1:345:A:LEU:HD21	1:355:A:ARG:HA	6	0.23
(1,2557)	1:341:A:VAL:HG12	1:403:A:ILE:HD13	10	0.23
(1,2554)	1:338:A:TRP:HA	1:338:A:TRP:HE3	10	0.23
(1,2545)	1:436:A:GLN:H	1:437:A:VAL:HG11	19	0.23
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD11	9	0.23
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD22	1	0.23
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD22	10	0.23
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG22	5	0.23
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG21	15	0.23
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	10	0.23
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB2	3	0.23
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB2	7	0.23
(1,2425)	1:440:A:GLU:H	1:440:A:GLU:HG2	4	0.23
(1,2425)	1:440:A:GLU:H	1:440:A:GLU:HG2	16	0.23
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	2	0.23
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	17	0.23
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	16	0.23
(1,2129)	1:447:A:GLU:H	1:447:A:GLU:HB3	19	0.23
(1,2126)	1:410:A:ARG:H	1:410:A:ARG:HB3	1	0.23
(1,2126)	1:410:A:ARG:H	1:410:A:ARG:HB3	2	0.23
(1,2126)	1:410:A:ARG:H	1:410:A:ARG:HB2	16	0.23
(1,2067)	1:365:A:ARG:H	1:355:A:ARG:HG2	19	0.23
(1,1954)	1:399:A:LYS:H	1:399:A:LYS:HG2	9	0.23
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	6	0.23
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	15	0.23
(1,1916)	1:366:A:ILE:HG22	1:411:A:LEU:HD13	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1909)	1:344:A:LEU:HD13	1:354:A:ILE:HG21	2	0.23
(1,1901)	1:433:A:LEU:HD22	1:433:A:LEU:HD11	11	0.23
(1,1901)	1:433:A:LEU:HD21	1:433:A:LEU:HD13	14	0.23
(1,1892)	1:403:A:ILE:HD13	1:402:A:ILE:HG23	1	0.23
(1,1892)	1:403:A:ILE:HD12	1:402:A:ILE:HG22	4	0.23
(1,1884)	1:394:A:LEU:HD13	1:394:A:LEU:HD22	18	0.23
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB3	7	0.23
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB2	17	0.23
(1,1821)	1:386:A:THR:H	1:389:A:LYS:HD2	10	0.23
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD13	1	0.23
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD13	6	0.23
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD11	9	0.23
(1,1778)	1:337:A:LEU:HD13	1:376:A:TRP:HB3	10	0.23
(1,1756)	1:402:A:ILE:HB	1:397:A:TYR:HB2	11	0.23
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD23	15	0.23
(1,1672)	1:403:A:ILE:HG22	1:405:A:LYS:H	15	0.23
(1,1666)	1:403:A:ILE:HG13	1:364:A:PHE:HZ	6	0.23
(1,1626)	1:406:A:GLU:H	1:406:A:GLU:HG3	5	0.23
(1,1626)	1:406:A:GLU:H	1:406:A:GLU:HG3	19	0.23
(1,1607)	1:411:A:LEU:HD13	1:366:A:ILE:H	4	0.23
(1,1604)	1:365:A:ARG:HB2	1:412:A:LEU:HD13	12	0.23
(1,1600)	1:412:A:LEU:HD22	1:412:A:LEU:H	2	0.23
(1,1600)	1:412:A:LEU:HD23	1:412:A:LEU:H	11	0.23
(1,1488)	1:431:A:GLU:HB2	1:336:A:LEU:HD22	2	0.23
(1,1485)	1:432:A:HIS:HD2	1:433:A:LEU:HD22	9	0.23
(1,1452)	1:361:A:SER:H	1:360:A:GLU:HG2	15	0.23
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG23	11	0.23
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	2	0.23
(1,1313)	1:375:A:LEU:HD11	1:376:A:TRP:H	18	0.23
(1,1250)	1:345:A:LEU:HD21	1:355:A:ARG:HA	11	0.23
(1,1250)	1:345:A:LEU:HD22	1:355:A:ARG:HA	18	0.23
(1,1217)	1:359:A:LYS:HD2	1:356:A:TRP:HZ2	5	0.23
(1,1217)	1:359:A:LYS:HD2	1:356:A:TRP:HZ2	9	0.23
(1,1217)	1:359:A:LYS:HD2	1:356:A:TRP:HZ2	12	0.23
(1,1207)	1:360:A:GLU:HB3	1:360:A:GLU:HG2	10	0.23
(1,1207)	1:360:A:GLU:HB3	1:360:A:GLU:HG2	14	0.23
(1,1207)	1:360:A:GLU:HB3	1:360:A:GLU:HG2	16	0.23
(1,1175)	1:363:A:ILE:HG23	1:363:A:ILE:HG13	7	0.23
(1,1175)	1:363:A:ILE:HG22	1:363:A:ILE:HG13	8	0.23
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	11	0.23
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG11	3	0.23
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG13	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG11	14	0.23
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG22	1	0.23
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG21	8	0.23
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG23	15	0.23
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG23	17	0.23
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	5	0.23
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	10	0.23
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	14	0.23
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	16	0.23
(1,1078)	1:372:A:LEU:HD11	1:340:A:TYR:HE2	4	0.23
(1,1078)	1:372:A:LEU:HD13	1:340:A:TYR:HE2	6	0.23
(1,1078)	1:372:A:LEU:HD12	1:340:A:TYR:HE2	9	0.23
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD11	4	0.23
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD12	9	0.23
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD12	13	0.23
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	11	0.23
(1,1060)	1:351:A:GLU:HB2	1:355:A:ARG:HD3	19	0.23
(1,1044)	1:349:A:ARG:HB2	1:349:A:ARG:HG2	19	0.23
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	5	0.23
(1,1033)	1:348:A:SER:HB3	1:351:A:GLU:HB3	6	0.23
(1,1016)	1:338:A:TRP:HH2	1:422:A:ILE:HG22	5	0.23
(1,1001)	1:409:A:GLN:HB2	1:409:A:GLN:HG2	14	0.23
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	1	0.23
(1,992)	1:457:A:PRO:HA	1:457:A:PRO:HG2	4	0.23
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG23	3	0.23
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG23	13	0.23
(1,970)	1:450:A:ILE:HG21	1:450:A:ILE:HG12	13	0.23
(1,926)	1:442:A:THR:H	1:441:A:GLN:HG2	1	0.23
(1,903)	1:438:A:LEU:HD22	1:438:A:LEU:HB3	5	0.23
(1,902)	1:438:A:LEU:HD12	1:376:A:TRP:HZ2	7	0.23
(1,890)	1:439:A:ASP:H	1:438:A:LEU:HB2	1	0.23
(1,890)	1:439:A:ASP:H	1:438:A:LEU:HB2	10	0.23
(1,890)	1:439:A:ASP:H	1:438:A:LEU:HB2	14	0.23
(1,887)	1:437:A:VAL:HG23	1:393:A:ALA:HA	17	0.23
(1,885)	1:437:A:VAL:HG13	1:393:A:ALA:HA	18	0.23
(1,876)	1:436:A:GLN:HB2	1:437:A:VAL:HG12	18	0.23
(1,871)	1:435:A:SER:HB2	1:435:A:SER:HA	10	0.23
(1,871)	1:435:A:SER:HB2	1:435:A:SER:HA	17	0.23
(1,870)	1:435:A:SER:HB3	1:435:A:SER:H	3	0.23
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB1	9	0.23
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB3	10	0.23
(1,850)	1:431:A:GLU:HG3	1:431:A:GLU:HB2	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:431:A:GLU:HG3	1:431:A:GLU:HB2	6	0.23
(1,836)	1:430:A:LEU:HD11	1:427:A:THR:HB	9	0.23
(1,836)	1:430:A:LEU:HD13	1:427:A:THR:HB	11	0.23
(1,822)	1:429:A:ARG:HA	1:429:A:ARG:HG2	15	0.23
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD22	12	0.23
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD3	15	0.23
(1,533)	1:394:A:LEU:HD23	1:403:A:ILE:HG22	4	0.23
(1,533)	1:394:A:LEU:HD23	1:403:A:ILE:HG23	5	0.23
(1,530)	1:394:A:LEU:HD23	1:397:A:TYR:HB3	18	0.23
(1,456)	1:386:A:THR:HG23	1:387:A:TYR:HB2	6	0.23
(1,454)	1:386:A:THR:HG21	1:370:A:ASN:HA	8	0.23
(1,443)	1:384:A:ASN:H	1:384:A:ASN:HB2	8	0.23
(1,429)	1:381:A:ASN:HA	1:381:A:ASN:HB2	5	0.23
(1,429)	1:381:A:ASN:HA	1:381:A:ASN:HB2	17	0.23
(1,400)	1:377:A:GLY:HA3	1:382:A:ARG:HB3	16	0.23
(1,367)	1:374:A:ARG:HB3	1:374:A:ARG:HD2	10	0.23
(1,306)	1:354:A:ILE:HD12	1:366:A:ILE:HG21	3	0.23
(1,205)	1:357:A:GLU:HB3	1:363:A:ILE:HG22	17	0.23
(1,138)	1:351:A:GLU:HG3	1:351:A:GLU:HB2	13	0.23
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD23	1	0.23
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD22	6	0.23
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	5	0.23
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	6	0.23
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	1	0.22
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	6	0.22
(1,2972)	1:435:A:SER:H	1:436:A:GLN:HG3	10	0.22
(1,2964)	1:446:A:ASP:H	1:445:A:GLU:HB3	9	0.22
(1,2952)	1:382:A:ARG:H	1:381:A:ASN:HB2	9	0.22
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD22	1	0.22
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	4	0.22
(1,2882)	1:402:A:ILE:HB	1:397:A:TYR:HD2	5	0.22
(1,2882)	1:402:A:ILE:HB	1:397:A:TYR:HD2	9	0.22
(1,2882)	1:402:A:ILE:HB	1:397:A:TYR:HD2	13	0.22
(1,2868)	1:366:A:ILE:HA	1:367:A:VAL:HB	18	0.22
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	4	0.22
(1,2850)	1:344:A:LEU:HD11	1:350:A:TYR:HD2	13	0.22
(1,2825)	1:413:A:PHE:HE2	1:366:A:ILE:HB	7	0.22
(1,2825)	1:413:A:PHE:HE2	1:366:A:ILE:HB	11	0.22
(1,2825)	1:413:A:PHE:HE2	1:366:A:ILE:HB	18	0.22
(1,2824)	1:413:A:PHE:HE2	1:411:A:LEU:HD22	1	0.22
(1,2818)	1:417:A:LYS:HG2	1:416:A:MET:HB2	3	0.22
(1,2805)	1:430:A:LEU:HD13	1:433:A:LEU:H	18	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2752)	1:392:A:ARG:H	1:392:A:ARG:HD3	9	0.22
(1,2752)	1:392:A:ARG:H	1:392:A:ARG:HD2	19	0.22
(1,2686)	1:430:A:LEU:HD11	1:430:A:LEU:HD22	15	0.22
(1,2667)	1:414:A:ARG:HA	1:414:A:ARG:HD2	12	0.22
(1,2663)	1:411:A:LEU:HD21	1:387:A:TYR:HE2	7	0.22
(1,2662)	1:411:A:LEU:HD21	1:366:A:ILE:HB	11	0.22
(1,2659)	1:366:A:ILE:HD13	1:411:A:LEU:HB3	7	0.22
(1,2656)	1:410:A:ARG:HB2	1:410:A:ARG:HD3	15	0.22
(1,2649)	1:403:A:ILE:HG22	1:364:A:PHE:HZ	4	0.22
(1,2649)	1:403:A:ILE:HG22	1:364:A:PHE:HZ	9	0.22
(1,2645)	1:402:A:ILE:HD13	1:338:A:TRP:HB3	14	0.22
(1,2637)	1:349:A:ARG:HB2	1:349:A:ARG:HA	1	0.22
(1,2637)	1:349:A:ARG:HB2	1:349:A:ARG:HA	5	0.22
(1,2637)	1:349:A:ARG:HB2	1:349:A:ARG:HA	14	0.22
(1,2637)	1:349:A:ARG:HB2	1:349:A:ARG:HA	18	0.22
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	4	0.22
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	12	0.22
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	13	0.22
(1,2567)	1:345:A:LEU:HD21	1:355:A:ARG:HA	17	0.22
(1,2557)	1:341:A:VAL:HG12	1:403:A:ILE:HD13	7	0.22
(1,2557)	1:341:A:VAL:HG12	1:403:A:ILE:HD12	13	0.22
(1,2557)	1:341:A:VAL:HG11	1:403:A:ILE:HD12	14	0.22
(1,2556)	1:341:A:VAL:HG13	1:364:A:PHE:HZ	18	0.22
(1,2539)	1:404:A:ARG:H	1:403:A:ILE:HG21	7	0.22
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD21	14	0.22
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG21	10	0.22
(1,2508)	1:434:A:GLU:H	1:434:A:GLU:HG2	7	0.22
(1,2508)	1:434:A:GLU:H	1:434:A:GLU:HG2	12	0.22
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB2	2	0.22
(1,2425)	1:440:A:GLU:H	1:440:A:GLU:HG2	18	0.22
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	10	0.22
(1,2259)	1:452:A:SER:H	1:451:A:ALA:HA	11	0.22
(1,2252)	1:442:A:THR:H	1:441:A:GLN:HB3	12	0.22
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	4	0.22
(1,2126)	1:410:A:ARG:H	1:410:A:ARG:HB3	8	0.22
(1,2126)	1:410:A:ARG:H	1:410:A:ARG:HB2	10	0.22
(1,2067)	1:365:A:ARG:H	1:355:A:ARG:HG2	8	0.22
(1,2051)	1:361:A:SER:H	1:361:A:SER:HB3	13	0.22
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD12	15	0.22
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG23	2	0.22
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG22	6	0.22
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	10	0.22
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	17	0.22
(1,1916)	1:366:A:ILE:HG22	1:411:A:LEU:HD13	4	0.22
(1,1909)	1:344:A:LEU:HD12	1:354:A:ILE:HG23	14	0.22
(1,1906)	1:451:A:ALA:HB1	1:449:A:THR:HG21	5	0.22
(1,1901)	1:433:A:LEU:HD23	1:433:A:LEU:HD12	9	0.22
(1,1894)	1:411:A:LEU:HD23	1:411:A:LEU:HD12	18	0.22
(1,1892)	1:403:A:ILE:HD13	1:402:A:ILE:HG23	10	0.22
(1,1892)	1:403:A:ILE:HD13	1:402:A:ILE:HG22	17	0.22
(1,1883)	1:393:A:ALA:HB3	1:437:A:VAL:HG22	2	0.22
(1,1883)	1:393:A:ALA:HB1	1:437:A:VAL:HG21	3	0.22
(1,1883)	1:393:A:ALA:HB1	1:437:A:VAL:HG22	9	0.22
(1,1883)	1:393:A:ALA:HB2	1:437:A:VAL:HG23	17	0.22
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB2	1	0.22
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB2	3	0.22
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB2	15	0.22
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB2	16	0.22
(1,1802)	1:336:A:LEU:HD13	1:431:A:GLU:HA	2	0.22
(1,1800)	1:336:A:LEU:HD11	1:338:A:TRP:HD1	19	0.22
(1,1795)	1:431:A:GLU:HG3	1:336:A:LEU:HD21	15	0.22
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD13	2	0.22
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD13	7	0.22
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD13	14	0.22
(1,1780)	1:337:A:LEU:HD13	1:376:A:TRP:HA	1	0.22
(1,1780)	1:337:A:LEU:HD11	1:376:A:TRP:HA	4	0.22
(1,1761)	1:340:A:TYR:HB2	1:337:A:LEU:HA	18	0.22
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD23	11	0.22
(1,1672)	1:403:A:ILE:HG23	1:405:A:LYS:H	3	0.22
(1,1626)	1:406:A:GLU:H	1:406:A:GLU:HG3	16	0.22
(1,1603)	1:357:A:GLU:HG2	1:412:A:LEU:HD13	17	0.22
(1,1571)	1:415:A:PHE:HE1	1:422:A:ILE:HD12	15	0.22
(1,1537)	1:421:A:GLU:HB2	1:418:A:THR:HG22	5	0.22
(1,1475)	1:433:A:LEU:HD23	1:434:A:GLU:H	6	0.22
(1,1452)	1:361:A:SER:H	1:360:A:GLU:HG2	16	0.22
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG22	14	0.22
(1,1442)	1:443:A:TYR:HE2	1:445:A:GLU:HG2	4	0.22
(1,1435)	1:445:A:GLU:HG3	1:445:A:GLU:HA	16	0.22
(1,1432)	1:445:A:GLU:HG2	1:445:A:GLU:HA	12	0.22
(1,1412)	1:454:A:VAL:HB	1:450:A:ILE:HA	15	0.22
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	19	0.22
(1,1372)	1:390:A:MET:HG2	1:390:A:MET:H	11	0.22
(1,1328)	1:399:A:LYS:H	1:400:A:LEU:HD12	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD23	4	0.22
(1,1267)	1:354:A:ILE:HD13	1:367:A:VAL:H	14	0.22
(1,1250)	1:345:A:LEU:HD21	1:355:A:ARG:HA	6	0.22
(1,1250)	1:345:A:LEU:HD22	1:355:A:ARG:HA	10	0.22
(1,1250)	1:345:A:LEU:HD21	1:355:A:ARG:HA	17	0.22
(1,1217)	1:359:A:LYS:HD2	1:356:A:TRP:HZ2	15	0.22
(1,1207)	1:360:A:GLU:HB2	1:360:A:GLU:HG3	3	0.22
(1,1207)	1:360:A:GLU:HB2	1:360:A:GLU:HG3	5	0.22
(1,1207)	1:360:A:GLU:HB3	1:360:A:GLU:HG2	9	0.22
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	2	0.22
(1,1179)	1:361:A:SER:HB3	1:363:A:ILE:HD13	2	0.22
(1,1179)	1:361:A:SER:HB3	1:363:A:ILE:HD12	15	0.22
(1,1175)	1:363:A:ILE:HG23	1:363:A:ILE:HG13	1	0.22
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG13	2	0.22
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG13	6	0.22
(1,1123)	1:354:A:ILE:H	1:367:A:VAL:HG23	14	0.22
(1,1102)	1:369:A:PRO:HB3	1:387:A:TYR:HD1	5	0.22
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	7	0.22
(1,1089)	1:370:A:ASN:HB3	1:370:A:ASN:HA	10	0.22
(1,1086)	1:371:A:GLY:HA3	1:374:A:ARG:HB3	3	0.22
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	1	0.22
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	4	0.22
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	7	0.22
(1,1084)	1:372:A:LEU:HD11	1:344:A:LEU:HD11	10	0.22
(1,1084)	1:372:A:LEU:HD12	1:344:A:LEU:HD12	17	0.22
(1,1077)	1:372:A:LEU:HD11	1:340:A:TYR:HD2	3	0.22
(1,1077)	1:372:A:LEU:HD12	1:340:A:TYR:HD2	12	0.22
(1,1077)	1:372:A:LEU:HD13	1:340:A:TYR:HD2	15	0.22
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD13	19	0.22
(1,1056)	1:349:A:ARG:HG2	1:350:A:TYR:HE1	3	0.22
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	7	0.22
(1,1011)	1:356:A:TRP:HH2	1:418:A:THR:HG23	12	0.22
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG22	4	0.22
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG22	10	0.22
(1,970)	1:450:A:ILE:HG22	1:450:A:ILE:HG12	1	0.22
(1,970)	1:450:A:ILE:HG23	1:450:A:ILE:HG12	2	0.22
(1,970)	1:450:A:ILE:HG23	1:450:A:ILE:HG12	6	0.22
(1,970)	1:450:A:ILE:HG22	1:450:A:ILE:HG12	7	0.22
(1,970)	1:450:A:ILE:HG21	1:450:A:ILE:HG12	8	0.22
(1,970)	1:450:A:ILE:HG21	1:450:A:ILE:HG12	14	0.22
(1,970)	1:450:A:ILE:HG23	1:450:A:ILE:HG12	16	0.22
(1,970)	1:450:A:ILE:HG22	1:450:A:ILE:HG12	18	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,937)	1:444:A:GLN:HE22	1:444:A:GLN:HG2	5	0.22
(1,937)	1:444:A:GLN:HE22	1:444:A:GLN:HG2	11	0.22
(1,923)	1:441:A:GLN:HG3	1:441:A:GLN:HB2	2	0.22
(1,903)	1:438:A:LEU:HD21	1:438:A:LEU:HB3	9	0.22
(1,903)	1:438:A:LEU:HD21	1:438:A:LEU:HB3	14	0.22
(1,902)	1:438:A:LEU:HD13	1:376:A:TRP:HZ2	11	0.22
(1,890)	1:439:A:ASP:H	1:438:A:LEU:HB2	6	0.22
(1,890)	1:439:A:ASP:H	1:438:A:LEU:HB2	12	0.22
(1,890)	1:439:A:ASP:H	1:438:A:LEU:HB2	16	0.22
(1,885)	1:437:A:VAL:HG12	1:393:A:ALA:HA	4	0.22
(1,876)	1:436:A:GLN:HB2	1:437:A:VAL:HG13	10	0.22
(1,871)	1:435:A:SER:HB2	1:435:A:SER:HA	13	0.22
(1,871)	1:435:A:SER:HB2	1:435:A:SER:HA	15	0.22
(1,871)	1:435:A:SER:HB2	1:435:A:SER:HA	16	0.22
(1,870)	1:435:A:SER:HB3	1:435:A:SER:H	1	0.22
(1,870)	1:435:A:SER:HB3	1:435:A:SER:H	2	0.22
(1,836)	1:430:A:LEU:HD12	1:427:A:THR:HB	5	0.22
(1,836)	1:430:A:LEU:HD11	1:427:A:THR:HB	6	0.22
(1,813)	1:427:A:THR:HG23	1:425:A:GLY:H	15	0.22
(1,813)	1:427:A:THR:HG22	1:425:A:GLY:H	18	0.22
(1,760)	1:338:A:TRP:HZ2	1:419:A:PRO:HA	1	0.22
(1,699)	1:413:A:PHE:HB2	1:364:A:PHE:HE2	18	0.22
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD12	5	0.22
(1,629)	1:403:A:ILE:HD13	1:415:A:PHE:HD1	2	0.22
(1,594)	1:400:A:LEU:HD23	1:426:A:ARG:HG3	8	0.22
(1,594)	1:400:A:LEU:HD22	1:426:A:ARG:HG3	14	0.22
(1,594)	1:400:A:LEU:HD21	1:426:A:ARG:HG3	17	0.22
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD3	2	0.22
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD3	11	0.22
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD3	18	0.22
(1,549)	1:396:A:HIS:HB3	1:430:A:LEU:HD21	2	0.22
(1,530)	1:394:A:LEU:HD23	1:397:A:TYR:HB3	16	0.22
(1,528)	1:394:A:LEU:HD21	1:364:A:PHE:HZ	16	0.22
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	2	0.22
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	5	0.22
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	2	0.22
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	3	0.22
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	7	0.22
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	8	0.22
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	9	0.22
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	13	0.22
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	18	0.22
(1,454)	1:386:A:THR:HG21	1:370:A:ASN:HA	2	0.22
(1,358)	1:374:A:ARG:HA	1:374:A:ARG:HD2	2	0.22
(1,309)	1:366:A:ILE:HD13	1:364:A:PHE:HZ	13	0.22
(1,309)	1:366:A:ILE:HD12	1:364:A:PHE:HZ	18	0.22
(1,268)	1:364:A:PHE:HA	1:345:A:LEU:HD22	1	0.22
(1,231)	1:359:A:LYS:HG3	1:359:A:LYS:HE2	3	0.22
(1,231)	1:359:A:LYS:HG3	1:359:A:LYS:HE2	9	0.22
(1,231)	1:359:A:LYS:HG3	1:359:A:LYS:HE2	16	0.22
(1,203)	1:357:A:GLU:HB2	1:412:A:LEU:HD23	2	0.22
(1,203)	1:357:A:GLU:HB2	1:412:A:LEU:HD22	8	0.22
(1,174)	1:354:A:ILE:HD12	1:341:A:VAL:HA	16	0.22
(1,174)	1:354:A:ILE:HD13	1:341:A:VAL:HA	19	0.22
(1,166)	1:354:A:ILE:HG21	1:372:A:LEU:HD22	15	0.22
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD21	14	0.22
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD21	16	0.22
(1,93)	1:345:A:LEU:HA	1:354:A:ILE:HG22	13	0.22
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD21	1	0.22
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD23	2	0.22
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD21	5	0.22
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD23	8	0.22
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD21	10	0.22
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD22	12	0.22
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD22	16	0.22
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD22	17	0.22
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD21	18	0.22
(1,63)	1:344:A:LEU:HA	1:347:A:ASP:HB2	12	0.22
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	15	0.22
(1,42)	1:341:A:VAL:HG21	1:415:A:PHE:HE2	9	0.22
(1,42)	1:341:A:VAL:HG22	1:415:A:PHE:HE2	19	0.22
(1,16)	1:340:A:TYR:HA	1:343:A:GLN:HB2	12	0.22
(1,15)	1:339:A:ASP:HB2	1:336:A:LEU:HB2	7	0.22
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	12	0.21
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG21	8	0.21
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	7	0.21
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	13	0.21
(1,2964)	1:446:A:ASP:H	1:445:A:GLU:HB3	17	0.21
(1,2940)	1:434:A:GLU:H	1:433:A:LEU:HB2	3	0.21
(1,2931)	1:420:A:ASP:H	1:421:A:GLU:HG3	19	0.21
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	10	0.21
(1,2871)	1:444:A:GLN:HB2	1:444:A:GLN:HG3	2	0.21
(1,2850)	1:344:A:LEU:HD12	1:350:A:TYR:HD1	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2825)	1:413:A:PHE:HE2	1:366:A:ILE:HB	5	0.21
(1,2824)	1:413:A:PHE:HE2	1:411:A:LEU:HD22	14	0.21
(1,2786)	1:431:A:GLU:H	1:431:A:GLU:HG2	8	0.21
(1,2745)	1:360:A:GLU:HA	1:359:A:LYS:HG2	14	0.21
(1,2740)	1:362:A:LYS:HG2	1:356:A:TRP:HZ3	17	0.21
(1,2705)	1:394:A:LEU:HA	1:397:A:TYR:HD1	5	0.21
(1,2686)	1:430:A:LEU:HD11	1:430:A:LEU:HD22	2	0.21
(1,2684)	1:429:A:ARG:HG2	1:433:A:LEU:HD22	6	0.21
(1,2663)	1:411:A:LEU:HD22	1:387:A:TYR:HE2	12	0.21
(1,2659)	1:366:A:ILE:HD12	1:411:A:LEU:HB3	3	0.21
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD2	4	0.21
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD2	19	0.21
(1,2655)	1:410:A:ARG:HB2	1:410:A:ARG:HD3	4	0.21
(1,2650)	1:403:A:ILE:HD11	1:338:A:TRP:HA	5	0.21
(1,2637)	1:349:A:ARG:HB2	1:349:A:ARG:HA	2	0.21
(1,2637)	1:349:A:ARG:HB2	1:349:A:ARG:HA	6	0.21
(1,2637)	1:349:A:ARG:HB2	1:349:A:ARG:HA	7	0.21
(1,2637)	1:349:A:ARG:HB2	1:349:A:ARG:HA	10	0.21
(1,2637)	1:349:A:ARG:HB2	1:349:A:ARG:HA	11	0.21
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	1	0.21
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	3	0.21
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	5	0.21
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	6	0.21
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	11	0.21
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	15	0.21
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	16	0.21
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	18	0.21
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	19	0.21
(1,2607)	1:367:A:VAL:HA	1:365:A:ARG:HD2	1	0.21
(1,2557)	1:341:A:VAL:HG11	1:403:A:ILE:HD12	4	0.21
(1,2539)	1:404:A:ARG:H	1:403:A:ILE:HG21	15	0.21
(1,2537)	1:394:A:LEU:H	1:394:A:LEU:HD11	11	0.21
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD22	17	0.21
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG23	14	0.21
(1,2508)	1:434:A:GLU:H	1:434:A:GLU:HG2	5	0.21
(1,2425)	1:440:A:GLU:H	1:440:A:GLU:HG2	1	0.21
(1,2425)	1:440:A:GLU:H	1:440:A:GLU:HG2	2	0.21
(1,2425)	1:440:A:GLU:H	1:440:A:GLU:HG2	13	0.21
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	1	0.21
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	5	0.21
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	6	0.21
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	8	0.21
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	12	0.21
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	13	0.21
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	15	0.21
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	17	0.21
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	18	0.21
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD23	6	0.21
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD21	7	0.21
(1,2276)	1:410:A:ARG:HE	1:365:A:ARG:HE	2	0.21
(1,2259)	1:452:A:SER:H	1:451:A:ALA:HA	15	0.21
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	19	0.21
(1,2150)	1:388:A:GLU:H	1:388:A:GLU:HB3	11	0.21
(1,2051)	1:361:A:SER:H	1:361:A:SER:HB3	9	0.21
(1,2051)	1:361:A:SER:H	1:361:A:SER:HB3	17	0.21
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD22	3	0.21
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD12	1	0.21
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD12	4	0.21
(1,1954)	1:399:A:LYS:H	1:399:A:LYS:HG2	16	0.21
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	3	0.21
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	18	0.21
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	19	0.21
(1,1931)	1:335:A:ARG:H	1:336:A:LEU:HB2	5	0.21
(1,1899)	1:430:A:LEU:HD11	1:400:A:LEU:HD23	19	0.21
(1,1892)	1:403:A:ILE:HD12	1:402:A:ILE:HG23	6	0.21
(1,1892)	1:403:A:ILE:HD13	1:402:A:ILE:HG22	18	0.21
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD13	8	0.21
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD12	13	0.21
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD13	19	0.21
(1,1780)	1:337:A:LEU:HD13	1:376:A:TRP:HA	15	0.21
(1,1778)	1:337:A:LEU:HD11	1:376:A:TRP:HB3	17	0.21
(1,1770)	1:394:A:LEU:HD21	1:337:A:LEU:HD12	10	0.21
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD23	12	0.21
(1,1710)	1:344:A:LEU:HD21	1:350:A:TYR:HB3	13	0.21
(1,1666)	1:403:A:ILE:HG13	1:364:A:PHE:HZ	3	0.21
(1,1659)	1:404:A:ARG:HB2	1:404:A:ARG:HD3	8	0.21
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	1	0.21
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	2	0.21
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	7	0.21
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	9	0.21
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	11	0.21
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	12	0.21
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	17	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	18	0.21
(1,1611)	1:410:A:ARG:HG3	1:410:A:ARG:H	15	0.21
(1,1603)	1:357:A:GLU:HG2	1:412:A:LEU:HD12	12	0.21
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	12	0.21
(1,1533)	1:378:A:ASN:HB2	1:375:A:LEU:HA	10	0.21
(1,1498)	1:429:A:ARG:HD2	1:429:A:ARG:HB2	18	0.21
(1,1475)	1:433:A:LEU:HD22	1:434:A:GLU:H	5	0.21
(1,1475)	1:433:A:LEU:HD21	1:434:A:GLU:H	12	0.21
(1,1475)	1:433:A:LEU:HD23	1:434:A:GLU:H	19	0.21
(1,1462)	1:435:A:SER:H	1:434:A:GLU:HB3	10	0.21
(1,1453)	1:438:A:LEU:HD11	1:435:A:SER:H	3	0.21
(1,1452)	1:361:A:SER:H	1:360:A:GLU:HG2	9	0.21
(1,1449)	1:442:A:THR:HG22	1:445:A:GLU:HB2	7	0.21
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG21	6	0.21
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	17	0.21
(1,1409)	1:435:A:SER:HB2	1:438:A:LEU:HB2	8	0.21
(1,1402)	1:383:A:THR:HG22	1:384:A:ASN:HD21	15	0.21
(1,1355)	1:395:A:ARG:HB3	1:395:A:ARG:HG2	1	0.21
(1,1340)	1:399:A:LYS:HD3	1:396:A:HIS:HA	18	0.21
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	7	0.21
(1,1267)	1:354:A:ILE:HD11	1:367:A:VAL:H	5	0.21
(1,1263)	1:354:A:ILE:HG22	1:345:A:LEU:H	19	0.21
(1,1217)	1:359:A:LYS:HD2	1:356:A:TRP:HZ2	2	0.21
(1,1217)	1:359:A:LYS:HD2	1:356:A:TRP:HZ2	4	0.21
(1,1217)	1:359:A:LYS:HD2	1:356:A:TRP:HZ2	10	0.21
(1,1217)	1:359:A:LYS:HD2	1:356:A:TRP:HZ2	16	0.21
(1,1179)	1:361:A:SER:HB3	1:363:A:ILE:HD12	6	0.21
(1,1179)	1:361:A:SER:HB3	1:363:A:ILE:HD12	12	0.21
(1,1175)	1:363:A:ILE:HG23	1:363:A:ILE:HG13	11	0.21
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG11	8	0.21
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG13	11	0.21
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG22	4	0.21
(1,1129)	1:367:A:VAL:HB	1:367:A:VAL:HG22	18	0.21
(1,1128)	1:355:A:ARG:HB3	1:367:A:VAL:HG22	14	0.21
(1,1078)	1:372:A:LEU:HD11	1:340:A:TYR:HE2	3	0.21
(1,1078)	1:372:A:LEU:HD11	1:340:A:TYR:HE2	8	0.21
(1,1078)	1:372:A:LEU:HD12	1:340:A:TYR:HE2	11	0.21
(1,1078)	1:372:A:LEU:HD13	1:340:A:TYR:HE2	17	0.21
(1,1078)	1:372:A:LEU:HD12	1:340:A:TYR:HE2	19	0.21
(1,1011)	1:356:A:TRP:HH2	1:418:A:THR:HG21	10	0.21
(1,979)	1:453:A:PRO:HG2	1:453:A:PRO:HB3	13	0.21
(1,979)	1:453:A:PRO:HG2	1:453:A:PRO:HB3	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:450:A:ILE:HG21	1:450:A:ILE:HG12	5	0.21
(1,970)	1:450:A:ILE:HG23	1:450:A:ILE:HG12	12	0.21
(1,970)	1:450:A:ILE:HG22	1:450:A:ILE:HG12	19	0.21
(1,956)	1:450:A:ILE:H	1:449:A:THR:HB	13	0.21
(1,937)	1:444:A:GLN:HE22	1:444:A:GLN:HG2	9	0.21
(1,937)	1:444:A:GLN:HE22	1:444:A:GLN:HG2	14	0.21
(1,929)	1:443:A:TYR:H	1:442:A:THR:HB	17	0.21
(1,903)	1:438:A:LEU:HD23	1:438:A:LEU:HB3	7	0.21
(1,903)	1:438:A:LEU:HD23	1:438:A:LEU:HB3	18	0.21
(1,902)	1:438:A:LEU:HD11	1:376:A:TRP:HZ2	6	0.21
(1,902)	1:438:A:LEU:HD13	1:376:A:TRP:HZ2	14	0.21
(1,888)	1:437:A:VAL:HG21	1:441:A:GLN:HE22	9	0.21
(1,885)	1:437:A:VAL:HG12	1:393:A:ALA:HA	14	0.21
(1,876)	1:436:A:GLN:HB2	1:437:A:VAL:HG13	3	0.21
(1,871)	1:435:A:SER:HB2	1:435:A:SER:HA	5	0.21
(1,871)	1:435:A:SER:HB2	1:435:A:SER:HA	9	0.21
(1,870)	1:435:A:SER:HB3	1:435:A:SER:H	10	0.21
(1,870)	1:435:A:SER:HB3	1:435:A:SER:H	12	0.21
(1,870)	1:435:A:SER:HB3	1:435:A:SER:H	13	0.21
(1,870)	1:435:A:SER:HB3	1:435:A:SER:H	17	0.21
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB2	6	0.21
(1,864)	1:433:A:LEU:HA	1:433:A:LEU:HD12	12	0.21
(1,836)	1:430:A:LEU:HD11	1:427:A:THR:HB	14	0.21
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG23	2	0.21
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG22	4	0.21
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG23	6	0.21
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG22	7	0.21
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG23	8	0.21
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG22	19	0.21
(1,800)	1:426:A:ARG:HB2	1:426:A:ARG:HG2	3	0.21
(1,760)	1:338:A:TRP:HZ2	1:419:A:PRO:HA	7	0.21
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	1	0.21
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	7	0.21
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	11	0.21
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	14	0.21
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	15	0.21
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	17	0.21
(1,713)	1:414:A:ARG:HE	1:414:A:ARG:HB3	18	0.21
(1,699)	1:413:A:PHE:HB2	1:364:A:PHE:HE2	17	0.21
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD11	15	0.21
(1,678)	1:411:A:LEU:HA	1:411:A:LEU:HD21	19	0.21
(1,650)	1:405:A:LYS:HE2	1:405:A:LYS:HG3	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,650)	1:405:A:LYS:HE2	1:405:A:LYS:HG3	13	0.21
(1,629)	1:403:A:ILE:HD13	1:415:A:PHE:HD1	15	0.21
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD3	10	0.21
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD3	12	0.21
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD3	13	0.21
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD3	14	0.21
(1,556)	1:397:A:TYR:HA	1:400:A:LEU:HB3	12	0.21
(1,533)	1:394:A:LEU:HD21	1:403:A:ILE:HG22	8	0.21
(1,533)	1:394:A:LEU:HD23	1:403:A:ILE:HG21	13	0.21
(1,530)	1:394:A:LEU:HD22	1:397:A:TYR:HB3	19	0.21
(1,528)	1:394:A:LEU:HD21	1:364:A:PHE:HZ	3	0.21
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD11	4	0.21
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	1	0.21
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	4	0.21
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	5	0.21
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	6	0.21
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	10	0.21
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	14	0.21
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	16	0.21
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	17	0.21
(1,306)	1:354:A:ILE:HD11	1:366:A:ILE:HG21	4	0.21
(1,306)	1:354:A:ILE:HD13	1:366:A:ILE:HG23	8	0.21
(1,301)	1:366:A:ILE:HG21	1:372:A:LEU:HB3	9	0.21
(1,301)	1:366:A:ILE:HG21	1:372:A:LEU:HB3	11	0.21
(1,231)	1:359:A:LYS:HG3	1:359:A:LYS:HE2	12	0.21
(1,204)	1:357:A:GLU:HB3	1:412:A:LEU:HD11	13	0.21
(1,203)	1:357:A:GLU:HB2	1:412:A:LEU:HD21	6	0.21
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	4	0.21
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	8	0.21
(1,174)	1:354:A:ILE:HD12	1:341:A:VAL:HA	13	0.21
(1,138)	1:351:A:GLU:HG3	1:351:A:GLU:HB2	3	0.21
(1,112)	1:347:A:ASP:H	1:347:A:ASP:HB3	17	0.21
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD23	6	0.21
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD23	7	0.21
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD23	4	0.21
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD22	7	0.21
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD23	9	0.21
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD21	11	0.21
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD23	14	0.21
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD23	15	0.21
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD23	19	0.21
(1,42)	1:341:A:VAL:HG21	1:415:A:PHE:HE2	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:341:A:VAL:HG23	1:415:A:PHE:HE2	18	0.21
(1,41)	1:341:A:VAL:HG22	1:364:A:PHE:HZ	13	0.21
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	18	0.2
(1,2977)	1:417:A:LYS:H	1:422:A:ILE:HG12	9	0.2
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG21	1	0.2
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG22	9	0.2
(1,2964)	1:446:A:ASP:H	1:445:A:GLU:HB3	5	0.2
(1,2958)	1:393:A:ALA:H	1:391:A:SER:HB3	8	0.2
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD21	11	0.2
(1,2890)	1:430:A:LEU:H	1:336:A:LEU:HD11	9	0.2
(1,2871)	1:445:A:GLU:HB3	1:445:A:GLU:HG2	9	0.2
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	12	0.2
(1,2825)	1:413:A:PHE:HE2	1:366:A:ILE:HB	6	0.2
(1,2797)	1:433:A:LEU:HD11	1:434:A:GLU:HA	19	0.2
(1,2794)	1:433:A:LEU:HD22	1:429:A:ARG:HD3	15	0.2
(1,2667)	1:414:A:ARG:HA	1:414:A:ARG:HD2	2	0.2
(1,2655)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	13	0.2
(1,2637)	1:349:A:ARG:HB2	1:349:A:ARG:HA	17	0.2
(1,2618)	1:375:A:LEU:HD22	1:378:A:ASN:HB2	2	0.2
(1,2612)	1:393:A:ALA:HB1	1:376:A:TRP:HZ3	9	0.2
(1,2612)	1:393:A:ALA:HB1	1:376:A:TRP:HZ3	16	0.2
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	2	0.2
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	7	0.2
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	8	0.2
(1,2607)	1:367:A:VAL:HA	1:365:A:ARG:HD2	13	0.2
(1,2587)	1:362:A:LYS:HA	1:415:A:PHE:HD2	19	0.2
(1,2567)	1:345:A:LEU:HD22	1:355:A:ARG:HA	4	0.2
(1,2567)	1:345:A:LEU:HD23	1:356:A:TRP:HA	10	0.2
(1,2556)	1:341:A:VAL:HG12	1:364:A:PHE:HZ	19	0.2
(1,2548)	1:443:A:TYR:H	1:442:A:THR:HG22	3	0.2
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD11	12	0.2
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG23	17	0.2
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD23	5	0.2
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD22	10	0.2
(1,2508)	1:434:A:GLU:H	1:434:A:GLU:HG2	15	0.2
(1,2425)	1:440:A:GLU:H	1:440:A:GLU:HG2	8	0.2
(1,2425)	1:440:A:GLU:H	1:440:A:GLU:HG2	9	0.2
(1,2425)	1:440:A:GLU:H	1:440:A:GLU:HG2	11	0.2
(1,2425)	1:440:A:GLU:H	1:440:A:GLU:HG2	14	0.2
(1,2425)	1:440:A:GLU:H	1:440:A:GLU:HG2	19	0.2
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	3	0.2
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	11	0.2
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	14	0.2
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	16	0.2
(1,2359)	1:382:A:ARG:H	1:382:A:ARG:HG3	6	0.2
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD23	1	0.2
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD23	5	0.2
(1,2324)	1:352:A:ASN:HD21	1:367:A:VAL:HG23	8	0.2
(1,2252)	1:442:A:THR:H	1:441:A:GLN:HB3	18	0.2
(1,2133)	1:383:A:THR:H	1:384:A:ASN:H	11	0.2
(1,2126)	1:410:A:ARG:H	1:410:A:ARG:HB3	11	0.2
(1,2126)	1:410:A:ARG:H	1:410:A:ARG:HB3	12	0.2
(1,2051)	1:361:A:SER:H	1:361:A:SER:HB3	1	0.2
(1,2051)	1:361:A:SER:H	1:361:A:SER:HB3	7	0.2
(1,2051)	1:361:A:SER:H	1:361:A:SER:HB3	8	0.2
(1,2051)	1:361:A:SER:H	1:361:A:SER:HB3	10	0.2
(1,2051)	1:361:A:SER:H	1:361:A:SER:HB3	16	0.2
(1,2051)	1:361:A:SER:H	1:361:A:SER:HB3	18	0.2
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD12	7	0.2
(1,1954)	1:399:A:LYS:H	1:399:A:LYS:HG2	8	0.2
(1,1931)	1:335:A:ARG:H	1:336:A:LEU:HB2	12	0.2
(1,1910)	1:354:A:ILE:HG23	1:345:A:LEU:HD23	19	0.2
(1,1909)	1:344:A:LEU:HD11	1:354:A:ILE:HG22	8	0.2
(1,1909)	1:344:A:LEU:HD11	1:354:A:ILE:HG21	13	0.2
(1,1906)	1:451:A:ALA:HB2	1:449:A:THR:HG21	12	0.2
(1,1883)	1:393:A:ALA:HB2	1:437:A:VAL:HG22	6	0.2
(1,1873)	1:383:A:THR:HG22	1:384:A:ASN:HD22	5	0.2
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB1	9	0.2
(1,1827)	1:430:A:LEU:HB3	1:430:A:LEU:HD21	7	0.2
(1,1827)	1:430:A:LEU:HB3	1:430:A:LEU:HD22	19	0.2
(1,1825)	1:418:A:THR:HB	1:419:A:PRO:HD2	5	0.2
(1,1825)	1:418:A:THR:HB	1:419:A:PRO:HD2	14	0.2
(1,1802)	1:336:A:LEU:HD13	1:431:A:GLU:HA	16	0.2
(1,1795)	1:431:A:GLU:HG3	1:336:A:LEU:HD22	2	0.2
(1,1795)	1:431:A:GLU:HG3	1:336:A:LEU:HD22	12	0.2
(1,1784)	1:337:A:LEU:HD11	1:340:A:TYR:H	4	0.2
(1,1784)	1:337:A:LEU:HD12	1:340:A:TYR:H	13	0.2
(1,1784)	1:337:A:LEU:HD13	1:340:A:TYR:H	19	0.2
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD12	19	0.2
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD12	3	0.2
(1,1781)	1:340:A:TYR:HD2	1:337:A:LEU:HD11	16	0.2
(1,1778)	1:337:A:LEU:HD11	1:376:A:TRP:HB3	13	0.2
(1,1756)	1:402:A:ILE:HB	1:397:A:TYR:HB2	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD21	16	0.2
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD11	6	0.2
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD11	14	0.2
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	3	0.2
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	4	0.2
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	5	0.2
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	6	0.2
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	8	0.2
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	10	0.2
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	13	0.2
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	14	0.2
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	15	0.2
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	16	0.2
(1,1622)	1:407:A:PRO:HG2	1:407:A:PRO:HD3	19	0.2
(1,1604)	1:365:A:ARG:HB2	1:412:A:LEU:HD11	14	0.2
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	6	0.2
(1,1505)	1:385:A:MET:HA	1:389:A:LYS:HB2	5	0.2
(1,1505)	1:385:A:MET:HA	1:389:A:LYS:HB2	7	0.2
(1,1498)	1:429:A:ARG:HD2	1:429:A:ARG:HB2	9	0.2
(1,1497)	1:429:A:ARG:HG2	1:429:A:ARG:HB3	19	0.2
(1,1488)	1:431:A:GLU:HB2	1:336:A:LEU:HD22	13	0.2
(1,1488)	1:431:A:GLU:HB2	1:336:A:LEU:HD22	16	0.2
(1,1475)	1:433:A:LEU:HD21	1:434:A:GLU:H	13	0.2
(1,1475)	1:433:A:LEU:HD23	1:434:A:GLU:H	15	0.2
(1,1470)	1:433:A:LEU:HA	1:436:A:GLN:HB2	4	0.2
(1,1462)	1:435:A:SER:H	1:434:A:GLU:HB3	9	0.2
(1,1454)	1:438:A:LEU:HD13	1:376:A:TRP:HH2	18	0.2
(1,1432)	1:445:A:GLU:HG2	1:445:A:GLU:HA	7	0.2
(1,1432)	1:445:A:GLU:HG2	1:445:A:GLU:HA	9	0.2
(1,1431)	1:448:A:PRO:HD3	1:447:A:GLU:HB3	5	0.2
(1,1427)	1:447:A:GLU:HA	1:448:A:PRO:HD3	1	0.2
(1,1412)	1:454:A:VAL:HB	1:450:A:ILE:HA	1	0.2
(1,1412)	1:454:A:VAL:HB	1:450:A:ILE:HA	14	0.2
(1,1344)	1:398:A:TYR:HD1	1:398:A:TYR:H	12	0.2
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	14	0.2
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD23	8	0.2
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD23	12	0.2
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD23	14	0.2
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD21	17	0.2
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD23	19	0.2
(1,1304)	1:376:A:TRP:HZ2	1:380:A:LYS:HE3	8	0.2
(1,1304)	1:376:A:TRP:HZ2	1:380:A:LYS:HE3	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1267)	1:354:A:ILE:HD11	1:367:A:VAL:H	19	0.2
(1,1211)	1:359:A:LYS:HG3	1:359:A:LYS:HA	17	0.2
(1,1207)	1:360:A:GLU:HB2	1:360:A:GLU:HG3	13	0.2
(1,1175)	1:363:A:ILE:HG23	1:363:A:ILE:HG13	12	0.2
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG23	19	0.2
(1,1164)	1:363:A:ILE:HG13	1:358:A:ASP:HB2	4	0.2
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	5	0.2
(1,1133)	1:367:A:VAL:HG11	1:352:A:ASN:HB3	10	0.2
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG13	7	0.2
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG12	9	0.2
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	3	0.2
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	5	0.2
(1,1084)	1:372:A:LEU:HD11	1:344:A:LEU:HD12	14	0.2
(1,1077)	1:372:A:LEU:HD12	1:340:A:TYR:HD2	9	0.2
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD11	10	0.2
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	12	0.2
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	17	0.2
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	4	0.2
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	9	0.2
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	10	0.2
(1,1026)	1:336:A:LEU:HD21	1:432:A:HIS:H	17	0.2
(1,1016)	1:338:A:TRP:HH2	1:422:A:ILE:HG21	13	0.2
(1,979)	1:453:A:PRO:HG2	1:453:A:PRO:HB3	1	0.2
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG23	14	0.2
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG21	19	0.2
(1,970)	1:450:A:ILE:HG21	1:450:A:ILE:HG12	9	0.2
(1,970)	1:450:A:ILE:HG21	1:450:A:ILE:HG12	11	0.2
(1,941)	1:447:A:GLU:H	1:446:A:ASP:HB2	14	0.2
(1,903)	1:438:A:LEU:HD23	1:438:A:LEU:HB3	19	0.2
(1,902)	1:438:A:LEU:HD12	1:376:A:TRP:HZ2	10	0.2
(1,902)	1:438:A:LEU:HD11	1:376:A:TRP:HZ2	13	0.2
(1,890)	1:439:A:ASP:H	1:438:A:LEU:HB2	9	0.2
(1,890)	1:439:A:ASP:H	1:438:A:LEU:HB2	15	0.2
(1,885)	1:437:A:VAL:HG12	1:393:A:ALA:HA	19	0.2
(1,884)	1:437:A:VAL:HG21	1:392:A:ARG:HG3	14	0.2
(1,884)	1:437:A:VAL:HG22	1:392:A:ARG:HG3	15	0.2
(1,871)	1:435:A:SER:HB2	1:435:A:SER:HA	2	0.2
(1,870)	1:435:A:SER:HB3	1:435:A:SER:H	9	0.2
(1,870)	1:435:A:SER:HB3	1:435:A:SER:H	15	0.2
(1,870)	1:435:A:SER:HB3	1:435:A:SER:H	16	0.2
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB2	17	0.2
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG22	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG21	3	0.2
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG21	10	0.2
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG21	11	0.2
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG23	12	0.2
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG22	13	0.2
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG21	15	0.2
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG21	18	0.2
(1,813)	1:427:A:THR:HG22	1:425:A:GLY:H	10	0.2
(1,800)	1:426:A:ARG:HB2	1:426:A:ARG:HG2	11	0.2
(1,800)	1:426:A:ARG:HB2	1:426:A:ARG:HG2	18	0.2
(1,760)	1:338:A:TRP:HZ2	1:419:A:PRO:HA	17	0.2
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	2	0.2
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	5	0.2
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	8	0.2
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	13	0.2
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	16	0.2
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	19	0.2
(1,699)	1:413:A:PHE:HB2	1:364:A:PHE:HE2	7	0.2
(1,666)	1:352:A:ASN:HA	1:351:A:GLU:HG2	10	0.2
(1,647)	1:405:A:LYS:HG2	1:405:A:LYS:HE3	6	0.2
(1,647)	1:405:A:LYS:HG2	1:405:A:LYS:HE3	11	0.2
(1,629)	1:403:A:ILE:HD13	1:415:A:PHE:HD1	10	0.2
(1,595)	1:400:A:LEU:HD22	1:400:A:LEU:HG	4	0.2
(1,595)	1:400:A:LEU:HD22	1:400:A:LEU:HG	5	0.2
(1,595)	1:400:A:LEU:HD22	1:400:A:LEU:HG	12	0.2
(1,595)	1:400:A:LEU:HD23	1:400:A:LEU:HG	17	0.2
(1,594)	1:400:A:LEU:HD22	1:426:A:ARG:HG3	16	0.2
(1,594)	1:400:A:LEU:HD21	1:426:A:ARG:HG3	18	0.2
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD2	9	0.2
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD2	16	0.2
(1,544)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	9	0.2
(1,544)	1:395:A:ARG:HB3	1:395:A:ARG:HD2	10	0.2
(1,544)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	11	0.2
(1,544)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	16	0.2
(1,533)	1:394:A:LEU:HD21	1:403:A:ILE:HG21	16	0.2
(1,530)	1:394:A:LEU:HD23	1:397:A:TYR:HB3	2	0.2
(1,530)	1:394:A:LEU:HD21	1:397:A:TYR:HB3	11	0.2
(1,497)	1:392:A:ARG:HA	1:392:A:ARG:HD2	18	0.2
(1,454)	1:386:A:THR:HG23	1:370:A:ASN:HA	4	0.2
(1,268)	1:364:A:PHE:HA	1:345:A:LEU:HD23	14	0.2
(1,236)	1:361:A:SER:HB3	1:358:A:ASP:HB2	8	0.2
(1,205)	1:357:A:GLU:HB3	1:363:A:ILE:HG22	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,166)	1:354:A:ILE:HG23	1:372:A:LEU:HD22	6	0.2
(1,121)	1:349:A:ARG:H	1:349:A:ARG:HB3	5	0.2
(1,121)	1:349:A:ARG:H	1:349:A:ARG:HB3	8	0.2
(1,121)	1:349:A:ARG:H	1:349:A:ARG:HB3	16	0.2
(1,121)	1:349:A:ARG:H	1:349:A:ARG:HB3	18	0.2
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD21	13	0.2
(1,88)	1:346:A:SER:HB2	1:346:A:SER:HA	19	0.2
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD21	3	0.2
(1,80)	1:344:A:LEU:HB2	1:344:A:LEU:HD21	13	0.2
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	3	0.2
(1,60)	1:344:A:LEU:H	1:343:A:GLN:HG3	8	0.2
(1,42)	1:341:A:VAL:HG21	1:415:A:PHE:HE2	8	0.2
(1,42)	1:341:A:VAL:HG23	1:415:A:PHE:HE2	12	0.2
(1,42)	1:341:A:VAL:HG22	1:415:A:PHE:HE2	17	0.2
(1,41)	1:341:A:VAL:HG23	1:364:A:PHE:HZ	3	0.2
(1,16)	1:340:A:TYR:HA	1:343:A:GLN:HB2	19	0.2
(1,5)	1:337:A:LEU:HD21	1:390:A:MET:HG3	2	0.2
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	8	0.19
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	2	0.19
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	9	0.19
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	19	0.19
(1,2972)	1:435:A:SER:H	1:436:A:GLN:HG3	17	0.19
(1,2964)	1:446:A:ASP:H	1:445:A:GLU:HB3	2	0.19
(1,2952)	1:382:A:ARG:H	1:382:A:ARG:HD3	10	0.19
(1,2940)	1:411:A:LEU:H	1:410:A:ARG:HG3	1	0.19
(1,2931)	1:420:A:ASP:H	1:421:A:GLU:HG3	4	0.19
(1,2931)	1:420:A:ASP:H	1:421:A:GLU:HG3	11	0.19
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	7	0.19
(1,2895)	1:353:A:PHE:H	1:367:A:VAL:HG22	9	0.19
(1,2882)	1:402:A:ILE:HB	1:397:A:TYR:HD2	7	0.19
(1,2871)	1:444:A:GLN:HB2	1:444:A:GLN:HG3	8	0.19
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	16	0.19
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	18	0.19
(1,2850)	1:344:A:LEU:HD12	1:350:A:TYR:HD1	6	0.19
(1,2825)	1:413:A:PHE:HE2	1:366:A:ILE:HB	14	0.19
(1,2824)	1:413:A:PHE:HE2	1:411:A:LEU:HD23	6	0.19
(1,2824)	1:413:A:PHE:HE2	1:411:A:LEU:HD23	7	0.19
(1,2800)	1:432:A:HIS:HB3	1:433:A:LEU:HD21	8	0.19
(1,2786)	1:431:A:GLU:H	1:431:A:GLU:HG2	4	0.19
(1,2758)	1:375:A:LEU:HD21	1:340:A:TYR:HE2	5	0.19
(1,2752)	1:392:A:ARG:H	1:392:A:ARG:HD3	15	0.19
(1,2752)	1:392:A:ARG:H	1:392:A:ARG:HD3	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE3	17	0.19
(1,2705)	1:394:A:LEU:HA	1:397:A:TYR:HD2	2	0.19
(1,2705)	1:394:A:LEU:HA	1:397:A:TYR:HD1	3	0.19
(1,2705)	1:394:A:LEU:HA	1:397:A:TYR:HD1	16	0.19
(1,2686)	1:430:A:LEU:HD11	1:430:A:LEU:HD21	4	0.19
(1,2686)	1:430:A:LEU:HD11	1:430:A:LEU:HD21	7	0.19
(1,2656)	1:410:A:ARG:HB2	1:410:A:ARG:HD3	5	0.19
(1,2655)	1:410:A:ARG:HB2	1:410:A:ARG:HD3	14	0.19
(1,2650)	1:403:A:ILE:HD12	1:338:A:TRP:HA	16	0.19
(1,2643)	1:402:A:ILE:HD12	1:397:A:TYR:HD1	18	0.19
(1,2637)	1:349:A:ARG:HB2	1:349:A:ARG:HA	15	0.19
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	9	0.19
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	10	0.19
(1,2610)	1:372:A:LEU:HA	1:372:A:LEU:HB3	14	0.19
(1,2567)	1:345:A:LEU:HD21	1:355:A:ARG:HA	9	0.19
(1,2548)	1:443:A:TYR:H	1:442:A:THR:HG23	1	0.19
(1,2548)	1:443:A:TYR:H	1:442:A:THR:HG22	4	0.19
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD12	4	0.19
(1,2531)	1:383:A:THR:H	1:383:A:THR:HG23	16	0.19
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD22	9	0.19
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB2	1	0.19
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	4	0.19
(1,2383)	1:397:A:TYR:H	1:397:A:TYR:HB3	19	0.19
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD23	4	0.19
(1,2067)	1:365:A:ARG:H	1:355:A:ARG:HG2	15	0.19
(1,2051)	1:361:A:SER:H	1:361:A:SER:HB3	3	0.19
(1,2051)	1:361:A:SER:H	1:361:A:SER:HB3	5	0.19
(1,2051)	1:361:A:SER:H	1:361:A:SER:HB3	11	0.19
(1,2051)	1:361:A:SER:H	1:361:A:SER:HB3	19	0.19
(1,2048)	1:361:A:SER:H	1:358:A:ASP:HB2	1	0.19
(1,2048)	1:361:A:SER:H	1:358:A:ASP:HB2	2	0.19
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD11	8	0.19
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG22	11	0.19
(1,1937)	1:341:A:VAL:H	1:340:A:TYR:HB2	9	0.19
(1,1931)	1:335:A:ARG:H	1:336:A:LEU:HB2	6	0.19
(1,1920)	1:372:A:LEU:HD12	1:366:A:ILE:HD13	18	0.19
(1,1909)	1:344:A:LEU:HD13	1:354:A:ILE:HG21	7	0.19
(1,1909)	1:344:A:LEU:HD11	1:354:A:ILE:HG23	16	0.19
(1,1903)	1:438:A:LEU:HD23	1:438:A:LEU:HD12	4	0.19
(1,1898)	1:427:A:THR:HG23	1:430:A:LEU:HD13	1	0.19
(1,1895)	1:411:A:LEU:HD21	1:366:A:ILE:HD11	12	0.19
(1,1892)	1:403:A:ILE:HD11	1:402:A:ILE:HG22	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1883)	1:393:A:ALA:HB3	1:437:A:VAL:HG21	15	0.19
(1,1876)	1:389:A:LYS:H	1:388:A:GLU:HB2	19	0.19
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB3	2	0.19
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB2	5	0.19
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB3	12	0.19
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB2	18	0.19
(1,1795)	1:431:A:GLU:HG3	1:336:A:LEU:HD22	11	0.19
(1,1795)	1:431:A:GLU:HG3	1:336:A:LEU:HD21	17	0.19
(1,1795)	1:431:A:GLU:HG3	1:336:A:LEU:HD23	19	0.19
(1,1784)	1:337:A:LEU:HD11	1:340:A:TYR:H	18	0.19
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD13	4	0.19
(1,1776)	1:337:A:LEU:HD11	1:390:A:MET:HG3	17	0.19
(1,1756)	1:402:A:ILE:HB	1:397:A:TYR:HB2	3	0.19
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD23	1	0.19
(1,1659)	1:404:A:ARG:HB2	1:404:A:ARG:HD3	2	0.19
(1,1659)	1:404:A:ARG:HB2	1:404:A:ARG:HD3	11	0.19
(1,1645)	1:404:A:ARG:HB3	1:404:A:ARG:HG3	1	0.19
(1,1645)	1:404:A:ARG:HB3	1:404:A:ARG:HG3	6	0.19
(1,1645)	1:404:A:ARG:HB3	1:404:A:ARG:HG3	17	0.19
(1,1635)	1:405:A:LYS:HG2	1:405:A:LYS:HD3	3	0.19
(1,1635)	1:405:A:LYS:HG2	1:405:A:LYS:HD3	7	0.19
(1,1635)	1:405:A:LYS:HG2	1:405:A:LYS:HD3	8	0.19
(1,1635)	1:405:A:LYS:HG2	1:405:A:LYS:HD3	13	0.19
(1,1635)	1:405:A:LYS:HG2	1:405:A:LYS:HD3	17	0.19
(1,1635)	1:405:A:LYS:HG2	1:405:A:LYS:HD3	19	0.19
(1,1626)	1:406:A:GLU:H	1:406:A:GLU:HG3	6	0.19
(1,1626)	1:406:A:GLU:H	1:406:A:GLU:HG3	10	0.19
(1,1626)	1:406:A:GLU:H	1:406:A:GLU:HG3	14	0.19
(1,1606)	1:411:A:LEU:HD13	1:369:A:PRO:HA	18	0.19
(1,1603)	1:357:A:GLU:HG2	1:412:A:LEU:HD12	8	0.19
(1,1600)	1:412:A:LEU:HD23	1:412:A:LEU:H	6	0.19
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	18	0.19
(1,1533)	1:378:A:ASN:HB2	1:375:A:LEU:HA	1	0.19
(1,1505)	1:385:A:MET:HA	1:389:A:LYS:HB2	14	0.19
(1,1505)	1:385:A:MET:HA	1:389:A:LYS:HB2	17	0.19
(1,1488)	1:431:A:GLU:HB2	1:336:A:LEU:HD22	1	0.19
(1,1486)	1:432:A:HIS:HD2	1:436:A:GLN:HB2	18	0.19
(1,1479)	1:433:A:LEU:HD13	1:393:A:ALA:HA	2	0.19
(1,1452)	1:361:A:SER:H	1:360:A:GLU:HG2	12	0.19
(1,1444)	1:442:A:THR:HG22	1:443:A:TYR:HA	9	0.19
(1,1412)	1:454:A:VAL:HB	1:450:A:ILE:HA	5	0.19
(1,1402)	1:383:A:THR:HG22	1:384:A:ASN:HD21	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1393)	1:386:A:THR:HG21	1:388:A:GLU:HB3	5	0.19
(1,1391)	1:387:A:TYR:HE1	1:369:A:PRO:HB3	17	0.19
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD21	16	0.19
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD22	17	0.19
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD21	18	0.19
(1,1313)	1:375:A:LEU:HD12	1:376:A:TRP:H	17	0.19
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	6	0.19
(1,1267)	1:354:A:ILE:HD11	1:367:A:VAL:H	7	0.19
(1,1250)	1:345:A:LEU:HD22	1:355:A:ARG:HA	4	0.19
(1,1225)	1:357:A:GLU:HG3	1:412:A:LEU:HD21	4	0.19
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	18	0.19
(1,1207)	1:360:A:GLU:HB2	1:360:A:GLU:HG3	4	0.19
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	19	0.19
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG11	1	0.19
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG12	16	0.19
(1,1102)	1:369:A:PRO:HB3	1:387:A:TYR:HD1	4	0.19
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	11	0.19
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	17	0.19
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD13	2	0.19
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD12	14	0.19
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	1	0.19
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	3	0.19
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	4	0.19
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	6	0.19
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	7	0.19
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	14	0.19
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	16	0.19
(1,1050)	1:350:A:TYR:HD2	1:350:A:TYR:HB3	12	0.19
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	1	0.19
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	14	0.19
(1,1026)	1:336:A:LEU:HD22	1:432:A:HIS:H	1	0.19
(1,1026)	1:336:A:LEU:HD23	1:432:A:HIS:H	4	0.19
(1,1026)	1:336:A:LEU:HD22	1:432:A:HIS:H	7	0.19
(1,1025)	1:336:A:LEU:HD23	1:430:A:LEU:H	8	0.19
(1,1016)	1:338:A:TRP:HH2	1:422:A:ILE:HG22	19	0.19
(1,1011)	1:356:A:TRP:HH2	1:418:A:THR:HG21	16	0.19
(1,1000)	1:409:A:GLN:HE21	1:409:A:GLN:HG2	4	0.19
(1,1000)	1:409:A:GLN:HE21	1:409:A:GLN:HG2	19	0.19
(1,979)	1:453:A:PRO:HG2	1:453:A:PRO:HB3	9	0.19
(1,978)	1:453:A:PRO:HA	1:450:A:ILE:HD13	4	0.19
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG21	1	0.19
(1,970)	1:450:A:ILE:HG22	1:450:A:ILE:HG12	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,960)	1:450:A:ILE:HA	1:450:A:ILE:HG13	3	0.19
(1,903)	1:438:A:LEU:HD21	1:438:A:LEU:HB3	11	0.19
(1,903)	1:438:A:LEU:HD23	1:438:A:LEU:HB3	16	0.19
(1,902)	1:438:A:LEU:HD12	1:376:A:TRP:HZ2	1	0.19
(1,871)	1:435:A:SER:HB2	1:435:A:SER:HA	4	0.19
(1,870)	1:435:A:SER:HB3	1:435:A:SER:H	5	0.19
(1,864)	1:433:A:LEU:HA	1:433:A:LEU:HD11	13	0.19
(1,836)	1:430:A:LEU:HD12	1:427:A:THR:HB	4	0.19
(1,836)	1:430:A:LEU:HD13	1:427:A:THR:HB	8	0.19
(1,836)	1:430:A:LEU:HD11	1:427:A:THR:HB	17	0.19
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG22	9	0.19
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG22	14	0.19
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG21	16	0.19
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG23	17	0.19
(1,813)	1:427:A:THR:HG22	1:425:A:GLY:H	17	0.19
(1,803)	1:426:A:ARG:H	1:426:A:ARG:HG2	19	0.19
(1,760)	1:338:A:TRP:HZ2	1:419:A:PRO:HA	15	0.19
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	3	0.19
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	4	0.19
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	6	0.19
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	9	0.19
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	10	0.19
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	18	0.19
(1,722)	1:414:A:ARG:HD3	1:363:A:ILE:HD11	17	0.19
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD13	19	0.19
(1,667)	1:409:A:GLN:HA	1:409:A:GLN:HG2	3	0.19
(1,603)	1:401:A:ASN:HA	1:401:A:ASN:HB2	2	0.19
(1,603)	1:401:A:ASN:HA	1:401:A:ASN:HB2	8	0.19
(1,603)	1:401:A:ASN:HA	1:401:A:ASN:HB2	9	0.19
(1,595)	1:400:A:LEU:HD23	1:400:A:LEU:HG	1	0.19
(1,595)	1:400:A:LEU:HD22	1:400:A:LEU:HG	14	0.19
(1,594)	1:400:A:LEU:HD21	1:426:A:ARG:HG3	15	0.19
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD2	8	0.19
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD2	19	0.19
(1,544)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	6	0.19
(1,533)	1:394:A:LEU:HD21	1:403:A:ILE:HG22	6	0.19
(1,533)	1:394:A:LEU:HD21	1:403:A:ILE:HG23	7	0.19
(1,530)	1:394:A:LEU:HD22	1:397:A:TYR:HB3	4	0.19
(1,528)	1:394:A:LEU:HD23	1:364:A:PHE:HZ	4	0.19
(1,528)	1:394:A:LEU:HD21	1:364:A:PHE:HZ	8	0.19
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD12	6	0.19
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD13	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD11	10	0.19
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	3	0.19
(1,469)	1:388:A:GLU:HA	1:388:A:GLU:HB2	11	0.19
(1,454)	1:386:A:THR:HG21	1:370:A:ASN:HA	7	0.19
(1,443)	1:384:A:ASN:H	1:384:A:ASN:HB2	9	0.19
(1,306)	1:354:A:ILE:HD11	1:366:A:ILE:HG22	10	0.19
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	7	0.19
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	8	0.19
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	17	0.19
(1,141)	1:352:A:ASN:HD22	1:352:A:ASN:HB3	5	0.19
(1,138)	1:351:A:GLU:HG3	1:351:A:GLU:HB2	9	0.19
(1,121)	1:349:A:ARG:H	1:349:A:ARG:HB3	1	0.19
(1,121)	1:349:A:ARG:H	1:349:A:ARG:HB3	4	0.19
(1,121)	1:349:A:ARG:H	1:349:A:ARG:HB3	9	0.19
(1,121)	1:349:A:ARG:H	1:349:A:ARG:HB3	14	0.19
(1,112)	1:347:A:ASP:H	1:347:A:ASP:HB3	13	0.19
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD21	2	0.19
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD22	5	0.19
(1,88)	1:346:A:SER:HB2	1:346:A:SER:HA	4	0.19
(1,49)	1:341:A:VAL:HG21	1:342:A:TYR:HA	6	0.19
(1,49)	1:341:A:VAL:HG23	1:342:A:TYR:HA	10	0.19
(1,42)	1:341:A:VAL:HG22	1:415:A:PHE:HE2	3	0.19
(1,42)	1:341:A:VAL:HG21	1:415:A:PHE:HE2	5	0.19
(1,41)	1:341:A:VAL:HG23	1:364:A:PHE:HZ	1	0.19
(1,41)	1:341:A:VAL:HG22	1:364:A:PHE:HZ	5	0.19
(1,41)	1:341:A:VAL:HG22	1:364:A:PHE:HZ	6	0.19
(1,41)	1:341:A:VAL:HG22	1:364:A:PHE:HZ	7	0.19
(1,41)	1:341:A:VAL:HG22	1:364:A:PHE:HZ	9	0.19
(1,41)	1:341:A:VAL:HG21	1:364:A:PHE:HZ	10	0.19
(1,41)	1:341:A:VAL:HG21	1:364:A:PHE:HZ	12	0.19
(1,41)	1:341:A:VAL:HG21	1:364:A:PHE:HZ	14	0.19
(1,37)	1:341:A:VAL:HG11	1:341:A:VAL:HG21	14	0.19
(1,37)	1:341:A:VAL:HG12	1:341:A:VAL:HG23	19	0.19
(1,15)	1:339:A:ASP:HB3	1:336:A:LEU:HB2	13	0.19
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	1	0.18
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	13	0.18
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG22	6	0.18
(1,2974)	1:433:A:LEU:H	1:436:A:GLN:HB2	17	0.18
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	18	0.18
(1,2945)	1:364:A:PHE:H	1:412:A:LEU:HG	12	0.18
(1,2940)	1:434:A:GLU:H	1:433:A:LEU:HB2	10	0.18
(1,2882)	1:402:A:ILE:HB	1:397:A:TYR:HD2	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2871)	1:445:A:GLU:HG3	1:445:A:GLU:HB3	14	0.18
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	7	0.18
(1,2850)	1:344:A:LEU:HD11	1:350:A:TYR:HD1	5	0.18
(1,2845)	1:402:A:ILE:HD12	1:338:A:TRP:HB2	9	0.18
(1,2844)	1:402:A:ILE:HG21	1:397:A:TYR:HD2	1	0.18
(1,2825)	1:413:A:PHE:HE2	1:366:A:ILE:HB	2	0.18
(1,2825)	1:413:A:PHE:HE2	1:366:A:ILE:HB	12	0.18
(1,2824)	1:413:A:PHE:HE2	1:411:A:LEU:HD22	2	0.18
(1,2811)	1:423:A:MET:HA	1:423:A:MET:HB2	5	0.18
(1,2811)	1:423:A:MET:HA	1:423:A:MET:HB2	7	0.18
(1,2811)	1:423:A:MET:HA	1:423:A:MET:HB2	9	0.18
(1,2811)	1:423:A:MET:HA	1:423:A:MET:HB2	10	0.18
(1,2811)	1:423:A:MET:HA	1:423:A:MET:HB2	13	0.18
(1,2752)	1:392:A:ARG:H	1:392:A:ARG:HD3	1	0.18
(1,2740)	1:362:A:LYS:HG2	1:356:A:TRP:HZ3	1	0.18
(1,2721)	1:354:A:ILE:HD13	1:372:A:LEU:HD22	14	0.18
(1,2707)	1:349:A:ARG:HG3	1:350:A:TYR:HD2	14	0.18
(1,2705)	1:394:A:LEU:HA	1:397:A:TYR:HD1	14	0.18
(1,2686)	1:430:A:LEU:HD13	1:430:A:LEU:HD22	10	0.18
(1,2675)	1:417:A:LYS:HD2	1:402:A:ILE:HG13	8	0.18
(1,2656)	1:410:A:ARG:HG3	1:410:A:ARG:HD2	14	0.18
(1,2656)	1:410:A:ARG:HB2	1:410:A:ARG:HD3	18	0.18
(1,2655)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	7	0.18
(1,2649)	1:403:A:ILE:HG23	1:364:A:PHE:HZ	10	0.18
(1,2643)	1:402:A:ILE:HD11	1:397:A:TYR:HD1	10	0.18
(1,2610)	1:372:A:LEU:HA	1:375:A:LEU:HG	17	0.18
(1,2603)	1:368:A:ASP:H	1:366:A:ILE:HA	12	0.18
(1,2597)	1:358:A:ASP:HB2	1:363:A:ILE:HG23	4	0.18
(1,2597)	1:358:A:ASP:HB2	1:363:A:ILE:HG22	12	0.18
(1,2597)	1:358:A:ASP:HB2	1:363:A:ILE:HG22	16	0.18
(1,2596)	1:363:A:ILE:HG21	1:364:A:PHE:HA	13	0.18
(1,2567)	1:345:A:LEU:HD21	1:355:A:ARG:HA	15	0.18
(1,2553)	1:454:A:VAL:H	1:454:A:VAL:HG22	9	0.18
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD12	2	0.18
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD11	14	0.18
(1,2537)	1:394:A:LEU:H	1:394:A:LEU:HD11	19	0.18
(1,2535)	1:392:A:ARG:H	1:437:A:VAL:HG21	8	0.18
(1,2531)	1:383:A:THR:H	1:383:A:THR:HG21	13	0.18
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD23	7	0.18
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG23	18	0.18
(1,2499)	1:421:A:GLU:H	1:420:A:ASP:HB2	11	0.18
(1,2425)	1:440:A:GLU:H	1:440:A:GLU:HG2	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2418)	1:444:A:GLN:H	1:441:A:GLN:HG2	2	0.18
(1,2406)	1:383:A:THR:H	1:382:A:ARG:HG2	8	0.18
(1,2405)	1:384:A:ASN:H	1:385:A:MET:HB2	15	0.18
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	14	0.18
(1,2216)	1:408:A:GLY:H	1:409:A:GLN:HG2	13	0.18
(1,2199)	1:412:A:LEU:H	1:412:A:LEU:HD12	13	0.18
(1,2158)	1:382:A:ARG:H	1:377:A:GLY:HA3	16	0.18
(1,2122)	1:410:A:ARG:H	1:409:A:GLN:HG2	15	0.18
(1,1984)	1:350:A:TYR:H	1:349:A:ARG:HG2	19	0.18
(1,1920)	1:372:A:LEU:HD12	1:366:A:ILE:HD11	3	0.18
(1,1910)	1:354:A:ILE:HG22	1:345:A:LEU:HD22	13	0.18
(1,1910)	1:354:A:ILE:HG22	1:345:A:LEU:HD21	17	0.18
(1,1903)	1:438:A:LEU:HD23	1:438:A:LEU:HD13	10	0.18
(1,1901)	1:433:A:LEU:HD23	1:433:A:LEU:HD12	15	0.18
(1,1883)	1:393:A:ALA:HB2	1:437:A:VAL:HG23	14	0.18
(1,1883)	1:393:A:ALA:HB3	1:437:A:VAL:HG23	18	0.18
(1,1882)	1:393:A:ALA:HB3	1:437:A:VAL:HG13	15	0.18
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB1	6	0.18
(1,1827)	1:430:A:LEU:HB3	1:430:A:LEU:HD23	8	0.18
(1,1825)	1:418:A:THR:HB	1:419:A:PRO:HD2	1	0.18
(1,1795)	1:431:A:GLU:HG3	1:336:A:LEU:HD21	14	0.18
(1,1787)	1:376:A:TRP:HZ2	1:337:A:LEU:HD21	8	0.18
(1,1783)	1:376:A:TRP:HZ2	1:337:A:LEU:HD12	6	0.18
(1,1780)	1:337:A:LEU:HD13	1:376:A:TRP:HA	14	0.18
(1,1780)	1:337:A:LEU:HD11	1:376:A:TRP:HA	16	0.18
(1,1709)	1:344:A:LEU:HD21	1:345:A:LEU:H	11	0.18
(1,1672)	1:403:A:ILE:HG23	1:405:A:LYS:H	2	0.18
(1,1672)	1:403:A:ILE:HG22	1:405:A:LYS:H	17	0.18
(1,1666)	1:403:A:ILE:HG13	1:364:A:PHE:HZ	1	0.18
(1,1666)	1:403:A:ILE:HG13	1:364:A:PHE:HZ	12	0.18
(1,1653)	1:404:A:ARG:HG2	1:414:A:ARG:HD3	3	0.18
(1,1637)	1:405:A:LYS:HE3	1:405:A:LYS:HG3	9	0.18
(1,1626)	1:406:A:GLU:H	1:406:A:GLU:HG3	3	0.18
(1,1603)	1:357:A:GLU:HG2	1:412:A:LEU:HD13	3	0.18
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	11	0.18
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	14	0.18
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	17	0.18
(1,1533)	1:378:A:ASN:HB2	1:375:A:LEU:HA	6	0.18
(1,1512)	1:424:A:SER:HA	1:424:A:SER:HB2	10	0.18
(1,1505)	1:385:A:MET:HA	1:389:A:LYS:HB2	1	0.18
(1,1497)	1:429:A:ARG:HG2	1:429:A:ARG:HB3	18	0.18
(1,1480)	1:412:A:LEU:HD23	1:357:A:GLU:HG2	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1456)	1:436:A:GLN:HB2	1:433:A:LEU:HD12	17	0.18
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG23	5	0.18
(1,1412)	1:454:A:VAL:HB	1:450:A:ILE:HA	13	0.18
(1,1372)	1:390:A:MET:HG2	1:390:A:MET:H	17	0.18
(1,1372)	1:390:A:MET:HG2	1:390:A:MET:H	19	0.18
(1,1370)	1:390:A:MET:HA	1:438:A:LEU:HD22	10	0.18
(1,1340)	1:399:A:LYS:HD3	1:396:A:HIS:HA	15	0.18
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	5	0.18
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD21	1	0.18
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD23	5	0.18
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD21	13	0.18
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD22	16	0.18
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	12	0.18
(1,1250)	1:345:A:LEU:HD21	1:355:A:ARG:HA	9	0.18
(1,1224)	1:363:A:ILE:HG21	1:357:A:GLU:HG2	2	0.18
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	19	0.18
(1,1217)	1:359:A:LYS:HD2	1:356:A:TRP:HZ2	7	0.18
(1,1217)	1:359:A:LYS:HD2	1:356:A:TRP:HZ2	18	0.18
(1,1207)	1:360:A:GLU:HB3	1:360:A:GLU:HG2	6	0.18
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD12	18	0.18
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG23	10	0.18
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG22	16	0.18
(1,1126)	1:355:A:ARG:HD3	1:367:A:VAL:HG22	9	0.18
(1,1126)	1:355:A:ARG:HD3	1:367:A:VAL:HG22	17	0.18
(1,1118)	1:367:A:VAL:HG21	1:366:A:ILE:HA	8	0.18
(1,1118)	1:367:A:VAL:HG21	1:366:A:ILE:HA	15	0.18
(1,1086)	1:371:A:GLY:HA3	1:374:A:ARG:HB2	4	0.18
(1,1077)	1:372:A:LEU:HD12	1:340:A:TYR:HD2	2	0.18
(1,1077)	1:372:A:LEU:HD12	1:340:A:TYR:HD2	14	0.18
(1,1077)	1:372:A:LEU:HD13	1:340:A:TYR:HD2	17	0.18
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD13	11	0.18
(1,1064)	1:352:A:ASN:HB3	1:352:A:ASN:HA	10	0.18
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	16	0.18
(1,1025)	1:336:A:LEU:HD21	1:430:A:LEU:H	14	0.18
(1,1025)	1:336:A:LEU:HD23	1:430:A:LEU:H	19	0.18
(1,1000)	1:409:A:GLN:HE21	1:409:A:GLN:HG2	9	0.18
(1,978)	1:453:A:PRO:HA	1:450:A:ILE:HD11	6	0.18
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG21	16	0.18
(1,970)	1:450:A:ILE:HG22	1:450:A:ILE:HG12	17	0.18
(1,960)	1:450:A:ILE:HA	1:450:A:ILE:HG13	13	0.18
(1,956)	1:450:A:ILE:H	1:449:A:THR:HB	1	0.18
(1,937)	1:444:A:GLN:HE22	1:444:A:GLN:HG2	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,903)	1:438:A:LEU:HD22	1:438:A:LEU:HB3	1	0.18
(1,887)	1:437:A:VAL:HG22	1:393:A:ALA:HA	19	0.18
(1,885)	1:437:A:VAL:HG13	1:393:A:ALA:HA	9	0.18
(1,884)	1:437:A:VAL:HG23	1:392:A:ARG:HG3	2	0.18
(1,884)	1:437:A:VAL:HG21	1:392:A:ARG:HG3	5	0.18
(1,872)	1:436:A:GLN:H	1:435:A:SER:HB2	14	0.18
(1,870)	1:435:A:SER:HB3	1:435:A:SER:H	4	0.18
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB1	1	0.18
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB2	11	0.18
(1,864)	1:433:A:LEU:HA	1:433:A:LEU:HD11	8	0.18
(1,864)	1:433:A:LEU:HA	1:433:A:LEU:HD11	19	0.18
(1,822)	1:429:A:ARG:HA	1:429:A:ARG:HG2	5	0.18
(1,815)	1:418:A:THR:HB	1:418:A:THR:HG23	5	0.18
(1,813)	1:427:A:THR:HG23	1:425:A:GLY:H	11	0.18
(1,813)	1:427:A:THR:HG23	1:425:A:GLY:H	16	0.18
(1,794)	1:423:A:MET:H	1:423:A:MET:HG2	13	0.18
(1,791)	1:428:A:ASP:HA	1:428:A:ASP:HB3	16	0.18
(1,760)	1:338:A:TRP:HZ2	1:419:A:PRO:HA	6	0.18
(1,760)	1:338:A:TRP:HZ2	1:419:A:PRO:HA	13	0.18
(1,730)	1:415:A:PHE:HB2	1:415:A:PHE:HD1	12	0.18
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD11	2	0.18
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD12	16	0.18
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD12	17	0.18
(1,678)	1:411:A:LEU:HA	1:411:A:LEU:HD22	15	0.18
(1,678)	1:411:A:LEU:HA	1:411:A:LEU:HD21	16	0.18
(1,603)	1:401:A:ASN:HA	1:401:A:ASN:HB2	13	0.18
(1,603)	1:401:A:ASN:HA	1:401:A:ASN:HB2	15	0.18
(1,590)	1:400:A:LEU:HD12	1:397:A:TYR:HE1	1	0.18
(1,556)	1:397:A:TYR:HA	1:400:A:LEU:HB3	5	0.18
(1,533)	1:394:A:LEU:HD23	1:403:A:ILE:HG22	9	0.18
(1,533)	1:394:A:LEU:HD21	1:403:A:ILE:HG22	14	0.18
(1,530)	1:394:A:LEU:HD23	1:397:A:TYR:HB3	14	0.18
(1,528)	1:394:A:LEU:HD21	1:364:A:PHE:HZ	2	0.18
(1,528)	1:394:A:LEU:HD22	1:364:A:PHE:HZ	15	0.18
(1,478)	1:389:A:LYS:HG3	1:389:A:LYS:HE2	10	0.18
(1,455)	1:386:A:THR:HG23	1:389:A:LYS:HE3	3	0.18
(1,443)	1:384:A:ASN:H	1:384:A:ASN:HB2	14	0.18
(1,400)	1:377:A:GLY:HA3	1:382:A:ARG:HB3	5	0.18
(1,364)	1:374:A:ARG:HA	1:374:A:ARG:HG3	9	0.18
(1,359)	1:374:A:ARG:HA	1:374:A:ARG:HB3	16	0.18
(1,301)	1:366:A:ILE:HG22	1:372:A:LEU:HB3	7	0.18
(1,268)	1:364:A:PHE:HA	1:345:A:LEU:HD22	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,266)	1:363:A:ILE:HG23	1:406:A:GLU:HG2	13	0.18
(1,215)	1:359:A:LYS:HA	1:359:A:LYS:HG2	6	0.18
(1,203)	1:357:A:GLU:HB2	1:412:A:LEU:HD22	7	0.18
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	1	0.18
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	2	0.18
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	5	0.18
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	6	0.18
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	9	0.18
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	10	0.18
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	11	0.18
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	12	0.18
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	13	0.18
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	15	0.18
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	16	0.18
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	18	0.18
(1,177)	1:345:A:LEU:HD11	1:354:A:ILE:HD12	5	0.18
(1,121)	1:349:A:ARG:H	1:349:A:ARG:HB3	10	0.18
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD23	11	0.18
(1,85)	1:344:A:LEU:HD22	1:350:A:TYR:HD1	16	0.18
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	10	0.18
(1,49)	1:341:A:VAL:HG21	1:342:A:TYR:HA	4	0.18
(1,49)	1:341:A:VAL:HG21	1:342:A:TYR:HA	13	0.18
(1,49)	1:341:A:VAL:HG21	1:342:A:TYR:HA	16	0.18
(1,49)	1:341:A:VAL:HG23	1:342:A:TYR:HA	18	0.18
(1,42)	1:341:A:VAL:HG23	1:415:A:PHE:HE2	14	0.18
(1,42)	1:341:A:VAL:HG21	1:415:A:PHE:HE2	15	0.18
(1,41)	1:341:A:VAL:HG21	1:364:A:PHE:HZ	2	0.18
(1,41)	1:341:A:VAL:HG22	1:364:A:PHE:HZ	4	0.18
(1,41)	1:341:A:VAL:HG22	1:364:A:PHE:HZ	8	0.18
(1,41)	1:341:A:VAL:HG21	1:364:A:PHE:HZ	11	0.18
(1,41)	1:341:A:VAL:HG21	1:364:A:PHE:HZ	18	0.18
(1,37)	1:341:A:VAL:HG11	1:341:A:VAL:HG23	3	0.18
(1,37)	1:341:A:VAL:HG12	1:341:A:VAL:HG23	17	0.18
(1,34)	1:341:A:VAL:HG12	1:337:A:LEU:HG	17	0.18
(1,15)	1:339:A:ASP:HB3	1:336:A:LEU:HB2	18	0.18
(1,5)	1:337:A:LEU:HD22	1:390:A:MET:HG3	8	0.18
(1,2992)	1:395:A:ARG:H	1:393:A:ALA:HB2	5	0.17
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	3	0.17
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	11	0.17
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG22	15	0.17
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	3	0.17
(1,2964)	1:446:A:ASP:H	1:445:A:GLU:HB3	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2964)	1:446:A:ASP:H	1:445:A:GLU:HB3	8	0.17
(1,2962)	1:454:A:VAL:H	1:450:A:ILE:HG22	8	0.17
(1,2957)	1:394:A:LEU:H	1:396:A:HIS:HD2	3	0.17
(1,2952)	1:382:A:ARG:H	1:381:A:ASN:HB2	7	0.17
(1,2952)	1:382:A:ARG:H	1:382:A:ARG:HD3	8	0.17
(1,2940)	1:434:A:GLU:H	1:433:A:LEU:HB2	11	0.17
(1,2918)	1:374:A:ARG:H	1:376:A:TRP:H	18	0.17
(1,2882)	1:402:A:ILE:HB	1:397:A:TYR:HD2	4	0.17
(1,2871)	1:444:A:GLN:HB2	1:444:A:GLN:HG3	15	0.17
(1,2871)	1:444:A:GLN:HB2	1:444:A:GLN:HG3	18	0.17
(1,2844)	1:402:A:ILE:HG21	1:397:A:TYR:HD2	6	0.17
(1,2838)	1:392:A:ARG:HG2	1:392:A:ARG:HD3	18	0.17
(1,2825)	1:413:A:PHE:HE2	1:366:A:ILE:HB	19	0.17
(1,2811)	1:423:A:MET:HA	1:423:A:MET:HB2	8	0.17
(1,2811)	1:428:A:ASP:HA	1:431:A:GLU:HB2	11	0.17
(1,2791)	1:438:A:LEU:HD21	1:385:A:MET:HG2	9	0.17
(1,2786)	1:445:A:GLU:HG3	1:446:A:ASP:H	16	0.17
(1,2758)	1:375:A:LEU:HD22	1:340:A:TYR:HE2	14	0.17
(1,2728)	1:366:A:ILE:HB	1:413:A:PHE:HZ	15	0.17
(1,2725)	1:367:A:VAL:HG21	1:365:A:ARG:HB3	2	0.17
(1,2721)	1:354:A:ILE:HD11	1:372:A:LEU:HD23	7	0.17
(1,2707)	1:349:A:ARG:HG3	1:350:A:TYR:HD2	16	0.17
(1,2686)	1:430:A:LEU:HD12	1:430:A:LEU:HD23	8	0.17
(1,2686)	1:430:A:LEU:HD11	1:430:A:LEU:HD23	13	0.17
(1,2686)	1:430:A:LEU:HD12	1:430:A:LEU:HD22	19	0.17
(1,2667)	1:414:A:ARG:HA	1:414:A:ARG:HD2	18	0.17
(1,2662)	1:411:A:LEU:HD21	1:366:A:ILE:HB	13	0.17
(1,2662)	1:411:A:LEU:HD23	1:366:A:ILE:HB	15	0.17
(1,2659)	1:366:A:ILE:HD12	1:411:A:LEU:HB3	5	0.17
(1,2637)	1:349:A:ARG:HB2	1:349:A:ARG:HA	3	0.17
(1,2603)	1:368:A:ASP:H	1:366:A:ILE:HA	16	0.17
(1,2580)	1:359:A:LYS:HA	1:359:A:LYS:HB3	14	0.17
(1,2555)	1:340:A:TYR:HA	1:343:A:GLN:HG2	19	0.17
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD12	15	0.17
(1,2539)	1:404:A:ARG:H	1:403:A:ILE:HG22	13	0.17
(1,2537)	1:394:A:LEU:H	1:394:A:LEU:HD12	12	0.17
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD21	16	0.17
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG23	11	0.17
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD22	2	0.17
(1,2516)	1:342:A:TYR:H	1:341:A:VAL:HG21	4	0.17
(1,2499)	1:421:A:GLU:H	1:420:A:ASP:HB2	3	0.17
(1,2425)	1:440:A:GLU:H	1:440:A:GLU:HG2	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2425)	1:440:A:GLU:H	1:440:A:GLU:HG2	17	0.17
(1,2418)	1:444:A:GLN:H	1:441:A:GLN:HG3	6	0.17
(1,2412)	1:451:A:ALA:H	1:456:A:TRP:HZ2	7	0.17
(1,2406)	1:383:A:THR:H	1:382:A:ARG:HG2	2	0.17
(1,2406)	1:383:A:THR:H	1:382:A:ARG:HG2	3	0.17
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD21	9	0.17
(1,2324)	1:352:A:ASN:HD21	1:367:A:VAL:HG21	4	0.17
(1,2259)	1:452:A:SER:H	1:451:A:ALA:HA	9	0.17
(1,2230)	1:417:A:LYS:H	1:415:A:PHE:HB2	12	0.17
(1,2199)	1:412:A:LEU:H	1:412:A:LEU:HD12	11	0.17
(1,2199)	1:412:A:LEU:H	1:412:A:LEU:HD13	12	0.17
(1,2141)	1:385:A:MET:H	1:384:A:ASN:H	7	0.17
(1,2126)	1:410:A:ARG:H	1:410:A:ARG:HB3	13	0.17
(1,2090)	1:371:A:GLY:H	1:370:A:ASN:HB2	3	0.17
(1,2067)	1:365:A:ARG:H	1:355:A:ARG:HG2	6	0.17
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD11	16	0.17
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG22	3	0.17
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG23	18	0.17
(1,1954)	1:399:A:LYS:H	1:399:A:LYS:HG2	19	0.17
(1,1920)	1:372:A:LEU:HD11	1:366:A:ILE:HD12	1	0.17
(1,1916)	1:366:A:ILE:HG23	1:411:A:LEU:HD13	18	0.17
(1,1909)	1:344:A:LEU:HD12	1:354:A:ILE:HG21	15	0.17
(1,1901)	1:433:A:LEU:HD21	1:433:A:LEU:HD11	17	0.17
(1,1883)	1:393:A:ALA:HB2	1:437:A:VAL:HG23	11	0.17
(1,1882)	1:393:A:ALA:HB2	1:437:A:VAL:HG12	4	0.17
(1,1882)	1:393:A:ALA:HB1	1:437:A:VAL:HG13	9	0.17
(1,1873)	1:383:A:THR:HG22	1:384:A:ASN:HD22	16	0.17
(1,1868)	1:376:A:TRP:HZ2	1:434:A:GLU:HG3	8	0.17
(1,1862)	1:434:A:GLU:HG2	1:434:A:GLU:HA	10	0.17
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB3	4	0.17
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB2	8	0.17
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB1	19	0.17
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	1	0.17
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	2	0.17
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	3	0.17
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	6	0.17
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	7	0.17
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	8	0.17
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	9	0.17
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	10	0.17
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	11	0.17
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	13	0.17
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	14	0.17
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	16	0.17
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	17	0.17
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	18	0.17
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	19	0.17
(1,1827)	1:430:A:LEU:HB3	1:430:A:LEU:HD23	13	0.17
(1,1820)	1:392:A:ARG:HB3	1:392:A:ARG:HA	16	0.17
(1,1795)	1:431:A:GLU:HG3	1:336:A:LEU:HD23	10	0.17
(1,1780)	1:337:A:LEU:HD13	1:376:A:TRP:HA	8	0.17
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	3	0.17
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	6	0.17
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	7	0.17
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD11	16	0.17
(1,1672)	1:403:A:ILE:HG22	1:405:A:LYS:H	5	0.17
(1,1666)	1:403:A:ILE:HG13	1:364:A:PHE:HZ	17	0.17
(1,1659)	1:404:A:ARG:HB2	1:404:A:ARG:HD3	7	0.17
(1,1659)	1:404:A:ARG:HB2	1:404:A:ARG:HD3	15	0.17
(1,1635)	1:405:A:LYS:HG2	1:405:A:LYS:HD3	9	0.17
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	5	0.17
(1,1604)	1:365:A:ARG:HB2	1:412:A:LEU:HD11	5	0.17
(1,1604)	1:365:A:ARG:HB2	1:412:A:LEU:HD12	11	0.17
(1,1604)	1:365:A:ARG:HB2	1:412:A:LEU:HD12	13	0.17
(1,1600)	1:412:A:LEU:HD21	1:412:A:LEU:H	9	0.17
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	2	0.17
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	15	0.17
(1,1533)	1:378:A:ASN:HB2	1:375:A:LEU:HA	4	0.17
(1,1533)	1:378:A:ASN:HB2	1:375:A:LEU:HA	16	0.17
(1,1502)	1:422:A:ILE:HA	1:427:A:THR:HG23	16	0.17
(1,1488)	1:431:A:GLU:HB2	1:336:A:LEU:HD23	8	0.17
(1,1480)	1:412:A:LEU:HD21	1:357:A:GLU:HG2	13	0.17
(1,1461)	1:435:A:SER:H	1:435:A:SER:HB2	19	0.17
(1,1447)	1:442:A:THR:HB	1:442:A:THR:HG22	19	0.17
(1,1432)	1:445:A:GLU:HG2	1:445:A:GLU:HA	1	0.17
(1,1432)	1:445:A:GLU:HG2	1:445:A:GLU:HA	15	0.17
(1,1427)	1:447:A:GLU:HA	1:448:A:PRO:HD3	13	0.17
(1,1372)	1:390:A:MET:HG2	1:390:A:MET:H	9	0.17
(1,1344)	1:398:A:TYR:HD1	1:398:A:TYR:H	8	0.17
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	9	0.17
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	11	0.17
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	16	0.17
(1,1332)	1:399:A:LYS:HA	1:399:A:LYS:HE2	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD22	6	0.17
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD23	11	0.17
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	8	0.17
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	13	0.17
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	19	0.17
(1,1267)	1:354:A:ILE:HD12	1:367:A:VAL:H	3	0.17
(1,1267)	1:354:A:ILE:HD11	1:367:A:VAL:H	10	0.17
(1,1267)	1:354:A:ILE:HD11	1:367:A:VAL:H	11	0.17
(1,1267)	1:354:A:ILE:HD11	1:367:A:VAL:H	15	0.17
(1,1267)	1:354:A:ILE:HD13	1:367:A:VAL:H	17	0.17
(1,1265)	1:354:A:ILE:HG22	1:355:A:ARG:H	9	0.17
(1,1265)	1:354:A:ILE:HG22	1:355:A:ARG:H	15	0.17
(1,1250)	1:345:A:LEU:HD21	1:355:A:ARG:HA	15	0.17
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	15	0.17
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	16	0.17
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD12	17	0.17
(1,1142)	1:450:A:ILE:HD11	1:454:A:VAL:HA	6	0.17
(1,1134)	1:367:A:VAL:HG11	1:354:A:ILE:H	10	0.17
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG12	12	0.17
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG13	13	0.17
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG12	17	0.17
(1,1128)	1:355:A:ARG:HB3	1:367:A:VAL:HG23	15	0.17
(1,1128)	1:355:A:ARG:HB3	1:367:A:VAL:HG21	18	0.17
(1,1118)	1:367:A:VAL:HG22	1:366:A:ILE:HA	4	0.17
(1,1118)	1:367:A:VAL:HG22	1:366:A:ILE:HA	18	0.17
(1,1078)	1:372:A:LEU:HD11	1:340:A:TYR:HE2	16	0.17
(1,1077)	1:372:A:LEU:HD13	1:340:A:TYR:HD2	6	0.17
(1,1000)	1:409:A:GLN:HE21	1:409:A:GLN:HG2	5	0.17
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG22	6	0.17
(1,960)	1:450:A:ILE:HA	1:450:A:ILE:HG13	17	0.17
(1,959)	1:449:A:THR:HG23	1:449:A:THR:HB	5	0.17
(1,959)	1:449:A:THR:HG21	1:449:A:THR:HB	9	0.17
(1,959)	1:449:A:THR:HG23	1:449:A:THR:HB	18	0.17
(1,956)	1:450:A:ILE:H	1:449:A:THR:HB	9	0.17
(1,947)	1:447:A:GLU:HG2	1:447:A:GLU:HA	4	0.17
(1,947)	1:447:A:GLU:HG2	1:447:A:GLU:HA	9	0.17
(1,941)	1:447:A:GLU:H	1:446:A:ASP:HB2	11	0.17
(1,930)	1:443:A:TYR:HA	1:443:A:TYR:HB3	17	0.17
(1,903)	1:438:A:LEU:HD21	1:438:A:LEU:HB3	3	0.17
(1,903)	1:438:A:LEU:HD23	1:438:A:LEU:HB3	6	0.17
(1,903)	1:438:A:LEU:HD21	1:438:A:LEU:HB3	12	0.17
(1,902)	1:438:A:LEU:HD11	1:376:A:TRP:HZ2	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,902)	1:438:A:LEU:HD11	1:376:A:TRP:HZ2	16	0.17
(1,885)	1:437:A:VAL:HG11	1:393:A:ALA:HA	5	0.17
(1,885)	1:437:A:VAL:HG12	1:393:A:ALA:HA	8	0.17
(1,884)	1:437:A:VAL:HG22	1:392:A:ARG:HG3	3	0.17
(1,884)	1:437:A:VAL:HG23	1:392:A:ARG:HG3	7	0.17
(1,884)	1:437:A:VAL:HG21	1:392:A:ARG:HG3	8	0.17
(1,884)	1:437:A:VAL:HG22	1:392:A:ARG:HG3	13	0.17
(1,864)	1:433:A:LEU:HA	1:433:A:LEU:HD12	6	0.17
(1,845)	1:431:A:GLU:HA	1:431:A:GLU:HG3	15	0.17
(1,836)	1:430:A:LEU:HD13	1:427:A:THR:HB	1	0.17
(1,813)	1:427:A:THR:HG23	1:425:A:GLY:H	8	0.17
(1,812)	1:418:A:THR:H	1:418:A:THR:HG22	2	0.17
(1,812)	1:418:A:THR:H	1:418:A:THR:HG22	6	0.17
(1,812)	1:418:A:THR:H	1:418:A:THR:HG22	12	0.17
(1,812)	1:418:A:THR:H	1:418:A:THR:HG21	19	0.17
(1,800)	1:426:A:ARG:HB2	1:426:A:ARG:HG2	19	0.17
(1,791)	1:428:A:ASP:HA	1:428:A:ASP:HB3	3	0.17
(1,760)	1:338:A:TRP:HZ2	1:419:A:PRO:HA	3	0.17
(1,760)	1:338:A:TRP:HZ2	1:419:A:PRO:HA	18	0.17
(1,742)	1:349:A:ARG:HB2	1:350:A:TYR:HA	12	0.17
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD12	14	0.17
(1,666)	1:352:A:ASN:HA	1:351:A:GLU:HG3	11	0.17
(1,629)	1:403:A:ILE:HD12	1:415:A:PHE:HD1	4	0.17
(1,603)	1:401:A:ASN:HA	1:401:A:ASN:HB2	4	0.17
(1,603)	1:401:A:ASN:HA	1:401:A:ASN:HB2	10	0.17
(1,595)	1:400:A:LEU:HD21	1:400:A:LEU:HG	6	0.17
(1,595)	1:400:A:LEU:HD23	1:400:A:LEU:HG	13	0.17
(1,595)	1:400:A:LEU:HD23	1:400:A:LEU:HG	18	0.17
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD2	1	0.17
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD2	5	0.17
(1,584)	1:399:A:LYS:HG3	1:399:A:LYS:HD2	7	0.17
(1,544)	1:395:A:ARG:HB3	1:395:A:ARG:HD2	17	0.17
(1,530)	1:394:A:LEU:HD23	1:397:A:TYR:HB3	15	0.17
(1,528)	1:394:A:LEU:HD23	1:364:A:PHE:HZ	11	0.17
(1,528)	1:394:A:LEU:HD21	1:364:A:PHE:HZ	14	0.17
(1,526)	1:394:A:LEU:H	1:394:A:LEU:HD23	18	0.17
(1,505)	1:385:A:MET:HG2	1:373:A:ALA:HB3	9	0.17
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	19	0.17
(1,455)	1:386:A:THR:HG23	1:389:A:LYS:HE2	2	0.17
(1,454)	1:386:A:THR:HG23	1:370:A:ASN:HA	5	0.17
(1,454)	1:386:A:THR:HG22	1:370:A:ASN:HA	14	0.17
(1,443)	1:384:A:ASN:H	1:384:A:ASN:HB2	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG21	2	0.17
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG21	10	0.17
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG23	14	0.17
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG21	15	0.17
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG21	18	0.17
(1,347)	1:373:A:ALA:HA	1:376:A:TRP:HB2	17	0.17
(1,306)	1:354:A:ILE:HD11	1:366:A:ILE:HG22	5	0.17
(1,301)	1:366:A:ILE:HG23	1:372:A:LEU:HB3	1	0.17
(1,301)	1:366:A:ILE:HG22	1:372:A:LEU:HB3	5	0.17
(1,301)	1:366:A:ILE:HG22	1:372:A:LEU:HB3	16	0.17
(1,268)	1:364:A:PHE:HA	1:345:A:LEU:HD22	15	0.17
(1,266)	1:363:A:ILE:HG23	1:406:A:GLU:HG2	16	0.17
(1,231)	1:359:A:LYS:HG3	1:359:A:LYS:HE2	13	0.17
(1,203)	1:357:A:GLU:HB2	1:412:A:LEU:HD22	19	0.17
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	3	0.17
(1,200)	1:357:A:GLU:HB3	1:357:A:GLU:HG2	19	0.17
(1,138)	1:351:A:GLU:HG3	1:351:A:GLU:HB2	19	0.17
(1,121)	1:349:A:ARG:H	1:349:A:ARG:HB3	7	0.17
(1,121)	1:349:A:ARG:H	1:349:A:ARG:HB3	11	0.17
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	13	0.17
(1,104)	1:345:A:LEU:HD23	1:356:A:TRP:HE3	10	0.17
(1,88)	1:346:A:SER:HB2	1:346:A:SER:HA	9	0.17
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	2	0.17
(1,60)	1:344:A:LEU:H	1:343:A:GLN:HG2	14	0.17
(1,49)	1:341:A:VAL:HG22	1:342:A:TYR:HA	1	0.17
(1,49)	1:341:A:VAL:HG21	1:342:A:TYR:HA	7	0.17
(1,49)	1:341:A:VAL:HG21	1:342:A:TYR:HA	8	0.17
(1,49)	1:341:A:VAL:HG23	1:342:A:TYR:HA	14	0.17
(1,49)	1:341:A:VAL:HG22	1:342:A:TYR:HA	17	0.17
(1,49)	1:341:A:VAL:HG22	1:342:A:TYR:HA	19	0.17
(1,42)	1:341:A:VAL:HG22	1:415:A:PHE:HE2	1	0.17
(1,42)	1:341:A:VAL:HG21	1:415:A:PHE:HE2	4	0.17
(1,41)	1:341:A:VAL:HG23	1:364:A:PHE:HZ	17	0.17
(1,37)	1:341:A:VAL:HG12	1:341:A:VAL:HG21	10	0.17
(1,37)	1:341:A:VAL:HG13	1:341:A:VAL:HG21	11	0.17
(1,37)	1:341:A:VAL:HG11	1:341:A:VAL:HG21	12	0.17
(1,37)	1:341:A:VAL:HG11	1:341:A:VAL:HG22	16	0.17
(1,37)	1:341:A:VAL:HG13	1:341:A:VAL:HG21	18	0.17
(1,15)	1:339:A:ASP:HB3	1:336:A:LEU:HB2	14	0.17
(1,5)	1:337:A:LEU:HD22	1:390:A:MET:HG3	15	0.17
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	7	0.16
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	19	0.16
(1,2931)	1:420:A:ASP:H	1:421:A:GLU:HG3	15	0.16
(1,2895)	1:353:A:PHE:H	1:367:A:VAL:HG21	1	0.16
(1,2871)	1:444:A:GLN:HB2	1:444:A:GLN:HG3	4	0.16
(1,2850)	1:344:A:LEU:HD12	1:350:A:TYR:HD1	2	0.16
(1,2836)	1:404:A:ARG:HG3	1:405:A:LYS:H	9	0.16
(1,2811)	1:428:A:ASP:HA	1:431:A:GLU:HB2	6	0.16
(1,2811)	1:428:A:ASP:HA	1:431:A:GLU:HB2	15	0.16
(1,2724)	1:367:A:VAL:HG23	1:352:A:ASN:HA	2	0.16
(1,2693)	1:437:A:VAL:HG22	1:441:A:GLN:HE22	11	0.16
(1,2686)	1:430:A:LEU:HD13	1:430:A:LEU:HD23	14	0.16
(1,2667)	1:414:A:ARG:HA	1:414:A:ARG:HD2	6	0.16
(1,2662)	1:411:A:LEU:HD21	1:366:A:ILE:HB	6	0.16
(1,2662)	1:411:A:LEU:HD23	1:366:A:ILE:HB	17	0.16
(1,2655)	1:395:A:ARG:HB3	1:395:A:ARG:HD2	12	0.16
(1,2597)	1:358:A:ASP:HB2	1:363:A:ILE:HG22	11	0.16
(1,2553)	1:454:A:VAL:H	1:454:A:VAL:HG23	6	0.16
(1,2537)	1:394:A:LEU:H	1:394:A:LEU:HD12	2	0.16
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG23	1	0.16
(1,2499)	1:421:A:GLU:H	1:420:A:ASP:HB2	8	0.16
(1,2477)	1:404:A:ARG:H	1:403:A:ILE:HD13	3	0.16
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB2	9	0.16
(1,2440)	1:431:A:GLU:H	1:432:A:HIS:HB2	12	0.16
(1,2424)	1:441:A:GLN:H	1:440:A:GLU:HB2	17	0.16
(1,2359)	1:382:A:ARG:H	1:382:A:ARG:HG3	16	0.16
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD21	8	0.16
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD22	16	0.16
(1,2324)	1:352:A:ASN:HD21	1:367:A:VAL:HG23	3	0.16
(1,2295)	1:356:A:TRP:HE1	1:345:A:LEU:HG	4	0.16
(1,2284)	1:414:A:ARG:HE	1:404:A:ARG:HE	15	0.16
(1,2276)	1:410:A:ARG:HE	1:365:A:ARG:HE	11	0.16
(1,2255)	1:445:A:GLU:H	1:444:A:GLN:HA	3	0.16
(1,2186)	1:402:A:ILE:H	1:397:A:TYR:HB2	6	0.16
(1,2139)	1:385:A:MET:H	1:385:A:MET:HB2	15	0.16
(1,2126)	1:410:A:ARG:H	1:410:A:ARG:HB3	17	0.16
(1,2122)	1:410:A:ARG:H	1:409:A:GLN:HG3	3	0.16
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD11	13	0.16
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD11	14	0.16
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG21	4	0.16
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG21	19	0.16
(1,1954)	1:399:A:LYS:H	1:399:A:LYS:HG2	4	0.16
(1,1910)	1:354:A:ILE:HG22	1:345:A:LEU:HD21	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1909)	1:344:A:LEU:HD12	1:354:A:ILE:HG21	9	0.16
(1,1903)	1:438:A:LEU:HD21	1:438:A:LEU:HD13	18	0.16
(1,1899)	1:430:A:LEU:HD12	1:400:A:LEU:HD23	14	0.16
(1,1892)	1:403:A:ILE:HD12	1:402:A:ILE:HG22	12	0.16
(1,1892)	1:403:A:ILE:HD12	1:402:A:ILE:HG21	19	0.16
(1,1882)	1:393:A:ALA:HB3	1:437:A:VAL:HG11	5	0.16
(1,1882)	1:393:A:ALA:HB3	1:437:A:VAL:HG13	18	0.16
(1,1877)	1:388:A:GLU:H	1:388:A:GLU:HG2	3	0.16
(1,1873)	1:383:A:THR:HG22	1:384:A:ASN:HD22	18	0.16
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	4	0.16
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	5	0.16
(1,1835)	1:369:A:PRO:HD2	1:369:A:PRO:HG3	15	0.16
(1,1828)	1:398:A:TYR:HA	1:399:A:LYS:HD2	17	0.16
(1,1827)	1:430:A:LEU:HB3	1:430:A:LEU:HD22	2	0.16
(1,1795)	1:431:A:GLU:HG3	1:336:A:LEU:HD22	18	0.16
(1,1756)	1:402:A:ILE:HB	1:397:A:TYR:HB2	2	0.16
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	13	0.16
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	15	0.16
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	17	0.16
(1,1645)	1:404:A:ARG:HB3	1:404:A:ARG:HG3	9	0.16
(1,1645)	1:404:A:ARG:HB3	1:404:A:ARG:HG3	19	0.16
(1,1626)	1:406:A:GLU:H	1:406:A:GLU:HG3	18	0.16
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	6	0.16
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	10	0.16
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	14	0.16
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	16	0.16
(1,1607)	1:411:A:LEU:HD13	1:366:A:ILE:H	19	0.16
(1,1603)	1:357:A:GLU:HG2	1:412:A:LEU:HD13	2	0.16
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	1	0.16
(1,1541)	1:445:A:GLU:HA	1:443:A:TYR:HD1	12	0.16
(1,1541)	1:445:A:GLU:HA	1:443:A:TYR:HD1	17	0.16
(1,1533)	1:378:A:ASN:HB2	1:375:A:LEU:HA	8	0.16
(1,1533)	1:378:A:ASN:HB2	1:375:A:LEU:HA	11	0.16
(1,1505)	1:385:A:MET:HA	1:389:A:LYS:HB2	9	0.16
(1,1488)	1:431:A:GLU:HB2	1:336:A:LEU:HD22	6	0.16
(1,1461)	1:435:A:SER:H	1:435:A:SER:HB2	14	0.16
(1,1461)	1:435:A:SER:H	1:435:A:SER:HB2	18	0.16
(1,1454)	1:438:A:LEU:HD11	1:376:A:TRP:HH2	17	0.16
(1,1444)	1:442:A:THR:HG23	1:443:A:TYR:HA	1	0.16
(1,1438)	1:444:A:GLN:HA	1:444:A:GLN:HB2	1	0.16
(1,1438)	1:444:A:GLN:HA	1:444:A:GLN:HB2	6	0.16
(1,1438)	1:444:A:GLN:HA	1:444:A:GLN:HB2	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1438)	1:444:A:GLN:HA	1:444:A:GLN:HB2	12	0.16
(1,1438)	1:444:A:GLN:HA	1:444:A:GLN:HB2	13	0.16
(1,1438)	1:444:A:GLN:HA	1:444:A:GLN:HB2	14	0.16
(1,1438)	1:444:A:GLN:HA	1:444:A:GLN:HB2	18	0.16
(1,1427)	1:447:A:GLU:HA	1:448:A:PRO:HD3	3	0.16
(1,1427)	1:447:A:GLU:HA	1:448:A:PRO:HD3	18	0.16
(1,1407)	1:456:A:TRP:HB3	1:456:A:TRP:HZ3	3	0.16
(1,1402)	1:383:A:THR:HG21	1:384:A:ASN:HD21	11	0.16
(1,1340)	1:399:A:LYS:HD3	1:396:A:HIS:HA	11	0.16
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	8	0.16
(1,1332)	1:399:A:LYS:HA	1:399:A:LYS:HE2	1	0.16
(1,1332)	1:399:A:LYS:HA	1:399:A:LYS:HE2	7	0.16
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD23	2	0.16
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD22	3	0.16
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD23	9	0.16
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD23	10	0.16
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	17	0.16
(1,1296)	1:379:A:HIS:HB3	1:380:A:LYS:HG2	19	0.16
(1,1267)	1:354:A:ILE:HD11	1:367:A:VAL:H	1	0.16
(1,1267)	1:354:A:ILE:HD12	1:367:A:VAL:H	2	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	1	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	2	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	3	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	4	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	5	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	6	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	7	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	8	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	9	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	10	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	11	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	12	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	13	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	14	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	15	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	16	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	18	0.16
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	19	0.16
(1,1224)	1:363:A:ILE:HG21	1:357:A:GLU:HG2	1	0.16
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	2	0.16
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	3	0.16
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	8	0.16
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	9	0.16
(1,1207)	1:360:A:GLU:HB3	1:360:A:GLU:HG2	15	0.16
(1,1207)	1:360:A:GLU:HB3	1:360:A:GLU:HG2	17	0.16
(1,1175)	1:363:A:ILE:HG23	1:363:A:ILE:HG13	3	0.16
(1,1126)	1:355:A:ARG:HD3	1:367:A:VAL:HG22	5	0.16
(1,1077)	1:372:A:LEU:HD12	1:340:A:TYR:HD2	11	0.16
(1,1077)	1:372:A:LEU:HD12	1:340:A:TYR:HD2	19	0.16
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD13	7	0.16
(1,1075)	1:372:A:LEU:HG	1:344:A:LEU:HD12	12	0.16
(1,1040)	1:349:A:ARG:HB2	1:349:A:ARG:HD2	13	0.16
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	18	0.16
(1,1033)	1:348:A:SER:HB3	1:351:A:GLU:HB3	10	0.16
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG22	12	0.16
(1,959)	1:449:A:THR:HG21	1:449:A:THR:HB	3	0.16
(1,959)	1:449:A:THR:HG22	1:449:A:THR:HB	4	0.16
(1,959)	1:449:A:THR:HG21	1:449:A:THR:HB	7	0.16
(1,959)	1:449:A:THR:HG23	1:449:A:THR:HB	12	0.16
(1,959)	1:449:A:THR:HG21	1:449:A:THR:HB	14	0.16
(1,946)	1:447:A:GLU:HG2	1:446:A:ASP:H	13	0.16
(1,929)	1:443:A:TYR:H	1:442:A:THR:HB	10	0.16
(1,929)	1:443:A:TYR:H	1:442:A:THR:HB	12	0.16
(1,903)	1:438:A:LEU:HD21	1:438:A:LEU:HB3	2	0.16
(1,903)	1:438:A:LEU:HD22	1:438:A:LEU:HB3	8	0.16
(1,903)	1:438:A:LEU:HD21	1:438:A:LEU:HB3	13	0.16
(1,898)	1:438:A:LEU:HD13	1:382:A:ARG:HG2	3	0.16
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD23	2	0.16
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD21	8	0.16
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD23	12	0.16
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD23	13	0.16
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD22	16	0.16
(1,888)	1:437:A:VAL:HG21	1:441:A:GLN:HE22	5	0.16
(1,887)	1:437:A:VAL:HG23	1:393:A:ALA:HA	11	0.16
(1,885)	1:437:A:VAL:HG11	1:393:A:ALA:HA	10	0.16
(1,884)	1:437:A:VAL:HG21	1:392:A:ARG:HG3	17	0.16
(1,872)	1:436:A:GLN:H	1:435:A:SER:HB2	7	0.16
(1,864)	1:433:A:LEU:HA	1:433:A:LEU:HD11	5	0.16
(1,864)	1:433:A:LEU:HA	1:433:A:LEU:HD13	16	0.16
(1,859)	1:436:A:GLN:H	1:434:A:GLU:HA	10	0.16
(1,850)	1:431:A:GLU:HG3	1:431:A:GLU:HB2	4	0.16
(1,850)	1:431:A:GLU:HG3	1:431:A:GLU:HB2	13	0.16
(1,845)	1:431:A:GLU:HA	1:431:A:GLU:HG3	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	17	0.16
(1,813)	1:427:A:THR:HG22	1:425:A:GLY:H	19	0.16
(1,812)	1:418:A:THR:H	1:418:A:THR:HG22	5	0.16
(1,812)	1:418:A:THR:H	1:418:A:THR:HG23	16	0.16
(1,800)	1:426:A:ARG:HB2	1:426:A:ARG:HG2	5	0.16
(1,760)	1:338:A:TRP:HZ2	1:419:A:PRO:HA	5	0.16
(1,760)	1:338:A:TRP:HZ2	1:419:A:PRO:HA	10	0.16
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD11	9	0.16
(1,678)	1:411:A:LEU:HA	1:411:A:LEU:HD23	5	0.16
(1,666)	1:352:A:ASN:HA	1:351:A:GLU:HG3	18	0.16
(1,601)	1:401:A:ASN:HD21	1:401:A:ASN:HB3	2	0.16
(1,601)	1:401:A:ASN:HD21	1:401:A:ASN:HB3	4	0.16
(1,595)	1:400:A:LEU:HD22	1:400:A:LEU:HG	10	0.16
(1,595)	1:400:A:LEU:HD22	1:400:A:LEU:HG	11	0.16
(1,595)	1:400:A:LEU:HD22	1:400:A:LEU:HG	19	0.16
(1,594)	1:400:A:LEU:HD23	1:426:A:ARG:HG3	2	0.16
(1,572)	1:399:A:LYS:HA	1:399:A:LYS:HB3	4	0.16
(1,556)	1:397:A:TYR:HA	1:400:A:LEU:HB3	9	0.16
(1,544)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	15	0.16
(1,455)	1:386:A:THR:HG22	1:389:A:LYS:HE3	4	0.16
(1,443)	1:384:A:ASN:H	1:384:A:ASN:HB2	18	0.16
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG22	1	0.16
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG23	4	0.16
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG22	6	0.16
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG21	7	0.16
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG22	9	0.16
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG23	11	0.16
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG23	17	0.16
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG23	19	0.16
(1,400)	1:377:A:GLY:HA3	1:382:A:ARG:HB3	13	0.16
(1,364)	1:374:A:ARG:HA	1:374:A:ARG:HG3	15	0.16
(1,359)	1:374:A:ARG:HA	1:374:A:ARG:HB3	13	0.16
(1,358)	1:374:A:ARG:HA	1:374:A:ARG:HD2	7	0.16
(1,353)	1:373:A:ALA:HB3	1:385:A:MET:HG3	19	0.16
(1,347)	1:373:A:ALA:HA	1:376:A:TRP:HB2	19	0.16
(1,318)	1:367:A:VAL:HA	1:367:A:VAL:HG21	5	0.16
(1,301)	1:366:A:ILE:HG21	1:372:A:LEU:HB3	4	0.16
(1,266)	1:363:A:ILE:HG21	1:406:A:GLU:HG2	10	0.16
(1,204)	1:357:A:GLU:HB3	1:412:A:LEU:HD12	1	0.16
(1,204)	1:357:A:GLU:HB3	1:412:A:LEU:HD12	8	0.16
(1,204)	1:357:A:GLU:HB3	1:412:A:LEU:HD13	17	0.16
(1,204)	1:357:A:GLU:HB3	1:412:A:LEU:HD13	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,203)	1:357:A:GLU:HB2	1:412:A:LEU:HD23	15	0.16
(1,179)	1:355:A:ARG:HB2	1:351:A:GLU:HA	12	0.16
(1,174)	1:354:A:ILE:HD12	1:341:A:VAL:HA	17	0.16
(1,166)	1:354:A:ILE:HG23	1:372:A:LEU:HD21	16	0.16
(1,138)	1:351:A:GLU:HG3	1:351:A:GLU:HB2	6	0.16
(1,127)	1:349:A:ARG:HD2	1:350:A:TYR:HE1	1	0.16
(1,121)	1:349:A:ARG:H	1:349:A:ARG:HB3	2	0.16
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	5	0.16
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	7	0.16
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	16	0.16
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	19	0.16
(1,115)	1:348:A:SER:HA	1:351:A:GLU:H	19	0.16
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD23	17	0.16
(1,104)	1:345:A:LEU:HD23	1:356:A:TRP:HE3	3	0.16
(1,104)	1:345:A:LEU:HD22	1:356:A:TRP:HE3	12	0.16
(1,104)	1:345:A:LEU:HD21	1:356:A:TRP:HE3	19	0.16
(1,93)	1:345:A:LEU:HA	1:354:A:ILE:HG22	17	0.16
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	14	0.16
(1,58)	1:343:A:GLN:HG3	1:343:A:GLN:HB2	18	0.16
(1,49)	1:341:A:VAL:HG23	1:342:A:TYR:HA	2	0.16
(1,49)	1:341:A:VAL:HG22	1:342:A:TYR:HA	3	0.16
(1,49)	1:341:A:VAL:HG23	1:342:A:TYR:HA	12	0.16
(1,49)	1:341:A:VAL:HG21	1:342:A:TYR:HA	15	0.16
(1,42)	1:341:A:VAL:HG23	1:415:A:PHE:HE2	10	0.16
(1,42)	1:341:A:VAL:HG21	1:415:A:PHE:HE2	16	0.16
(1,37)	1:341:A:VAL:HG11	1:341:A:VAL:HG22	8	0.16
(1,37)	1:341:A:VAL:HG13	1:341:A:VAL:HG22	9	0.16
(1,27)	1:341:A:VAL:HA	1:372:A:LEU:HD12	13	0.16
(1,1)	1:337:A:LEU:HD22	1:394:A:LEU:HD13	13	0.16
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	5	0.15
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	17	0.15
(1,2972)	1:435:A:SER:H	1:436:A:GLN:HG3	2	0.15
(1,2967)	1:444:A:GLN:H	1:444:A:GLN:HB3	15	0.15
(1,2952)	1:382:A:ARG:H	1:381:A:ASN:HB2	15	0.15
(1,2945)	1:364:A:PHE:H	1:412:A:LEU:HG	7	0.15
(1,2931)	1:420:A:ASP:H	1:421:A:GLU:HG3	1	0.15
(1,2931)	1:420:A:ASP:H	1:421:A:GLU:HG3	2	0.15
(1,2918)	1:374:A:ARG:H	1:376:A:TRP:H	3	0.15
(1,2875)	1:373:A:ALA:H	1:372:A:LEU:HD13	9	0.15
(1,2871)	1:444:A:GLN:HB2	1:444:A:GLN:HG3	19	0.15
(1,2850)	1:344:A:LEU:HD12	1:350:A:TYR:HD1	1	0.15
(1,2836)	1:404:A:ARG:HG3	1:405:A:LYS:H	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2811)	1:428:A:ASP:HA	1:431:A:GLU:HB2	1	0.15
(1,2792)	1:375:A:LEU:H	1:375:A:LEU:HD22	2	0.15
(1,2762)	1:394:A:LEU:HD23	1:398:A:TYR:HE1	4	0.15
(1,2758)	1:375:A:LEU:HD22	1:340:A:TYR:HE2	3	0.15
(1,2728)	1:366:A:ILE:HB	1:413:A:PHE:HZ	13	0.15
(1,2724)	1:367:A:VAL:HG23	1:352:A:ASN:HA	7	0.15
(1,2721)	1:354:A:ILE:HD13	1:372:A:LEU:HD21	8	0.15
(1,2705)	1:394:A:LEU:HA	1:397:A:TYR:HD2	9	0.15
(1,2684)	1:429:A:ARG:HG2	1:433:A:LEU:HD22	1	0.15
(1,2682)	1:418:A:THR:HG21	1:362:A:LYS:HE2	8	0.15
(1,2663)	1:411:A:LEU:HD23	1:387:A:TYR:HE2	1	0.15
(1,2663)	1:411:A:LEU:HD21	1:387:A:TYR:HE2	6	0.15
(1,2663)	1:411:A:LEU:HD23	1:387:A:TYR:HE1	13	0.15
(1,2663)	1:411:A:LEU:HD22	1:387:A:TYR:HE2	16	0.15
(1,2662)	1:411:A:LEU:HD23	1:366:A:ILE:HB	2	0.15
(1,2662)	1:411:A:LEU:HD21	1:366:A:ILE:HB	7	0.15
(1,2662)	1:411:A:LEU:HD21	1:366:A:ILE:HB	8	0.15
(1,2662)	1:411:A:LEU:HD23	1:366:A:ILE:HB	14	0.15
(1,2662)	1:411:A:LEU:HD22	1:366:A:ILE:HB	19	0.15
(1,2661)	1:411:A:LEU:HD13	1:410:A:ARG:HD3	14	0.15
(1,2659)	1:366:A:ILE:HD11	1:411:A:LEU:HB3	10	0.15
(1,2618)	1:375:A:LEU:HD21	1:378:A:ASN:HB2	14	0.15
(1,2596)	1:363:A:ILE:HG22	1:364:A:PHE:HA	19	0.15
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD12	1	0.15
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD12	6	0.15
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD11	9	0.15
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD13	12	0.15
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD11	13	0.15
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD12	15	0.15
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD11	17	0.15
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD11	18	0.15
(1,2567)	1:345:A:LEU:HD21	1:355:A:ARG:HA	12	0.15
(1,2557)	1:341:A:VAL:HG13	1:403:A:ILE:HD13	18	0.15
(1,2553)	1:454:A:VAL:H	1:454:A:VAL:HG22	1	0.15
(1,2537)	1:394:A:LEU:H	1:394:A:LEU:HD12	3	0.15
(1,2537)	1:394:A:LEU:H	1:394:A:LEU:HD13	16	0.15
(1,2521)	1:355:A:ARG:H	1:345:A:LEU:HD22	3	0.15
(1,2516)	1:342:A:TYR:H	1:341:A:VAL:HG23	11	0.15
(1,2499)	1:421:A:GLU:H	1:420:A:ASP:HB2	5	0.15
(1,2499)	1:421:A:GLU:H	1:420:A:ASP:HB2	13	0.15
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD22	15	0.15
(1,2295)	1:356:A:TRP:HE1	1:345:A:LEU:HG	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2295)	1:356:A:TRP:HE1	1:345:A:LEU:HG	13	0.15
(1,2284)	1:414:A:ARG:HE	1:404:A:ARG:HE	8	0.15
(1,2276)	1:410:A:ARG:HE	1:365:A:ARG:HE	3	0.15
(1,2258)	1:450:A:ILE:H	1:450:A:ILE:HG13	15	0.15
(1,2208)	1:406:A:GLU:H	1:412:A:LEU:HD12	5	0.15
(1,2199)	1:412:A:LEU:H	1:412:A:LEU:HD13	1	0.15
(1,2199)	1:412:A:LEU:H	1:412:A:LEU:HD13	8	0.15
(1,2184)	1:435:A:SER:H	1:432:A:HIS:HA	10	0.15
(1,2139)	1:385:A:MET:H	1:385:A:MET:HB2	19	0.15
(1,2126)	1:410:A:ARG:H	1:410:A:ARG:HB3	7	0.15
(1,2122)	1:410:A:ARG:H	1:409:A:GLN:HG2	7	0.15
(1,2090)	1:371:A:GLY:H	1:370:A:ASN:HB2	6	0.15
(1,2090)	1:371:A:GLY:H	1:370:A:ASN:HB2	12	0.15
(1,2090)	1:371:A:GLY:H	1:370:A:ASN:HB2	17	0.15
(1,2090)	1:371:A:GLY:H	1:370:A:ASN:HB2	18	0.15
(1,2090)	1:371:A:GLY:H	1:370:A:ASN:HB2	19	0.15
(1,2067)	1:365:A:ARG:H	1:355:A:ARG:HG2	14	0.15
(1,2048)	1:361:A:SER:H	1:358:A:ASP:HB2	3	0.15
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD12	11	0.15
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG23	7	0.15
(1,1920)	1:372:A:LEU:HD13	1:366:A:ILE:HD11	5	0.15
(1,1920)	1:372:A:LEU:HD12	1:366:A:ILE:HD11	16	0.15
(1,1882)	1:393:A:ALA:HB2	1:437:A:VAL:HG11	17	0.15
(1,1874)	1:382:A:ARG:HD3	1:382:A:ARG:HA	8	0.15
(1,1874)	1:382:A:ARG:HD3	1:382:A:ARG:HA	9	0.15
(1,1874)	1:382:A:ARG:HD3	1:382:A:ARG:HA	15	0.15
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB3	10	0.15
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB3	14	0.15
(1,1828)	1:398:A:TYR:HA	1:399:A:LYS:HD2	2	0.15
(1,1802)	1:336:A:LEU:HD13	1:431:A:GLU:HA	4	0.15
(1,1795)	1:431:A:GLU:HG3	1:336:A:LEU:HD22	7	0.15
(1,1787)	1:376:A:TRP:HZ2	1:337:A:LEU:HD23	10	0.15
(1,1784)	1:337:A:LEU:HD12	1:340:A:TYR:H	3	0.15
(1,1784)	1:337:A:LEU:HD13	1:340:A:TYR:H	14	0.15
(1,1756)	1:402:A:ILE:HB	1:397:A:TYR:HB2	4	0.15
(1,1756)	1:402:A:ILE:HB	1:397:A:TYR:HB2	5	0.15
(1,1740)	1:339:A:ASP:HB2	1:419:A:PRO:HG3	3	0.15
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	6	0.15
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	2	0.15
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	8	0.15
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	12	0.15
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	18	0.15
(1,1672)	1:403:A:ILE:HG21	1:405:A:LYS:H	12	0.15
(1,1647)	1:404:A:ARG:HB2	1:404:A:ARG:HG2	1	0.15
(1,1647)	1:404:A:ARG:HB2	1:404:A:ARG:HG2	6	0.15
(1,1647)	1:404:A:ARG:HB2	1:404:A:ARG:HG2	17	0.15
(1,1645)	1:404:A:ARG:HB3	1:404:A:ARG:HG3	13	0.15
(1,1626)	1:406:A:GLU:H	1:406:A:GLU:HG3	4	0.15
(1,1626)	1:406:A:GLU:H	1:406:A:GLU:HG3	8	0.15
(1,1626)	1:406:A:GLU:H	1:406:A:GLU:HG3	13	0.15
(1,1626)	1:406:A:GLU:H	1:406:A:GLU:HG3	15	0.15
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	3	0.15
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	13	0.15
(1,1607)	1:411:A:LEU:HD12	1:366:A:ILE:H	10	0.15
(1,1604)	1:365:A:ARG:HB2	1:412:A:LEU:HD13	1	0.15
(1,1604)	1:365:A:ARG:HB2	1:412:A:LEU:HD11	2	0.15
(1,1603)	1:357:A:GLU:HG2	1:412:A:LEU:HD13	6	0.15
(1,1600)	1:412:A:LEU:HD22	1:412:A:LEU:H	3	0.15
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	7	0.15
(1,1533)	1:378:A:ASN:HB2	1:375:A:LEU:HA	18	0.15
(1,1505)	1:385:A:MET:HA	1:389:A:LYS:HB2	13	0.15
(1,1462)	1:435:A:SER:H	1:434:A:GLU:HB3	19	0.15
(1,1461)	1:435:A:SER:H	1:435:A:SER:HB2	7	0.15
(1,1453)	1:438:A:LEU:HD13	1:435:A:SER:H	16	0.15
(1,1452)	1:361:A:SER:H	1:360:A:GLU:HG2	1	0.15
(1,1438)	1:444:A:GLN:HA	1:444:A:GLN:HB2	2	0.15
(1,1438)	1:444:A:GLN:HA	1:444:A:GLN:HB2	3	0.15
(1,1438)	1:444:A:GLN:HA	1:444:A:GLN:HB2	4	0.15
(1,1438)	1:444:A:GLN:HA	1:444:A:GLN:HB2	5	0.15
(1,1438)	1:444:A:GLN:HA	1:444:A:GLN:HB2	9	0.15
(1,1438)	1:444:A:GLN:HA	1:444:A:GLN:HB2	10	0.15
(1,1438)	1:444:A:GLN:HA	1:444:A:GLN:HB2	16	0.15
(1,1412)	1:454:A:VAL:HB	1:450:A:ILE:HA	3	0.15
(1,1412)	1:454:A:VAL:HB	1:450:A:ILE:HA	11	0.15
(1,1412)	1:454:A:VAL:HB	1:450:A:ILE:HA	12	0.15
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	18	0.15
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD21	15	0.15
(1,1311)	1:421:A:GLU:HA	1:421:A:GLU:HG3	7	0.15
(1,1311)	1:421:A:GLU:HA	1:421:A:GLU:HG3	10	0.15
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	7	0.15
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	10	0.15
(1,1276)	1:382:A:ARG:HG2	1:382:A:ARG:HB2	7	0.15
(1,1276)	1:382:A:ARG:HG2	1:382:A:ARG:HB2	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1267)	1:354:A:ILE:HD13	1:367:A:VAL:H	9	0.15
(1,1250)	1:345:A:LEU:HD21	1:355:A:ARG:HA	12	0.15
(1,1233)	1:356:A:TRP:HZ2	1:356:A:TRP:HE3	17	0.15
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	10	0.15
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	17	0.15
(1,1217)	1:359:A:LYS:HD2	1:356:A:TRP:HZ2	1	0.15
(1,1175)	1:363:A:ILE:HG21	1:363:A:ILE:HG13	19	0.15
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG22	7	0.15
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	1	0.15
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	2	0.15
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	10	0.15
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG11	12	0.15
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG11	18	0.15
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG12	10	0.15
(1,1123)	1:354:A:ILE:H	1:367:A:VAL:HG22	4	0.15
(1,1102)	1:369:A:PRO:HB3	1:387:A:TYR:HD1	11	0.15
(1,1086)	1:371:A:GLY:HA3	1:374:A:ARG:HB2	6	0.15
(1,1086)	1:371:A:GLY:HA3	1:374:A:ARG:HB2	12	0.15
(1,1086)	1:371:A:GLY:HA3	1:374:A:ARG:HB2	13	0.15
(1,1084)	1:372:A:LEU:HD12	1:344:A:LEU:HD13	7	0.15
(1,1038)	1:349:A:ARG:HA	1:349:A:ARG:HD3	8	0.15
(1,1026)	1:336:A:LEU:HD22	1:432:A:HIS:H	16	0.15
(1,1000)	1:409:A:GLN:HE21	1:409:A:GLN:HG2	3	0.15
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG22	2	0.15
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG22	10	0.15
(1,960)	1:450:A:ILE:HA	1:450:A:ILE:HG13	1	0.15
(1,960)	1:450:A:ILE:HA	1:450:A:ILE:HG13	7	0.15
(1,960)	1:450:A:ILE:HA	1:450:A:ILE:HG13	14	0.15
(1,959)	1:449:A:THR:HG22	1:449:A:THR:HB	2	0.15
(1,959)	1:449:A:THR:HG21	1:449:A:THR:HB	6	0.15
(1,959)	1:449:A:THR:HG22	1:449:A:THR:HB	8	0.15
(1,959)	1:449:A:THR:HG23	1:449:A:THR:HB	10	0.15
(1,959)	1:449:A:THR:HG21	1:449:A:THR:HB	15	0.15
(1,959)	1:449:A:THR:HG21	1:449:A:THR:HB	16	0.15
(1,959)	1:449:A:THR:HG21	1:449:A:THR:HB	17	0.15
(1,959)	1:449:A:THR:HG23	1:449:A:THR:HB	19	0.15
(1,956)	1:450:A:ILE:H	1:449:A:THR:HB	12	0.15
(1,947)	1:447:A:GLU:HG2	1:447:A:GLU:HA	13	0.15
(1,947)	1:447:A:GLU:HG2	1:447:A:GLU:HA	14	0.15
(1,941)	1:447:A:GLU:H	1:446:A:ASP:HB2	17	0.15
(1,927)	1:441:A:GLN:H	1:441:A:GLN:HG2	1	0.15
(1,923)	1:441:A:GLN:HB2	1:441:A:GLN:HG2	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,898)	1:438:A:LEU:HD11	1:382:A:ARG:HG2	9	0.15
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD21	1	0.15
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD23	3	0.15
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD22	6	0.15
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD22	10	0.15
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD23	11	0.15
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD23	14	0.15
(1,890)	1:439:A:ASP:H	1:438:A:LEU:HB2	7	0.15
(1,887)	1:437:A:VAL:HG22	1:393:A:ALA:HA	2	0.15
(1,887)	1:437:A:VAL:HG22	1:393:A:ALA:HA	9	0.15
(1,885)	1:437:A:VAL:HG11	1:393:A:ALA:HA	3	0.15
(1,885)	1:437:A:VAL:HG11	1:393:A:ALA:HA	7	0.15
(1,884)	1:437:A:VAL:HG23	1:392:A:ARG:HG3	1	0.15
(1,884)	1:437:A:VAL:HG21	1:392:A:ARG:HG3	12	0.15
(1,872)	1:436:A:GLN:H	1:435:A:SER:HB2	19	0.15
(1,845)	1:431:A:GLU:HA	1:431:A:GLU:HG3	11	0.15
(1,834)	1:430:A:LEU:HD12	1:397:A:TYR:HD1	8	0.15
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	1	0.15
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	6	0.15
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	13	0.15
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	14	0.15
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	16	0.15
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	19	0.15
(1,812)	1:418:A:THR:H	1:418:A:THR:HG21	1	0.15
(1,812)	1:418:A:THR:H	1:418:A:THR:HG21	7	0.15
(1,760)	1:338:A:TRP:HZ2	1:419:A:PRO:HA	11	0.15
(1,760)	1:338:A:TRP:HZ2	1:419:A:PRO:HA	12	0.15
(1,760)	1:338:A:TRP:HZ2	1:419:A:PRO:HA	19	0.15
(1,713)	1:414:A:ARG:HE	1:414:A:ARG:HB3	2	0.15
(1,699)	1:413:A:PHE:HB2	1:364:A:PHE:HE2	2	0.15
(1,699)	1:413:A:PHE:HB2	1:364:A:PHE:HE2	10	0.15
(1,699)	1:413:A:PHE:HB2	1:364:A:PHE:HE2	19	0.15
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD13	4	0.15
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD13	8	0.15
(1,678)	1:411:A:LEU:HA	1:411:A:LEU:HD22	17	0.15
(1,629)	1:403:A:ILE:HD12	1:415:A:PHE:HD1	16	0.15
(1,612)	1:402:A:ILE:HD12	1:400:A:LEU:HB3	10	0.15
(1,601)	1:401:A:ASN:HD21	1:401:A:ASN:HB3	8	0.15
(1,601)	1:401:A:ASN:HD21	1:401:A:ASN:HB3	9	0.15
(1,601)	1:401:A:ASN:HD21	1:401:A:ASN:HB3	10	0.15
(1,601)	1:401:A:ASN:HD21	1:401:A:ASN:HB3	13	0.15
(1,595)	1:400:A:LEU:HD21	1:400:A:LEU:HG	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:400:A:LEU:HD23	1:426:A:ARG:HG3	10	0.15
(1,556)	1:397:A:TYR:HA	1:400:A:LEU:HB3	7	0.15
(1,556)	1:397:A:TYR:HA	1:400:A:LEU:HB3	10	0.15
(1,544)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	2	0.15
(1,533)	1:394:A:LEU:HD21	1:403:A:ILE:HG21	3	0.15
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	12	0.15
(1,505)	1:385:A:MET:HG2	1:373:A:ALA:HB2	7	0.15
(1,505)	1:385:A:MET:HG2	1:373:A:ALA:HB2	12	0.15
(1,455)	1:386:A:THR:HG21	1:389:A:LYS:HE3	12	0.15
(1,454)	1:386:A:THR:HG23	1:370:A:ASN:HA	6	0.15
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG23	3	0.15
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG22	5	0.15
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG21	8	0.15
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG22	12	0.15
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG22	13	0.15
(1,442)	1:383:A:THR:HB	1:383:A:THR:HG21	16	0.15
(1,364)	1:374:A:ARG:HA	1:374:A:ARG:HG3	14	0.15
(1,358)	1:374:A:ARG:HA	1:374:A:ARG:HD2	18	0.15
(1,266)	1:363:A:ILE:HG22	1:406:A:GLU:HG2	6	0.15
(1,266)	1:363:A:ILE:HG21	1:406:A:GLU:HG2	19	0.15
(1,231)	1:359:A:LYS:HG3	1:359:A:LYS:HE2	5	0.15
(1,205)	1:357:A:GLU:HB3	1:363:A:ILE:HG23	8	0.15
(1,166)	1:354:A:ILE:HG21	1:372:A:LEU:HD23	12	0.15
(1,138)	1:351:A:GLU:HG3	1:351:A:GLU:HB2	1	0.15
(1,138)	1:351:A:GLU:HG3	1:351:A:GLU:HB2	8	0.15
(1,138)	1:351:A:GLU:HG3	1:351:A:GLU:HB2	14	0.15
(1,127)	1:349:A:ARG:HD2	1:350:A:TYR:HE1	7	0.15
(1,121)	1:349:A:ARG:H	1:349:A:ARG:HB3	6	0.15
(1,115)	1:348:A:SER:HA	1:351:A:GLU:H	13	0.15
(1,104)	1:345:A:LEU:HD22	1:356:A:TRP:HE3	9	0.15
(1,88)	1:346:A:SER:HB2	1:346:A:SER:HA	10	0.15
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	13	0.15
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	16	0.15
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	18	0.15
(1,58)	1:343:A:GLN:HG3	1:343:A:GLN:HB2	1	0.15
(1,58)	1:343:A:GLN:HG2	1:343:A:GLN:HB3	3	0.15
(1,58)	1:343:A:GLN:HG2	1:343:A:GLN:HB2	13	0.15
(1,58)	1:343:A:GLN:HG3	1:343:A:GLN:HB2	16	0.15
(1,57)	1:343:A:GLN:HG2	1:344:A:LEU:HD23	10	0.15
(1,49)	1:341:A:VAL:HG21	1:342:A:TYR:HA	5	0.15
(1,49)	1:341:A:VAL:HG21	1:342:A:TYR:HA	9	0.15
(1,49)	1:341:A:VAL:HG23	1:342:A:TYR:HA	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:341:A:VAL:HG23	1:415:A:PHE:HE2	2	0.15
(1,42)	1:341:A:VAL:HG21	1:415:A:PHE:HE2	7	0.15
(1,42)	1:341:A:VAL:HG23	1:415:A:PHE:HE2	11	0.15
(1,37)	1:341:A:VAL:HG12	1:341:A:VAL:HG23	1	0.15
(1,37)	1:341:A:VAL:HG13	1:341:A:VAL:HG22	15	0.15
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	6	0.14
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	9	0.14
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	10	0.14
(1,2989)	1:450:A:ILE:H	1:449:A:THR:HG23	1	0.14
(1,2989)	1:450:A:ILE:H	1:449:A:THR:HG21	12	0.14
(1,2976)	1:423:A:MET:H	1:422:A:ILE:HG21	17	0.14
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	10	0.14
(1,2945)	1:364:A:PHE:H	1:412:A:LEU:HG	15	0.14
(1,2936)	1:436:A:GLN:H	1:435:A:SER:HB2	14	0.14
(1,2935)	1:433:A:LEU:H	1:433:A:LEU:HD22	2	0.14
(1,2930)	1:418:A:THR:H	1:417:A:LYS:HB3	11	0.14
(1,2871)	1:444:A:GLN:HB2	1:444:A:GLN:HG3	3	0.14
(1,2871)	1:444:A:GLN:HB2	1:444:A:GLN:HG3	5	0.14
(1,2862)	1:379:A:HIS:HB3	1:340:A:TYR:HE1	15	0.14
(1,2845)	1:402:A:ILE:HD13	1:338:A:TRP:HB2	1	0.14
(1,2836)	1:414:A:ARG:HG3	1:363:A:ILE:H	10	0.14
(1,2825)	1:413:A:PHE:HE2	1:366:A:ILE:HB	9	0.14
(1,2811)	1:428:A:ASP:HA	1:431:A:GLU:HB2	4	0.14
(1,2774)	1:443:A:TYR:HD1	1:445:A:GLU:HB2	11	0.14
(1,2758)	1:375:A:LEU:HD22	1:340:A:TYR:HE2	16	0.14
(1,2744)	1:417:A:LYS:HE3	1:417:A:LYS:HD3	10	0.14
(1,2739)	1:362:A:LYS:HB2	1:356:A:TRP:HZ3	18	0.14
(1,2728)	1:366:A:ILE:HB	1:413:A:PHE:HZ	6	0.14
(1,2728)	1:366:A:ILE:HB	1:413:A:PHE:HZ	7	0.14
(1,2719)	1:372:A:LEU:HD11	1:340:A:TYR:HD2	16	0.14
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD12	4	0.14
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD11	13	0.14
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD11	17	0.14
(1,2696)	1:438:A:LEU:HD21	1:382:A:ARG:HD2	14	0.14
(1,2693)	1:437:A:VAL:HG22	1:441:A:GLN:HE22	14	0.14
(1,2682)	1:418:A:THR:HG22	1:419:A:PRO:HD2	1	0.14
(1,2682)	1:418:A:THR:HG21	1:419:A:PRO:HD2	10	0.14
(1,2663)	1:411:A:LEU:HD23	1:387:A:TYR:HE2	2	0.14
(1,2663)	1:411:A:LEU:HD22	1:387:A:TYR:HE2	19	0.14
(1,2659)	1:366:A:ILE:HD11	1:411:A:LEU:HB3	8	0.14
(1,2649)	1:403:A:ILE:HG22	1:364:A:PHE:HZ	11	0.14
(1,2618)	1:375:A:LEU:HD21	1:378:A:ASN:HB2	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2598)	1:363:A:ILE:HG22	1:357:A:GLU:HG2	4	0.14
(1,2597)	1:358:A:ASP:HB2	1:363:A:ILE:HG21	18	0.14
(1,2595)	1:451:A:ALA:H	1:450:A:ILE:HG23	1	0.14
(1,2587)	1:362:A:LYS:HA	1:415:A:PHE:HD2	13	0.14
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD13	2	0.14
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD13	3	0.14
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD12	5	0.14
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD12	7	0.14
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD11	8	0.14
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD11	14	0.14
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD11	16	0.14
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD12	19	0.14
(1,2537)	1:394:A:LEU:H	1:394:A:LEU:HD13	4	0.14
(1,2537)	1:394:A:LEU:H	1:394:A:LEU:HD13	15	0.14
(1,2529)	1:373:A:ALA:H	1:373:A:ALA:HB3	11	0.14
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG23	7	0.14
(1,2524)	1:364:A:PHE:H	1:363:A:ILE:HG21	12	0.14
(1,2499)	1:421:A:GLU:H	1:420:A:ASP:HB2	12	0.14
(1,2412)	1:451:A:ALA:H	1:456:A:TRP:HZ2	8	0.14
(1,2406)	1:383:A:THR:H	1:382:A:ARG:HG2	4	0.14
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD22	2	0.14
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD22	3	0.14
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD22	12	0.14
(1,2295)	1:356:A:TRP:HE1	1:345:A:LEU:HG	8	0.14
(1,2295)	1:356:A:TRP:HE1	1:345:A:LEU:HG	19	0.14
(1,2216)	1:408:A:GLY:H	1:409:A:GLN:HG3	5	0.14
(1,2213)	1:405:A:LYS:H	1:405:A:LYS:HG2	6	0.14
(1,2199)	1:412:A:LEU:H	1:412:A:LEU:HD11	18	0.14
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD13	3	0.14
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD11	17	0.14
(1,1990)	1:353:A:PHE:H	1:354:A:ILE:HG23	12	0.14
(1,1892)	1:403:A:ILE:HD12	1:402:A:ILE:HG22	14	0.14
(1,1892)	1:403:A:ILE:HD13	1:402:A:ILE:HG23	15	0.14
(1,1883)	1:393:A:ALA:HB1	1:437:A:VAL:HG22	1	0.14
(1,1883)	1:393:A:ALA:HB2	1:437:A:VAL:HG22	7	0.14
(1,1874)	1:382:A:ARG:HD3	1:382:A:ARG:HA	7	0.14
(1,1828)	1:398:A:TYR:HA	1:399:A:LYS:HD2	13	0.14
(1,1827)	1:430:A:LEU:HB3	1:430:A:LEU:HD21	4	0.14
(1,1827)	1:430:A:LEU:HB3	1:430:A:LEU:HD22	10	0.14
(1,1827)	1:430:A:LEU:HB3	1:430:A:LEU:HD22	15	0.14
(1,1820)	1:392:A:ARG:HB3	1:392:A:ARG:HA	10	0.14
(1,1802)	1:336:A:LEU:HD11	1:431:A:GLU:HA	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1778)	1:337:A:LEU:HD13	1:376:A:TRP:HB3	18	0.14
(1,1756)	1:402:A:ILE:HB	1:397:A:TYR:HB2	7	0.14
(1,1756)	1:402:A:ILE:HB	1:397:A:TYR:HB2	9	0.14
(1,1740)	1:339:A:ASP:HB2	1:419:A:PRO:HG3	8	0.14
(1,1740)	1:339:A:ASP:HB2	1:419:A:PRO:HG3	11	0.14
(1,1740)	1:339:A:ASP:HB2	1:419:A:PRO:HG3	12	0.14
(1,1740)	1:339:A:ASP:HB2	1:419:A:PRO:HG3	16	0.14
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	2	0.14
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	4	0.14
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	7	0.14
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	15	0.14
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	16	0.14
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	17	0.14
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	19	0.14
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	1	0.14
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	5	0.14
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	11	0.14
(1,1672)	1:403:A:ILE:HG21	1:405:A:LYS:H	1	0.14
(1,1672)	1:403:A:ILE:HG21	1:405:A:LYS:H	14	0.14
(1,1672)	1:403:A:ILE:HG23	1:405:A:LYS:H	16	0.14
(1,1667)	1:403:A:ILE:HG12	1:403:A:ILE:H	19	0.14
(1,1645)	1:404:A:ARG:HB3	1:404:A:ARG:HG3	10	0.14
(1,1645)	1:404:A:ARG:HB3	1:404:A:ARG:HG3	18	0.14
(1,1629)	1:406:A:GLU:HG3	1:412:A:LEU:HD12	19	0.14
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	4	0.14
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	8	0.14
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	15	0.14
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	19	0.14
(1,1611)	1:410:A:ARG:HG3	1:410:A:ARG:H	5	0.14
(1,1606)	1:411:A:LEU:HD13	1:369:A:PRO:HA	3	0.14
(1,1606)	1:411:A:LEU:HD12	1:369:A:PRO:HA	12	0.14
(1,1604)	1:365:A:ARG:HB2	1:412:A:LEU:HD13	10	0.14
(1,1603)	1:357:A:GLU:HG2	1:412:A:LEU:HD11	13	0.14
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	5	0.14
(1,1541)	1:445:A:GLU:HA	1:443:A:TYR:HD1	15	0.14
(1,1533)	1:378:A:ASN:HB2	1:375:A:LEU:HA	17	0.14
(1,1505)	1:385:A:MET:HA	1:389:A:LYS:HB2	3	0.14
(1,1485)	1:432:A:HIS:HD2	1:433:A:LEU:HD22	10	0.14
(1,1462)	1:435:A:SER:H	1:434:A:GLU:HB3	11	0.14
(1,1453)	1:438:A:LEU:HD12	1:435:A:SER:H	9	0.14
(1,1452)	1:361:A:SER:H	1:360:A:GLU:HG2	7	0.14
(1,1438)	1:444:A:GLN:HA	1:444:A:GLN:HB2	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1372)	1:390:A:MET:HG2	1:390:A:MET:H	16	0.14
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	19	0.14
(1,1323)	1:400:A:LEU:HB2	1:400:A:LEU:HD22	7	0.14
(1,1320)	1:374:A:ARG:H	1:374:A:ARG:HG2	18	0.14
(1,1311)	1:421:A:GLU:HA	1:421:A:GLU:HG3	4	0.14
(1,1311)	1:421:A:GLU:HA	1:421:A:GLU:HG3	13	0.14
(1,1311)	1:421:A:GLU:HA	1:421:A:GLU:HG3	14	0.14
(1,1311)	1:421:A:GLU:HA	1:421:A:GLU:HG3	18	0.14
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	15	0.14
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	18	0.14
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	7	0.14
(1,1267)	1:354:A:ILE:HD11	1:367:A:VAL:H	6	0.14
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	6	0.14
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	7	0.14
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	11	0.14
(1,1207)	1:360:A:GLU:HB3	1:360:A:GLU:HG2	1	0.14
(1,1182)	1:363:A:ILE:HD13	1:406:A:GLU:HG2	6	0.14
(1,1175)	1:363:A:ILE:HG21	1:363:A:ILE:HG13	4	0.14
(1,1175)	1:363:A:ILE:HG22	1:363:A:ILE:HG13	5	0.14
(1,1175)	1:363:A:ILE:HG23	1:363:A:ILE:HG13	13	0.14
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	3	0.14
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	13	0.14
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG12	4	0.14
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG13	5	0.14
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG12	8	0.14
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG11	9	0.14
(1,1134)	1:367:A:VAL:HG11	1:354:A:ILE:H	5	0.14
(1,1128)	1:355:A:ARG:HB3	1:367:A:VAL:HG21	4	0.14
(1,1123)	1:354:A:ILE:H	1:367:A:VAL:HG23	15	0.14
(1,1118)	1:367:A:VAL:HG22	1:366:A:ILE:HA	1	0.14
(1,1118)	1:367:A:VAL:HG21	1:366:A:ILE:HA	3	0.14
(1,1118)	1:367:A:VAL:HG23	1:366:A:ILE:HA	14	0.14
(1,1118)	1:367:A:VAL:HG21	1:366:A:ILE:HA	19	0.14
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	12	0.14
(1,1085)	1:373:A:ALA:HA	1:390:A:MET:HA	18	0.14
(1,1084)	1:372:A:LEU:HD11	1:344:A:LEU:HD13	19	0.14
(1,1077)	1:372:A:LEU:HD11	1:340:A:TYR:HD2	4	0.14
(1,1045)	1:349:A:ARG:HG2	1:349:A:ARG:HD2	13	0.14
(1,1016)	1:338:A:TRP:HH2	1:422:A:ILE:HG23	7	0.14
(1,979)	1:453:A:PRO:HG2	1:453:A:PRO:HB3	7	0.14
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG23	9	0.14
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG23	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,960)	1:450:A:ILE:HA	1:450:A:ILE:HG13	6	0.14
(1,959)	1:449:A:THR:HG22	1:449:A:THR:HB	1	0.14
(1,959)	1:449:A:THR:HG23	1:449:A:THR:HB	11	0.14
(1,956)	1:450:A:ILE:H	1:449:A:THR:HB	2	0.14
(1,947)	1:447:A:GLU:HG2	1:447:A:GLU:HA	1	0.14
(1,947)	1:447:A:GLU:HG2	1:447:A:GLU:HA	6	0.14
(1,903)	1:438:A:LEU:HD23	1:438:A:LEU:HB3	10	0.14
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD21	5	0.14
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD22	7	0.14
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD22	18	0.14
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD22	19	0.14
(1,885)	1:437:A:VAL:HG13	1:393:A:ALA:HA	11	0.14
(1,885)	1:437:A:VAL:HG13	1:393:A:ALA:HA	13	0.14
(1,885)	1:437:A:VAL:HG13	1:393:A:ALA:HA	15	0.14
(1,885)	1:437:A:VAL:HG11	1:393:A:ALA:HA	16	0.14
(1,884)	1:437:A:VAL:HG23	1:392:A:ARG:HG3	9	0.14
(1,876)	1:436:A:GLN:HB2	1:437:A:VAL:HG12	13	0.14
(1,859)	1:436:A:GLN:H	1:434:A:GLU:HA	12	0.14
(1,859)	1:436:A:GLN:H	1:434:A:GLU:HA	16	0.14
(1,845)	1:431:A:GLU:HA	1:431:A:GLU:HG3	12	0.14
(1,845)	1:431:A:GLU:HA	1:431:A:GLU:HG3	19	0.14
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	2	0.14
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	3	0.14
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	5	0.14
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	7	0.14
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	8	0.14
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	9	0.14
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	10	0.14
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	11	0.14
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	12	0.14
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	15	0.14
(1,812)	1:418:A:THR:H	1:418:A:THR:HG22	11	0.14
(1,812)	1:418:A:THR:H	1:418:A:THR:HG23	18	0.14
(1,802)	1:426:A:ARG:H	1:426:A:ARG:HG3	6	0.14
(1,713)	1:414:A:ARG:HE	1:414:A:ARG:HB3	17	0.14
(1,699)	1:413:A:PHE:HB2	1:364:A:PHE:HE2	4	0.14
(1,699)	1:413:A:PHE:HB2	1:364:A:PHE:HE2	13	0.14
(1,699)	1:413:A:PHE:HB2	1:364:A:PHE:HE2	16	0.14
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD13	3	0.14
(1,678)	1:411:A:LEU:HA	1:411:A:LEU:HD22	2	0.14
(1,666)	1:352:A:ASN:HA	1:351:A:GLU:HG3	4	0.14
(1,666)	1:352:A:ASN:HA	1:351:A:GLU:HG2	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,645)	1:406:A:GLU:H	1:405:A:LYS:HG2	1	0.14
(1,629)	1:403:A:ILE:HD12	1:415:A:PHE:HD1	3	0.14
(1,601)	1:401:A:ASN:HD21	1:401:A:ASN:HB3	15	0.14
(1,595)	1:400:A:LEU:HD22	1:400:A:LEU:HG	2	0.14
(1,595)	1:400:A:LEU:HD22	1:400:A:LEU:HG	9	0.14
(1,594)	1:400:A:LEU:HD23	1:426:A:ARG:HG3	9	0.14
(1,590)	1:400:A:LEU:HD11	1:397:A:TYR:HE1	3	0.14
(1,590)	1:400:A:LEU:HD12	1:397:A:TYR:HE1	6	0.14
(1,589)	1:400:A:LEU:HA	1:400:A:LEU:HD22	19	0.14
(1,556)	1:397:A:TYR:HA	1:400:A:LEU:HB3	4	0.14
(1,547)	1:395:A:ARG:HD2	1:395:A:ARG:H	6	0.14
(1,544)	1:395:A:ARG:HB2	1:395:A:ARG:HD3	18	0.14
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	5	0.14
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	12	0.14
(1,454)	1:386:A:THR:HG21	1:370:A:ASN:HA	10	0.14
(1,435)	1:382:A:ARG:HB2	1:382:A:ARG:HD2	18	0.14
(1,364)	1:374:A:ARG:HA	1:374:A:ARG:HG3	17	0.14
(1,359)	1:374:A:ARG:HA	1:374:A:ARG:HB3	2	0.14
(1,359)	1:374:A:ARG:HA	1:374:A:ARG:HB2	3	0.14
(1,359)	1:374:A:ARG:HA	1:374:A:ARG:HB3	5	0.14
(1,359)	1:374:A:ARG:HA	1:374:A:ARG:HB3	12	0.14
(1,301)	1:366:A:ILE:HG22	1:372:A:LEU:HB3	2	0.14
(1,301)	1:366:A:ILE:HG21	1:372:A:LEU:HB3	12	0.14
(1,266)	1:363:A:ILE:HG23	1:406:A:GLU:HG2	3	0.14
(1,266)	1:363:A:ILE:HG22	1:406:A:GLU:HG2	8	0.14
(1,266)	1:363:A:ILE:HG21	1:406:A:GLU:HG2	15	0.14
(1,138)	1:351:A:GLU:HG3	1:351:A:GLU:HB2	2	0.14
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	1	0.14
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	10	0.14
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	15	0.14
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	18	0.14
(1,112)	1:347:A:ASP:H	1:347:A:ASP:HB3	19	0.14
(1,58)	1:343:A:GLN:HG3	1:343:A:GLN:HB2	6	0.14
(1,58)	1:343:A:GLN:HG3	1:343:A:GLN:HB2	7	0.14
(1,41)	1:341:A:VAL:HG22	1:364:A:PHE:HZ	15	0.14
(1,37)	1:341:A:VAL:HG12	1:341:A:VAL:HG22	6	0.14
(1,37)	1:341:A:VAL:HG12	1:341:A:VAL:HG22	13	0.14
(1,15)	1:339:A:ASP:HB3	1:336:A:LEU:HB2	17	0.14
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	2	0.13
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	4	0.13
(1,2973)	1:434:A:GLU:H	1:433:A:LEU:HB2	11	0.13
(1,2945)	1:364:A:PHE:H	1:412:A:LEU:HG	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2945)	1:364:A:PHE:H	1:412:A:LEU:HG	2	0.13
(1,2945)	1:364:A:PHE:H	1:412:A:LEU:HG	3	0.13
(1,2945)	1:364:A:PHE:H	1:412:A:LEU:HG	8	0.13
(1,2945)	1:364:A:PHE:H	1:412:A:LEU:HG	18	0.13
(1,2931)	1:420:A:ASP:H	1:421:A:GLU:HG3	5	0.13
(1,2895)	1:353:A:PHE:H	1:367:A:VAL:HG22	6	0.13
(1,2871)	1:447:A:GLU:HG2	1:447:A:GLU:HB3	11	0.13
(1,2867)	1:372:A:LEU:HD12	1:340:A:TYR:HE2	12	0.13
(1,2850)	1:344:A:LEU:HD11	1:350:A:TYR:HD2	17	0.13
(1,2845)	1:402:A:ILE:HD13	1:338:A:TRP:HB2	16	0.13
(1,2837)	1:404:A:ARG:HD3	1:404:A:ARG:HB3	13	0.13
(1,2812)	1:421:A:GLU:HB3	1:421:A:GLU:HA	12	0.13
(1,2811)	1:428:A:ASP:HA	1:431:A:GLU:HB2	2	0.13
(1,2811)	1:428:A:ASP:HA	1:431:A:GLU:HB2	12	0.13
(1,2811)	1:428:A:ASP:HA	1:431:A:GLU:HB2	17	0.13
(1,2786)	1:446:A:ASP:H	1:445:A:GLU:HG2	1	0.13
(1,2762)	1:394:A:LEU:HD21	1:398:A:TYR:HE1	6	0.13
(1,2739)	1:362:A:LYS:HB2	1:356:A:TRP:HZ3	5	0.13
(1,2739)	1:362:A:LYS:HB2	1:356:A:TRP:HZ3	17	0.13
(1,2725)	1:367:A:VAL:HG21	1:365:A:ARG:HB3	8	0.13
(1,2724)	1:367:A:VAL:HG21	1:352:A:ASN:HA	13	0.13
(1,2719)	1:372:A:LEU:HD13	1:340:A:TYR:HD2	13	0.13
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD12	3	0.13
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD12	16	0.13
(1,2705)	1:394:A:LEU:HA	1:397:A:TYR:HD2	15	0.13
(1,2693)	1:437:A:VAL:HG21	1:441:A:GLN:HE22	8	0.13
(1,2686)	1:430:A:LEU:HD13	1:402:A:ILE:HD13	5	0.13
(1,2682)	1:418:A:THR:HG23	1:419:A:PRO:HD2	6	0.13
(1,2682)	1:418:A:THR:HG21	1:419:A:PRO:HD2	18	0.13
(1,2662)	1:411:A:LEU:HD23	1:366:A:ILE:HB	9	0.13
(1,2662)	1:411:A:LEU:HD22	1:366:A:ILE:HB	12	0.13
(1,2650)	1:403:A:ILE:HD12	1:338:A:TRP:HA	3	0.13
(1,2649)	1:403:A:ILE:HG23	1:364:A:PHE:HZ	5	0.13
(1,2649)	1:403:A:ILE:HG21	1:364:A:PHE:HZ	13	0.13
(1,2603)	1:368:A:ASP:H	1:366:A:ILE:HA	6	0.13
(1,2603)	1:368:A:ASP:H	1:366:A:ILE:HA	11	0.13
(1,2599)	1:363:A:ILE:HG22	1:363:A:ILE:HB	3	0.13
(1,2599)	1:363:A:ILE:HG21	1:363:A:ILE:HB	5	0.13
(1,2599)	1:363:A:ILE:HG21	1:363:A:ILE:HB	6	0.13
(1,2599)	1:363:A:ILE:HG22	1:363:A:ILE:HB	13	0.13
(1,2599)	1:363:A:ILE:HG22	1:363:A:ILE:HB	15	0.13
(1,2599)	1:363:A:ILE:HG23	1:363:A:ILE:HB	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2598)	1:363:A:ILE:HG21	1:357:A:GLU:HG3	16	0.13
(1,2597)	1:358:A:ASP:HB2	1:363:A:ILE:HG21	5	0.13
(1,2596)	1:363:A:ILE:HG21	1:364:A:PHE:HA	2	0.13
(1,2595)	1:451:A:ALA:H	1:450:A:ILE:HG23	13	0.13
(1,2587)	1:362:A:LYS:HA	1:415:A:PHE:HD2	5	0.13
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD12	4	0.13
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD12	10	0.13
(1,2576)	1:354:A:ILE:HG12	1:354:A:ILE:HD12	11	0.13
(1,2567)	1:345:A:LEU:HD22	1:355:A:ARG:HA	2	0.13
(1,2557)	1:341:A:VAL:HG13	1:403:A:ILE:HD13	15	0.13
(1,2552)	1:452:A:SER:H	1:451:A:ALA:HB3	13	0.13
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD11	10	0.13
(1,2537)	1:394:A:LEU:H	1:394:A:LEU:HD13	10	0.13
(1,2529)	1:373:A:ALA:H	1:373:A:ALA:HB2	15	0.13
(1,2499)	1:421:A:GLU:H	1:420:A:ASP:HB2	10	0.13
(1,2499)	1:421:A:GLU:H	1:420:A:ASP:HB2	17	0.13
(1,2476)	1:404:A:ARG:H	1:413:A:PHE:HB2	3	0.13
(1,2415)	1:447:A:GLU:H	1:448:A:PRO:HD3	5	0.13
(1,2412)	1:451:A:ALA:H	1:456:A:TRP:HZ2	18	0.13
(1,2406)	1:383:A:THR:H	1:382:A:ARG:HG2	19	0.13
(1,2359)	1:382:A:ARG:H	1:382:A:ARG:HG3	18	0.13
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD21	17	0.13
(1,2295)	1:356:A:TRP:HE1	1:345:A:LEU:HG	1	0.13
(1,2295)	1:356:A:TRP:HE1	1:345:A:LEU:HG	7	0.13
(1,2295)	1:356:A:TRP:HE1	1:345:A:LEU:HG	17	0.13
(1,2266)	1:355:A:ARG:HE	1:367:A:VAL:HB	8	0.13
(1,2234)	1:417:A:LYS:H	1:417:A:LYS:HB3	14	0.13
(1,2199)	1:412:A:LEU:H	1:412:A:LEU:HD11	7	0.13
(1,2199)	1:412:A:LEU:H	1:412:A:LEU:HD13	10	0.13
(1,2162)	1:389:A:LYS:H	1:389:A:LYS:HG2	11	0.13
(1,2131)	1:380:A:LYS:H	1:380:A:LYS:HG2	18	0.13
(1,2122)	1:410:A:ARG:H	1:409:A:GLN:HG2	13	0.13
(1,2122)	1:410:A:ARG:H	1:409:A:GLN:HG2	17	0.13
(1,2120)	1:377:A:GLY:H	1:385:A:MET:HB3	15	0.13
(1,2106)	1:374:A:ARG:H	1:374:A:ARG:HG3	16	0.13
(1,2090)	1:371:A:GLY:H	1:370:A:ASN:HB2	2	0.13
(1,2090)	1:371:A:GLY:H	1:370:A:ASN:HB2	8	0.13
(1,2090)	1:371:A:GLY:H	1:370:A:ASN:HB2	13	0.13
(1,2090)	1:371:A:GLY:H	1:370:A:ASN:HB2	14	0.13
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD12	12	0.13
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD13	18	0.13
(1,1931)	1:335:A:ARG:H	1:336:A:LEU:HB2	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1920)	1:372:A:LEU:HD12	1:366:A:ILE:HD13	8	0.13
(1,1920)	1:372:A:LEU:HD11	1:366:A:ILE:HD13	17	0.13
(1,1901)	1:433:A:LEU:HD23	1:433:A:LEU:HD12	2	0.13
(1,1898)	1:427:A:THR:HG21	1:430:A:LEU:HD12	3	0.13
(1,1898)	1:427:A:THR:HG21	1:430:A:LEU:HD13	8	0.13
(1,1865)	1:431:A:GLU:HA	1:431:A:GLU:HB2	6	0.13
(1,1865)	1:431:A:GLU:HA	1:431:A:GLU:HB2	8	0.13
(1,1828)	1:398:A:TYR:HA	1:399:A:LYS:HD2	6	0.13
(1,1828)	1:398:A:TYR:HA	1:399:A:LYS:HD2	11	0.13
(1,1828)	1:398:A:TYR:HA	1:399:A:LYS:HD2	15	0.13
(1,1827)	1:430:A:LEU:HB3	1:430:A:LEU:HD23	14	0.13
(1,1825)	1:418:A:THR:HB	1:419:A:PRO:HD2	13	0.13
(1,1802)	1:336:A:LEU:HD11	1:431:A:GLU:HA	10	0.13
(1,1784)	1:337:A:LEU:HD13	1:340:A:TYR:H	6	0.13
(1,1784)	1:337:A:LEU:HD13	1:340:A:TYR:H	12	0.13
(1,1740)	1:339:A:ASP:HB2	1:419:A:PRO:HG3	10	0.13
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	5	0.13
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	11	0.13
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	12	0.13
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	18	0.13
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD21	2	0.13
(1,1717)	1:342:A:TYR:HA	1:345:A:LEU:HD21	13	0.13
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	4	0.13
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	10	0.13
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	14	0.13
(1,1673)	1:394:A:LEU:HB3	1:403:A:ILE:HD12	7	0.13
(1,1672)	1:403:A:ILE:HG21	1:405:A:LYS:H	6	0.13
(1,1667)	1:403:A:ILE:HG12	1:403:A:ILE:H	11	0.13
(1,1667)	1:403:A:ILE:HG12	1:403:A:ILE:H	18	0.13
(1,1645)	1:404:A:ARG:HB3	1:404:A:ARG:HG3	2	0.13
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	18	0.13
(1,1606)	1:411:A:LEU:HD12	1:369:A:PRO:HA	6	0.13
(1,1603)	1:357:A:GLU:HG2	1:412:A:LEU:HD13	7	0.13
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	4	0.13
(1,1556)	1:417:A:LYS:HE3	1:417:A:LYS:HG3	8	0.13
(1,1533)	1:378:A:ASN:HB2	1:375:A:LEU:HA	2	0.13
(1,1505)	1:385:A:MET:HA	1:389:A:LYS:HB2	2	0.13
(1,1438)	1:444:A:GLN:HA	1:444:A:GLN:HB2	15	0.13
(1,1429)	1:447:A:GLU:HA	1:447:A:GLU:HB2	11	0.13
(1,1429)	1:447:A:GLU:HA	1:447:A:GLU:HB2	15	0.13
(1,1429)	1:447:A:GLU:HA	1:447:A:GLU:HB2	18	0.13
(1,1412)	1:454:A:VAL:HB	1:450:A:ILE:HA	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1372)	1:390:A:MET:HG2	1:390:A:MET:H	2	0.13
(1,1372)	1:390:A:MET:HG2	1:390:A:MET:H	13	0.13
(1,1372)	1:390:A:MET:HG2	1:390:A:MET:H	14	0.13
(1,1332)	1:399:A:LYS:HA	1:399:A:LYS:HE2	5	0.13
(1,1328)	1:399:A:LYS:H	1:400:A:LEU:HD13	16	0.13
(1,1311)	1:421:A:GLU:HA	1:421:A:GLU:HG3	2	0.13
(1,1311)	1:421:A:GLU:HA	1:421:A:GLU:HG3	8	0.13
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	1	0.13
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	4	0.13
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	5	0.13
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	14	0.13
(1,1267)	1:354:A:ILE:HD13	1:367:A:VAL:H	8	0.13
(1,1263)	1:354:A:ILE:HG21	1:345:A:LEU:H	13	0.13
(1,1255)	1:355:A:ARG:HD2	1:355:A:ARG:HB3	12	0.13
(1,1224)	1:363:A:ILE:HG22	1:357:A:GLU:HG2	9	0.13
(1,1224)	1:363:A:ILE:HG21	1:357:A:GLU:HG2	16	0.13
(1,1218)	1:359:A:LYS:H	1:359:A:LYS:HD2	17	0.13
(1,1203)	1:360:A:GLU:H	1:360:A:GLU:HA	14	0.13
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	12	0.13
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	15	0.13
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD13	8	0.13
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD11	19	0.13
(1,1175)	1:363:A:ILE:HG23	1:363:A:ILE:HG13	16	0.13
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG23	17	0.13
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	8	0.13
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	12	0.13
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	16	0.13
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG12	1	0.13
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG13	3	0.13
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG12	7	0.13
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG11	13	0.13
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG13	14	0.13
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG11	17	0.13
(1,1011)	1:356:A:TRP:HH2	1:418:A:THR:HG21	18	0.13
(1,1003)	1:409:A:GLN:HG2	1:406:A:GLU:HB2	14	0.13
(1,1000)	1:409:A:GLN:HE21	1:409:A:GLN:HG2	17	0.13
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG23	3	0.13
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG23	14	0.13
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG22	16	0.13
(1,960)	1:450:A:ILE:HA	1:450:A:ILE:HG13	12	0.13
(1,960)	1:450:A:ILE:HA	1:450:A:ILE:HG13	16	0.13
(1,960)	1:450:A:ILE:HA	1:450:A:ILE:HG13	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,959)	1:449:A:THR:HG21	1:449:A:THR:HB	13	0.13
(1,956)	1:450:A:ILE:H	1:449:A:THR:HB	8	0.13
(1,954)	1:450:A:ILE:H	1:449:A:THR:HA	7	0.13
(1,947)	1:447:A:GLU:HG2	1:447:A:GLU:HA	7	0.13
(1,947)	1:447:A:GLU:HG2	1:447:A:GLU:HA	12	0.13
(1,946)	1:447:A:GLU:HG2	1:446:A:ASP:H	1	0.13
(1,926)	1:442:A:THR:H	1:441:A:GLN:HG2	12	0.13
(1,902)	1:438:A:LEU:HD12	1:376:A:TRP:HZ2	2	0.13
(1,898)	1:438:A:LEU:HD13	1:382:A:ARG:HG2	7	0.13
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD22	4	0.13
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD23	9	0.13
(1,887)	1:437:A:VAL:HG22	1:393:A:ALA:HA	1	0.13
(1,877)	1:436:A:GLN:H	1:436:A:GLN:HG2	19	0.13
(1,864)	1:433:A:LEU:HA	1:433:A:LEU:HD11	7	0.13
(1,859)	1:436:A:GLN:H	1:434:A:GLU:HA	1	0.13
(1,859)	1:436:A:GLN:H	1:434:A:GLU:HA	5	0.13
(1,859)	1:436:A:GLN:H	1:434:A:GLU:HA	13	0.13
(1,855)	1:432:A:HIS:HB2	1:432:A:HIS:HD2	11	0.13
(1,845)	1:431:A:GLU:HA	1:431:A:GLU:HG3	18	0.13
(1,828)	1:430:A:LEU:H	1:430:A:LEU:HB3	4	0.13
(1,822)	1:429:A:ARG:HA	1:429:A:ARG:HG2	6	0.13
(1,812)	1:418:A:THR:H	1:418:A:THR:HG23	3	0.13
(1,812)	1:418:A:THR:H	1:418:A:THR:HG21	4	0.13
(1,812)	1:418:A:THR:H	1:418:A:THR:HG21	9	0.13
(1,812)	1:418:A:THR:H	1:418:A:THR:HG23	10	0.13
(1,812)	1:418:A:THR:H	1:418:A:THR:HG21	13	0.13
(1,812)	1:418:A:THR:H	1:418:A:THR:HG21	14	0.13
(1,812)	1:418:A:THR:H	1:418:A:THR:HG23	15	0.13
(1,800)	1:426:A:ARG:HB2	1:426:A:ARG:HG2	14	0.13
(1,760)	1:338:A:TRP:HZ2	1:419:A:PRO:HA	4	0.13
(1,760)	1:338:A:TRP:HZ2	1:419:A:PRO:HA	14	0.13
(1,699)	1:413:A:PHE:HB2	1:364:A:PHE:HE2	1	0.13
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD13	7	0.13
(1,678)	1:411:A:LEU:HA	1:411:A:LEU:HD22	3	0.13
(1,595)	1:400:A:LEU:HD21	1:400:A:LEU:HG	7	0.13
(1,595)	1:400:A:LEU:HD22	1:400:A:LEU:HG	8	0.13
(1,595)	1:400:A:LEU:HD21	1:400:A:LEU:HG	16	0.13
(1,590)	1:400:A:LEU:HD11	1:397:A:TYR:HE1	2	0.13
(1,573)	1:399:A:LYS:HB2	1:396:A:HIS:HA	11	0.13
(1,528)	1:394:A:LEU:HD21	1:364:A:PHE:HZ	19	0.13
(1,508)	1:394:A:LEU:HA	1:397:A:TYR:HB3	10	0.13
(1,475)	1:389:A:LYS:HA	1:389:A:LYS:HG3	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,444)	1:384:A:ASN:HD21	1:384:A:ASN:HB2	5	0.13
(1,364)	1:374:A:ARG:HA	1:374:A:ARG:HG3	8	0.13
(1,364)	1:374:A:ARG:HA	1:374:A:ARG:HG3	10	0.13
(1,364)	1:374:A:ARG:HA	1:374:A:ARG:HG3	19	0.13
(1,360)	1:374:A:ARG:HA	1:374:A:ARG:HG2	16	0.13
(1,359)	1:374:A:ARG:HA	1:374:A:ARG:HB3	7	0.13
(1,266)	1:363:A:ILE:HG22	1:406:A:GLU:HG2	14	0.13
(1,232)	1:359:A:LYS:HG2	1:359:A:LYS:HE2	2	0.13
(1,203)	1:357:A:GLU:HB2	1:412:A:LEU:HD21	11	0.13
(1,177)	1:345:A:LEU:HD11	1:354:A:ILE:HD11	9	0.13
(1,138)	1:351:A:GLU:HG3	1:351:A:GLU:HB2	7	0.13
(1,138)	1:351:A:GLU:HG3	1:351:A:GLU:HB2	15	0.13
(1,138)	1:351:A:GLU:HG3	1:351:A:GLU:HB2	16	0.13
(1,127)	1:349:A:ARG:HD2	1:350:A:TYR:HE1	4	0.13
(1,127)	1:349:A:ARG:HD2	1:350:A:TYR:HE1	6	0.13
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	3	0.13
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	4	0.13
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	12	0.13
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD23	9	0.13
(1,104)	1:345:A:LEU:HD23	1:356:A:TRP:HE3	18	0.13
(1,93)	1:345:A:LEU:HA	1:354:A:ILE:HG22	15	0.13
(1,88)	1:346:A:SER:HB2	1:346:A:SER:HA	17	0.13
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	17	0.13
(1,58)	1:343:A:GLN:HG3	1:343:A:GLN:HB2	5	0.13
(1,58)	1:343:A:GLN:HG2	1:343:A:GLN:HB3	8	0.13
(1,58)	1:343:A:GLN:HG2	1:343:A:GLN:HB3	17	0.13
(1,41)	1:341:A:VAL:HG22	1:364:A:PHE:HZ	16	0.13
(1,37)	1:341:A:VAL:HG13	1:341:A:VAL:HG21	2	0.13
(1,37)	1:341:A:VAL:HG11	1:341:A:VAL:HG22	5	0.13
(1,2967)	1:444:A:GLN:H	1:444:A:GLN:HB3	9	0.12
(1,2945)	1:364:A:PHE:H	1:412:A:LEU:HG	5	0.12
(1,2945)	1:364:A:PHE:H	1:412:A:LEU:HG	6	0.12
(1,2945)	1:364:A:PHE:H	1:412:A:LEU:HG	11	0.12
(1,2945)	1:364:A:PHE:H	1:412:A:LEU:HG	13	0.12
(1,2945)	1:364:A:PHE:H	1:412:A:LEU:HG	16	0.12
(1,2945)	1:364:A:PHE:H	1:412:A:LEU:HG	17	0.12
(1,2945)	1:364:A:PHE:H	1:412:A:LEU:HG	19	0.12
(1,2936)	1:436:A:GLN:H	1:435:A:SER:HB2	7	0.12
(1,2931)	1:420:A:ASP:H	1:421:A:GLU:HG3	8	0.12
(1,2924)	1:442:A:THR:H	1:441:A:GLN:HA	17	0.12
(1,2918)	1:374:A:ARG:H	1:376:A:TRP:H	1	0.12
(1,2918)	1:374:A:ARG:H	1:376:A:TRP:H	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2871)	1:444:A:GLN:HB2	1:444:A:GLN:HG3	1	0.12
(1,2856)	1:342:A:TYR:HE1	1:342:A:TYR:HA	19	0.12
(1,2852)	1:343:A:GLN:HB3	1:340:A:TYR:HD1	3	0.12
(1,2850)	1:344:A:LEU:HD11	1:350:A:TYR:HD1	12	0.12
(1,2845)	1:402:A:ILE:HD12	1:338:A:TRP:HB2	6	0.12
(1,2838)	1:410:A:ARG:HG2	1:410:A:ARG:HD2	16	0.12
(1,2811)	1:428:A:ASP:HA	1:431:A:GLU:HB2	3	0.12
(1,2758)	1:375:A:LEU:HD21	1:340:A:TYR:HE2	18	0.12
(1,2758)	1:375:A:LEU:HD23	1:340:A:TYR:HE2	19	0.12
(1,2755)	1:354:A:ILE:HD13	1:345:A:LEU:H	19	0.12
(1,2748)	1:359:A:LYS:HA	1:359:A:LYS:HE2	6	0.12
(1,2739)	1:362:A:LYS:HB2	1:356:A:TRP:HZ3	11	0.12
(1,2739)	1:362:A:LYS:HB2	1:356:A:TRP:HZ3	14	0.12
(1,2728)	1:366:A:ILE:HB	1:413:A:PHE:HZ	10	0.12
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD11	6	0.12
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD11	7	0.12
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD13	9	0.12
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD13	11	0.12
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD11	15	0.12
(1,2682)	1:418:A:THR:HG22	1:419:A:PRO:HD2	4	0.12
(1,2667)	1:414:A:ARG:HA	1:414:A:ARG:HD2	13	0.12
(1,2662)	1:411:A:LEU:HD21	1:366:A:ILE:HB	4	0.12
(1,2650)	1:403:A:ILE:HD13	1:338:A:TRP:HA	7	0.12
(1,2649)	1:403:A:ILE:HG23	1:364:A:PHE:HZ	15	0.12
(1,2618)	1:375:A:LEU:HD22	1:378:A:ASN:HB2	13	0.12
(1,2612)	1:393:A:ALA:HB1	1:376:A:TRP:HZ3	13	0.12
(1,2603)	1:368:A:ASP:H	1:366:A:ILE:HA	10	0.12
(1,2599)	1:363:A:ILE:HG21	1:363:A:ILE:HB	1	0.12
(1,2599)	1:363:A:ILE:HG22	1:363:A:ILE:HB	4	0.12
(1,2599)	1:363:A:ILE:HG23	1:363:A:ILE:HB	10	0.12
(1,2599)	1:363:A:ILE:HG21	1:363:A:ILE:HB	11	0.12
(1,2599)	1:363:A:ILE:HG22	1:363:A:ILE:HB	16	0.12
(1,2597)	1:358:A:ASP:HB2	1:363:A:ILE:HG23	8	0.12
(1,2597)	1:358:A:ASP:HB2	1:363:A:ILE:HG23	19	0.12
(1,2557)	1:341:A:VAL:HG13	1:403:A:ILE:HD13	2	0.12
(1,2537)	1:394:A:LEU:H	1:394:A:LEU:HD12	9	0.12
(1,2529)	1:373:A:ALA:H	1:373:A:ALA:HB1	14	0.12
(1,2516)	1:342:A:TYR:H	1:341:A:VAL:HG23	10	0.12
(1,2516)	1:342:A:TYR:H	1:341:A:VAL:HG23	12	0.12
(1,2516)	1:342:A:TYR:H	1:341:A:VAL:HG21	15	0.12
(1,2493)	1:440:A:GLU:H	1:439:A:ASP:HB3	6	0.12
(1,2413)	1:449:A:THR:H	1:448:A:PRO:HB3	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2412)	1:451:A:ALA:H	1:456:A:TRP:HZ2	11	0.12
(1,2406)	1:383:A:THR:H	1:382:A:ARG:HG2	9	0.12
(1,2406)	1:383:A:THR:H	1:382:A:ARG:HG2	12	0.12
(1,2359)	1:382:A:ARG:H	1:382:A:ARG:HG3	9	0.12
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD21	19	0.12
(1,2295)	1:356:A:TRP:HE1	1:345:A:LEU:HG	14	0.12
(1,2295)	1:356:A:TRP:HE1	1:345:A:LEU:HG	15	0.12
(1,2276)	1:410:A:ARG:HE	1:365:A:ARG:HE	10	0.12
(1,2216)	1:408:A:GLY:H	1:409:A:GLN:HG3	4	0.12
(1,2184)	1:435:A:SER:H	1:432:A:HIS:HA	4	0.12
(1,2143)	1:386:A:THR:H	1:373:A:ALA:HB3	6	0.12
(1,2126)	1:410:A:ARG:H	1:410:A:ARG:HB3	19	0.12
(1,2067)	1:365:A:ARG:H	1:355:A:ARG:HG2	11	0.12
(1,2044)	1:411:A:LEU:H	1:412:A:LEU:HD21	19	0.12
(1,2025)	1:381:A:ASN:H	1:381:A:ASN:HB3	5	0.12
(1,1920)	1:372:A:LEU:HD12	1:366:A:ILE:HD12	4	0.12
(1,1920)	1:372:A:LEU:HD13	1:366:A:ILE:HD13	12	0.12
(1,1877)	1:388:A:GLU:H	1:388:A:GLU:HG2	5	0.12
(1,1873)	1:383:A:THR:HG21	1:384:A:ASN:HD22	9	0.12
(1,1865)	1:431:A:GLU:HA	1:431:A:GLU:HB2	1	0.12
(1,1865)	1:431:A:GLU:HA	1:431:A:GLU:HB2	3	0.12
(1,1865)	1:431:A:GLU:HA	1:431:A:GLU:HB2	4	0.12
(1,1865)	1:431:A:GLU:HA	1:431:A:GLU:HB2	5	0.12
(1,1865)	1:431:A:GLU:HA	1:431:A:GLU:HB2	9	0.12
(1,1865)	1:431:A:GLU:HA	1:431:A:GLU:HB2	16	0.12
(1,1833)	1:340:A:TYR:HE2	1:375:A:LEU:HG	13	0.12
(1,1828)	1:398:A:TYR:HA	1:399:A:LYS:HD2	10	0.12
(1,1827)	1:430:A:LEU:HB3	1:430:A:LEU:HD21	12	0.12
(1,1827)	1:430:A:LEU:HB3	1:430:A:LEU:HD23	17	0.12
(1,1780)	1:337:A:LEU:HD13	1:376:A:TRP:HA	2	0.12
(1,1761)	1:340:A:TYR:HB2	1:337:A:LEU:HA	14	0.12
(1,1756)	1:402:A:ILE:HB	1:397:A:TYR:HB2	12	0.12
(1,1756)	1:402:A:ILE:HB	1:397:A:TYR:HB2	16	0.12
(1,1740)	1:339:A:ASP:HB2	1:419:A:PRO:HG3	1	0.12
(1,1740)	1:339:A:ASP:HB2	1:419:A:PRO:HG3	6	0.12
(1,1740)	1:339:A:ASP:HB2	1:419:A:PRO:HG3	15	0.12
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	3	0.12
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	8	0.12
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	9	0.12
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	19	0.12
(1,1666)	1:403:A:ILE:HG13	1:364:A:PHE:HZ	8	0.12
(1,1666)	1:403:A:ILE:HG13	1:364:A:PHE:HZ	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1659)	1:404:A:ARG:HB2	1:404:A:ARG:HD3	5	0.12
(1,1645)	1:404:A:ARG:HB3	1:404:A:ARG:HG3	4	0.12
(1,1645)	1:404:A:ARG:HB3	1:404:A:ARG:HG3	11	0.12
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	1	0.12
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	2	0.12
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	9	0.12
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	11	0.12
(1,1580)	1:413:A:PHE:HB2	1:413:A:PHE:HD1	10	0.12
(1,1567)	1:422:A:ILE:HD11	1:415:A:PHE:HD1	11	0.12
(1,1505)	1:385:A:MET:HA	1:389:A:LYS:HB2	6	0.12
(1,1502)	1:422:A:ILE:HA	1:427:A:THR:HG22	18	0.12
(1,1488)	1:431:A:GLU:HB2	1:336:A:LEU:HD21	15	0.12
(1,1479)	1:433:A:LEU:HD12	1:393:A:ALA:HA	10	0.12
(1,1452)	1:361:A:SER:H	1:360:A:GLU:HG2	11	0.12
(1,1444)	1:442:A:THR:HG22	1:443:A:TYR:HA	14	0.12
(1,1429)	1:447:A:GLU:HA	1:447:A:GLU:HB2	16	0.12
(1,1429)	1:447:A:GLU:HA	1:447:A:GLU:HB2	19	0.12
(1,1423)	1:450:A:ILE:H	1:450:A:ILE:HG12	7	0.12
(1,1390)	1:387:A:TYR:HE2	1:390:A:MET:HG2	5	0.12
(1,1349)	1:443:A:TYR:HE1	1:445:A:GLU:HA	7	0.12
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	12	0.12
(1,1332)	1:399:A:LYS:HA	1:399:A:LYS:HE2	19	0.12
(1,1311)	1:421:A:GLU:HA	1:421:A:GLU:HG3	1	0.12
(1,1311)	1:421:A:GLU:HA	1:421:A:GLU:HG3	5	0.12
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	3	0.12
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	9	0.12
(1,1265)	1:354:A:ILE:HG22	1:355:A:ARG:H	7	0.12
(1,1250)	1:345:A:LEU:HD22	1:355:A:ARG:HA	2	0.12
(1,1224)	1:363:A:ILE:HG21	1:357:A:GLU:HG2	18	0.12
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	1	0.12
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	12	0.12
(1,1219)	1:357:A:GLU:HG3	1:357:A:GLU:HA	13	0.12
(1,1203)	1:360:A:GLU:H	1:360:A:GLU:HA	4	0.12
(1,1203)	1:360:A:GLU:H	1:360:A:GLU:HA	12	0.12
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	4	0.12
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	14	0.12
(1,1181)	1:358:A:ASP:HB2	1:363:A:ILE:HD13	16	0.12
(1,1180)	1:363:A:ILE:HD13	1:414:A:ARG:HD2	1	0.12
(1,1175)	1:363:A:ILE:HG21	1:363:A:ILE:HG13	10	0.12
(1,1175)	1:363:A:ILE:HG21	1:363:A:ILE:HG13	15	0.12
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG22	1	0.12
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG22	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG22	11	0.12
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	7	0.12
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG11	10	0.12
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG13	15	0.12
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG11	16	0.12
(1,1130)	1:365:A:ARG:HG2	1:367:A:VAL:HG21	8	0.12
(1,1121)	1:367:A:VAL:HG21	1:365:A:ARG:HA	15	0.12
(1,1121)	1:367:A:VAL:HG22	1:365:A:ARG:HA	18	0.12
(1,1118)	1:367:A:VAL:HG21	1:366:A:ILE:HA	7	0.12
(1,1084)	1:372:A:LEU:HD11	1:344:A:LEU:HD12	9	0.12
(1,1044)	1:349:A:ARG:HB2	1:349:A:ARG:HG3	2	0.12
(1,1044)	1:349:A:ARG:HB2	1:349:A:ARG:HG3	11	0.12
(1,1016)	1:338:A:TRP:HH2	1:422:A:ILE:HG23	2	0.12
(1,1011)	1:356:A:TRP:HH2	1:418:A:THR:HG22	9	0.12
(1,1011)	1:356:A:TRP:HH2	1:418:A:THR:HG22	13	0.12
(1,995)	1:457:A:PRO:HD2	1:456:A:TRP:HA	7	0.12
(1,978)	1:453:A:PRO:HA	1:450:A:ILE:HD12	10	0.12
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG21	1	0.12
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG22	4	0.12
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG22	6	0.12
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG23	8	0.12
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG23	9	0.12
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG23	11	0.12
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG22	12	0.12
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG23	13	0.12
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG21	19	0.12
(1,956)	1:450:A:ILE:H	1:449:A:THR:HB	14	0.12
(1,947)	1:447:A:GLU:HG2	1:447:A:GLU:HA	2	0.12
(1,947)	1:447:A:GLU:HG2	1:447:A:GLU:HA	3	0.12
(1,930)	1:443:A:TYR:HA	1:443:A:TYR:HB3	11	0.12
(1,893)	1:438:A:LEU:HB2	1:438:A:LEU:HD21	15	0.12
(1,887)	1:437:A:VAL:HG22	1:393:A:ALA:HA	6	0.12
(1,887)	1:437:A:VAL:HG21	1:393:A:ALA:HA	15	0.12
(1,885)	1:437:A:VAL:HG11	1:393:A:ALA:HA	12	0.12
(1,876)	1:436:A:GLN:HB2	1:437:A:VAL:HG13	7	0.12
(1,859)	1:436:A:GLN:H	1:434:A:GLU:HA	15	0.12
(1,855)	1:432:A:HIS:HB2	1:432:A:HIS:HD2	1	0.12
(1,855)	1:432:A:HIS:HB2	1:432:A:HIS:HD2	12	0.12
(1,850)	1:431:A:GLU:HG3	1:431:A:GLU:HB2	8	0.12
(1,845)	1:431:A:GLU:HA	1:431:A:GLU:HG3	2	0.12
(1,842)	1:430:A:LEU:HG	1:430:A:LEU:HD22	6	0.12
(1,812)	1:418:A:THR:H	1:418:A:THR:HG22	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,812)	1:418:A:THR:H	1:418:A:THR:HG22	17	0.12
(1,801)	1:426:A:ARG:HG3	1:426:A:ARG:HA	4	0.12
(1,800)	1:426:A:ARG:HB2	1:426:A:ARG:HG2	4	0.12
(1,791)	1:428:A:ASP:HA	1:428:A:ASP:HB3	2	0.12
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD13	1	0.12
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD12	6	0.12
(1,681)	1:411:A:LEU:HB3	1:411:A:LEU:HD13	11	0.12
(1,667)	1:409:A:GLN:HA	1:409:A:GLN:HG2	7	0.12
(1,667)	1:409:A:GLN:HA	1:409:A:GLN:HG2	17	0.12
(1,666)	1:352:A:ASN:HA	1:351:A:GLU:HG3	16	0.12
(1,645)	1:406:A:GLU:H	1:405:A:LYS:HG2	8	0.12
(1,645)	1:406:A:GLU:H	1:405:A:LYS:HG2	13	0.12
(1,629)	1:403:A:ILE:HD11	1:415:A:PHE:HD1	9	0.12
(1,612)	1:402:A:ILE:HD13	1:400:A:LEU:HB3	2	0.12
(1,612)	1:402:A:ILE:HD11	1:400:A:LEU:HB3	12	0.12
(1,593)	1:400:A:LEU:H	1:400:A:LEU:HD22	19	0.12
(1,589)	1:400:A:LEU:HA	1:400:A:LEU:HD21	7	0.12
(1,547)	1:395:A:ARG:HD2	1:395:A:ARG:H	9	0.12
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	13	0.12
(1,471)	1:388:A:GLU:HB3	1:388:A:GLU:HG2	17	0.12
(1,468)	1:388:A:GLU:HA	1:391:A:SER:HB3	13	0.12
(1,441)	1:384:A:ASN:H	1:383:A:THR:HB	9	0.12
(1,342)	1:372:A:LEU:HA	1:372:A:LEU:HD12	12	0.12
(1,342)	1:372:A:LEU:HA	1:372:A:LEU:HD13	13	0.12
(1,301)	1:366:A:ILE:HG23	1:372:A:LEU:HB3	6	0.12
(1,266)	1:363:A:ILE:HG21	1:406:A:GLU:HG2	4	0.12
(1,232)	1:359:A:LYS:HG2	1:359:A:LYS:HE2	11	0.12
(1,203)	1:357:A:GLU:HB2	1:412:A:LEU:HD22	9	0.12
(1,203)	1:357:A:GLU:HB2	1:412:A:LEU:HD23	16	0.12
(1,138)	1:351:A:GLU:HG3	1:351:A:GLU:HB2	18	0.12
(1,121)	1:349:A:ARG:H	1:349:A:ARG:HB3	3	0.12
(1,121)	1:349:A:ARG:H	1:349:A:ARG:HB3	15	0.12
(1,118)	1:348:A:SER:H	1:348:A:SER:HB3	11	0.12
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	6	0.12
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	9	0.12
(1,104)	1:345:A:LEU:HD22	1:356:A:TRP:HE3	17	0.12
(1,93)	1:345:A:LEU:HA	1:354:A:ILE:HG23	8	0.12
(1,88)	1:346:A:SER:HB2	1:346:A:SER:HA	8	0.12
(1,88)	1:346:A:SER:HB2	1:346:A:SER:HA	15	0.12
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	12	0.12
(1,58)	1:343:A:GLN:HG3	1:343:A:GLN:HB2	2	0.12
(1,58)	1:343:A:GLN:HG2	1:343:A:GLN:HB3	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:343:A:GLN:HG3	1:343:A:GLN:HB2	15	0.12
(1,37)	1:341:A:VAL:HG12	1:341:A:VAL:HG22	7	0.12
(1,27)	1:341:A:VAL:HA	1:372:A:LEU:HD13	3	0.12
(1,27)	1:341:A:VAL:HA	1:372:A:LEU:HD12	15	0.12
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	14	0.11
(1,2990)	1:364:A:PHE:H	1:363:A:ILE:HB	15	0.11
(1,2974)	1:433:A:LEU:H	1:436:A:GLN:HB3	4	0.11
(1,2971)	1:436:A:GLN:H	1:433:A:LEU:HA	12	0.11
(1,2964)	1:446:A:ASP:H	1:445:A:GLU:HB3	6	0.11
(1,2945)	1:364:A:PHE:H	1:412:A:LEU:HG	9	0.11
(1,2936)	1:436:A:GLN:H	1:435:A:SER:HB2	19	0.11
(1,2931)	1:420:A:ASP:H	1:421:A:GLU:HG3	10	0.11
(1,2924)	1:442:A:THR:H	1:441:A:GLN:HA	3	0.11
(1,2895)	1:353:A:PHE:H	1:367:A:VAL:HG23	2	0.11
(1,2890)	1:430:A:LEU:H	1:336:A:LEU:HD13	17	0.11
(1,2871)	1:447:A:GLU:HG2	1:447:A:GLU:HB3	10	0.11
(1,2867)	1:372:A:LEU:HD13	1:340:A:TYR:HE2	7	0.11
(1,2867)	1:372:A:LEU:HD13	1:340:A:TYR:HE2	15	0.11
(1,2836)	1:404:A:ARG:HG3	1:405:A:LYS:H	13	0.11
(1,2812)	1:375:A:LEU:HB3	1:375:A:LEU:HA	3	0.11
(1,2812)	1:421:A:GLU:HB3	1:421:A:GLU:HA	4	0.11
(1,2812)	1:421:A:GLU:HB3	1:421:A:GLU:HA	6	0.11
(1,2812)	1:375:A:LEU:HB3	1:375:A:LEU:HA	14	0.11
(1,2812)	1:375:A:LEU:HB3	1:375:A:LEU:HA	16	0.11
(1,2812)	1:375:A:LEU:HB3	1:375:A:LEU:HA	18	0.11
(1,2798)	1:412:A:LEU:HD22	1:410:A:ARG:HD2	14	0.11
(1,2763)	1:398:A:TYR:HD1	1:398:A:TYR:HE1	11	0.11
(1,2758)	1:375:A:LEU:HD22	1:340:A:TYR:HE2	6	0.11
(1,2739)	1:362:A:LYS:HB2	1:356:A:TRP:HZ3	15	0.11
(1,2739)	1:362:A:LYS:HB2	1:356:A:TRP:HZ3	16	0.11
(1,2728)	1:366:A:ILE:HB	1:413:A:PHE:HZ	1	0.11
(1,2728)	1:366:A:ILE:HB	1:413:A:PHE:HZ	18	0.11
(1,2721)	1:354:A:ILE:HD13	1:372:A:LEU:HD23	13	0.11
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD11	1	0.11
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD13	5	0.11
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD12	8	0.11
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD13	12	0.11
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD12	18	0.11
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD13	19	0.11
(1,2707)	1:349:A:ARG:HG3	1:350:A:TYR:HD2	8	0.11
(1,2707)	1:349:A:ARG:HG3	1:350:A:TYR:HD2	18	0.11
(1,2684)	1:429:A:ARG:HG2	1:433:A:LEU:HD23	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2682)	1:418:A:THR:HG22	1:419:A:PRO:HD2	9	0.11
(1,2682)	1:418:A:THR:HG22	1:419:A:PRO:HD2	14	0.11
(1,2682)	1:418:A:THR:HG22	1:419:A:PRO:HD2	19	0.11
(1,2663)	1:411:A:LEU:HD23	1:387:A:TYR:HE2	17	0.11
(1,2662)	1:411:A:LEU:HD23	1:366:A:ILE:HB	1	0.11
(1,2662)	1:411:A:LEU:HD23	1:366:A:ILE:HB	10	0.11
(1,2659)	1:366:A:ILE:HD11	1:411:A:LEU:HB3	18	0.11
(1,2618)	1:375:A:LEU:HD22	1:378:A:ASN:HB2	9	0.11
(1,2612)	1:393:A:ALA:HB3	1:376:A:TRP:HZ3	10	0.11
(1,2599)	1:363:A:ILE:HG21	1:363:A:ILE:HB	7	0.11
(1,2599)	1:363:A:ILE:HG22	1:363:A:ILE:HB	9	0.11
(1,2599)	1:363:A:ILE:HG21	1:363:A:ILE:HB	14	0.11
(1,2596)	1:363:A:ILE:HG22	1:364:A:PHE:HA	4	0.11
(1,2595)	1:451:A:ALA:H	1:450:A:ILE:HG22	10	0.11
(1,2544)	1:430:A:LEU:H	1:430:A:LEU:HD13	8	0.11
(1,2530)	1:375:A:LEU:H	1:375:A:LEU:HD23	5	0.11
(1,2529)	1:373:A:ALA:H	1:373:A:ALA:HB3	5	0.11
(1,2529)	1:373:A:ALA:H	1:373:A:ALA:HB1	9	0.11
(1,2516)	1:342:A:TYR:H	1:341:A:VAL:HG22	3	0.11
(1,2516)	1:342:A:TYR:H	1:341:A:VAL:HG21	8	0.11
(1,2516)	1:342:A:TYR:H	1:341:A:VAL:HG21	16	0.11
(1,2516)	1:342:A:TYR:H	1:341:A:VAL:HG22	19	0.11
(1,2513)	1:442:A:THR:H	1:441:A:GLN:HB2	4	0.11
(1,2499)	1:421:A:GLU:H	1:420:A:ASP:HB2	7	0.11
(1,2493)	1:440:A:GLU:H	1:439:A:ASP:HB3	4	0.11
(1,2419)	1:443:A:TYR:H	1:442:A:THR:HA	5	0.11
(1,2418)	1:444:A:GLN:H	1:441:A:GLN:HG2	9	0.11
(1,2406)	1:383:A:THR:H	1:382:A:ARG:HG2	14	0.11
(1,2347)	1:356:A:TRP:HE1	1:346:A:SER:HB3	5	0.11
(1,2331)	1:366:A:ILE:H	1:412:A:LEU:HD23	11	0.11
(1,2295)	1:356:A:TRP:HE1	1:345:A:LEU:HG	3	0.11
(1,2295)	1:356:A:TRP:HE1	1:345:A:LEU:HG	11	0.11
(1,2295)	1:356:A:TRP:HE1	1:345:A:LEU:HG	18	0.11
(1,2284)	1:414:A:ARG:HE	1:404:A:ARG:HE	6	0.11
(1,2284)	1:414:A:ARG:HE	1:404:A:ARG:HE	17	0.11
(1,2276)	1:410:A:ARG:HE	1:365:A:ARG:HE	5	0.11
(1,2266)	1:355:A:ARG:HE	1:367:A:VAL:HB	14	0.11
(1,2251)	1:446:A:ASP:H	1:445:A:GLU:HG2	9	0.11
(1,2199)	1:412:A:LEU:H	1:412:A:LEU:HD11	16	0.11
(1,2191)	1:403:A:ILE:H	1:397:A:TYR:HB2	16	0.11
(1,2184)	1:435:A:SER:H	1:432:A:HIS:HA	8	0.11
(1,2158)	1:382:A:ARG:H	1:377:A:GLY:HA3	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2132)	1:380:A:LYS:H	1:380:A:LYS:HB3	17	0.11
(1,2126)	1:410:A:ARG:H	1:410:A:ARG:HB3	6	0.11
(1,2122)	1:410:A:ARG:H	1:409:A:GLN:HG2	16	0.11
(1,2120)	1:377:A:GLY:H	1:385:A:MET:HB3	19	0.11
(1,2067)	1:365:A:ARG:H	1:355:A:ARG:HG2	7	0.11
(1,2067)	1:365:A:ARG:H	1:355:A:ARG:HG2	16	0.11
(1,1978)	1:349:A:ARG:H	1:347:A:ASP:HB2	12	0.11
(1,1920)	1:372:A:LEU:HD13	1:366:A:ILE:HD13	19	0.11
(1,1910)	1:354:A:ILE:HG22	1:345:A:LEU:HD21	15	0.11
(1,1885)	1:400:A:LEU:HD22	1:402:A:ILE:HD12	16	0.11
(1,1881)	1:434:A:GLU:HG3	1:393:A:ALA:HB2	3	0.11
(1,1875)	1:389:A:LYS:H	1:388:A:GLU:HB3	12	0.11
(1,1865)	1:431:A:GLU:HA	1:431:A:GLU:HB2	7	0.11
(1,1865)	1:431:A:GLU:HA	1:431:A:GLU:HB2	13	0.11
(1,1827)	1:430:A:LEU:HB3	1:430:A:LEU:HD23	5	0.11
(1,1787)	1:376:A:TRP:HZ2	1:337:A:LEU:HD21	15	0.11
(1,1784)	1:337:A:LEU:HD12	1:340:A:TYR:H	5	0.11
(1,1751)	1:338:A:TRP:HZ2	1:423:A:MET:HG2	4	0.11
(1,1729)	1:340:A:TYR:HD2	1:340:A:TYR:HB2	15	0.11
(1,1729)	1:340:A:TYR:HD2	1:340:A:TYR:HB2	18	0.11
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	1	0.11
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	14	0.11
(1,1697)	1:345:A:LEU:HA	1:344:A:LEU:H	9	0.11
(1,1667)	1:403:A:ILE:HG12	1:403:A:ILE:H	5	0.11
(1,1667)	1:403:A:ILE:HG12	1:403:A:ILE:H	9	0.11
(1,1667)	1:403:A:ILE:HG12	1:403:A:ILE:H	10	0.11
(1,1667)	1:403:A:ILE:HG12	1:403:A:ILE:H	16	0.11
(1,1661)	1:404:A:ARG:HG2	1:404:A:ARG:HD3	19	0.11
(1,1659)	1:404:A:ARG:HB2	1:404:A:ARG:HD3	9	0.11
(1,1659)	1:404:A:ARG:HB2	1:404:A:ARG:HD3	12	0.11
(1,1659)	1:404:A:ARG:HB2	1:404:A:ARG:HD3	18	0.11
(1,1659)	1:404:A:ARG:HB2	1:404:A:ARG:HD3	19	0.11
(1,1645)	1:404:A:ARG:HB3	1:404:A:ARG:HG3	8	0.11
(1,1645)	1:404:A:ARG:HB3	1:404:A:ARG:HG3	12	0.11
(1,1640)	1:405:A:LYS:H	1:404:A:ARG:HB3	7	0.11
(1,1640)	1:405:A:LYS:H	1:404:A:ARG:HB3	11	0.11
(1,1629)	1:406:A:GLU:HG3	1:412:A:LEU:HD11	8	0.11
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	7	0.11
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	12	0.11
(1,1618)	1:407:A:PRO:HB2	1:407:A:PRO:HD3	17	0.11
(1,1603)	1:357:A:GLU:HG2	1:412:A:LEU:HD13	19	0.11
(1,1600)	1:412:A:LEU:HD21	1:412:A:LEU:H	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1580)	1:413:A:PHE:HB2	1:413:A:PHE:HD1	3	0.11
(1,1580)	1:413:A:PHE:HB2	1:413:A:PHE:HD1	8	0.11
(1,1580)	1:413:A:PHE:HB2	1:413:A:PHE:HD1	13	0.11
(1,1580)	1:413:A:PHE:HB2	1:413:A:PHE:HD1	17	0.11
(1,1580)	1:413:A:PHE:HB2	1:413:A:PHE:HD1	18	0.11
(1,1573)	1:414:A:ARG:HG2	1:403:A:ILE:HA	9	0.11
(1,1555)	1:417:A:LYS:HG3	1:417:A:LYS:HE2	9	0.11
(1,1533)	1:378:A:ASN:HB2	1:375:A:LEU:HA	3	0.11
(1,1505)	1:385:A:MET:HA	1:389:A:LYS:HB2	10	0.11
(1,1505)	1:385:A:MET:HA	1:389:A:LYS:HB2	11	0.11
(1,1488)	1:431:A:GLU:HB2	1:336:A:LEU:HD22	12	0.11
(1,1479)	1:433:A:LEU:HD13	1:393:A:ALA:HA	18	0.11
(1,1426)	1:448:A:PRO:HB2	1:448:A:PRO:HA	17	0.11
(1,1407)	1:456:A:TRP:HB3	1:456:A:TRP:HZ3	13	0.11
(1,1402)	1:383:A:THR:HG22	1:384:A:ASN:HD21	18	0.11
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	1	0.11
(1,1338)	1:400:A:LEU:H	1:399:A:LYS:HG3	17	0.11
(1,1320)	1:374:A:ARG:H	1:374:A:ARG:HG2	4	0.11
(1,1311)	1:421:A:GLU:HA	1:421:A:GLU:HG3	11	0.11
(1,1311)	1:421:A:GLU:HA	1:421:A:GLU:HG3	12	0.11
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	2	0.11
(1,1301)	1:376:A:TRP:HD1	1:341:A:VAL:HB	16	0.11
(1,1267)	1:354:A:ILE:HD11	1:367:A:VAL:H	4	0.11
(1,1265)	1:354:A:ILE:HG22	1:355:A:ARG:H	1	0.11
(1,1236)	1:356:A:TRP:HZ3	1:356:A:TRP:HA	3	0.11
(1,1203)	1:360:A:GLU:H	1:360:A:GLU:HA	1	0.11
(1,1203)	1:360:A:GLU:H	1:360:A:GLU:HA	6	0.11
(1,1203)	1:360:A:GLU:H	1:360:A:GLU:HA	15	0.11
(1,1194)	1:361:A:SER:HB3	1:360:A:GLU:H	6	0.11
(1,1193)	1:362:A:LYS:HE2	1:362:A:LYS:HA	12	0.11
(1,1180)	1:363:A:ILE:HD13	1:414:A:ARG:HD2	5	0.11
(1,1174)	1:361:A:SER:HB2	1:363:A:ILE:HG23	9	0.11
(1,1143)	1:366:A:ILE:H	1:365:A:ARG:HB2	6	0.11
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG12	2	0.11
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG12	6	0.11
(1,1136)	1:367:A:VAL:HB	1:367:A:VAL:HG11	19	0.11
(1,1123)	1:354:A:ILE:H	1:367:A:VAL:HG21	1	0.11
(1,1118)	1:367:A:VAL:HG23	1:366:A:ILE:HA	9	0.11
(1,1080)	1:372:A:LEU:HD21	1:353:A:PHE:HD1	17	0.11
(1,1044)	1:349:A:ARG:HB2	1:349:A:ARG:HG3	6	0.11
(1,1044)	1:349:A:ARG:HB2	1:349:A:ARG:HG3	7	0.11
(1,1026)	1:336:A:LEU:HD22	1:432:A:HIS:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,971)	1:450:A:ILE:H	1:450:A:ILE:HG23	5	0.11
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG22	2	0.11
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG21	15	0.11
(1,960)	1:450:A:ILE:HA	1:450:A:ILE:HG13	2	0.11
(1,960)	1:450:A:ILE:HA	1:450:A:ILE:HG13	5	0.11
(1,956)	1:450:A:ILE:H	1:449:A:THR:HB	4	0.11
(1,956)	1:450:A:ILE:H	1:449:A:THR:HB	19	0.11
(1,947)	1:447:A:GLU:HG2	1:447:A:GLU:HA	8	0.11
(1,943)	1:446:A:ASP:HB3	1:446:A:ASP:HA	1	0.11
(1,943)	1:446:A:ASP:HB3	1:446:A:ASP:HA	10	0.11
(1,943)	1:446:A:ASP:HB3	1:446:A:ASP:HA	11	0.11
(1,941)	1:447:A:GLU:H	1:446:A:ASP:HB2	8	0.11
(1,926)	1:442:A:THR:H	1:441:A:GLN:HG2	5	0.11
(1,924)	1:441:A:GLN:HE22	1:441:A:GLN:HG2	13	0.11
(1,924)	1:441:A:GLN:HE22	1:441:A:GLN:HG2	19	0.11
(1,898)	1:438:A:LEU:HD12	1:382:A:ARG:HG2	15	0.11
(1,887)	1:437:A:VAL:HG21	1:393:A:ALA:HA	3	0.11
(1,887)	1:437:A:VAL:HG23	1:393:A:ALA:HA	8	0.11
(1,887)	1:437:A:VAL:HG23	1:393:A:ALA:HA	10	0.11
(1,876)	1:436:A:GLN:HB2	1:437:A:VAL:HG13	5	0.11
(1,876)	1:436:A:GLN:HB2	1:437:A:VAL:HG12	15	0.11
(1,872)	1:436:A:GLN:H	1:435:A:SER:HB2	6	0.11
(1,872)	1:436:A:GLN:H	1:435:A:SER:HB2	8	0.11
(1,864)	1:433:A:LEU:HA	1:433:A:LEU:HD11	1	0.11
(1,864)	1:433:A:LEU:HA	1:433:A:LEU:HD12	3	0.11
(1,864)	1:433:A:LEU:HA	1:433:A:LEU:HD13	14	0.11
(1,859)	1:436:A:GLN:H	1:434:A:GLU:HA	3	0.11
(1,859)	1:436:A:GLN:H	1:434:A:GLU:HA	7	0.11
(1,859)	1:436:A:GLN:H	1:434:A:GLU:HA	8	0.11
(1,855)	1:432:A:HIS:HB2	1:432:A:HIS:HD2	10	0.11
(1,855)	1:432:A:HIS:HB2	1:432:A:HIS:HD2	16	0.11
(1,845)	1:431:A:GLU:HA	1:431:A:GLU:HG3	14	0.11
(1,842)	1:430:A:LEU:HG	1:430:A:LEU:HD21	17	0.11
(1,813)	1:427:A:THR:HG21	1:425:A:GLY:H	6	0.11
(1,813)	1:427:A:THR:HG22	1:425:A:GLY:H	7	0.11
(1,800)	1:426:A:ARG:HB2	1:426:A:ARG:HG2	12	0.11
(1,791)	1:428:A:ASP:HA	1:428:A:ASP:HB3	18	0.11
(1,699)	1:413:A:PHE:HB2	1:364:A:PHE:HE2	6	0.11
(1,666)	1:352:A:ASN:HA	1:351:A:GLU:HG3	7	0.11
(1,666)	1:352:A:ASN:HA	1:351:A:GLU:HG3	8	0.11
(1,666)	1:352:A:ASN:HA	1:351:A:GLU:HG3	12	0.11
(1,666)	1:352:A:ASN:HA	1:351:A:GLU:HG3	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,666)	1:352:A:ASN:HA	1:351:A:GLU:HG3	15	0.11
(1,666)	1:352:A:ASN:HA	1:351:A:GLU:HG3	19	0.11
(1,657)	1:406:A:GLU:HB2	1:412:A:LEU:HB2	8	0.11
(1,595)	1:400:A:LEU:HD23	1:400:A:LEU:HG	15	0.11
(1,573)	1:399:A:LYS:HB2	1:396:A:HIS:HA	2	0.11
(1,547)	1:395:A:ARG:HD2	1:395:A:ARG:H	15	0.11
(1,528)	1:394:A:LEU:HD23	1:364:A:PHE:HZ	12	0.11
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	11	0.11
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	14	0.11
(1,495)	1:392:A:ARG:HA	1:392:A:ARG:HG2	6	0.11
(1,488)	1:392:A:ARG:H	1:391:A:SER:HB2	5	0.11
(1,439)	1:382:A:ARG:HB3	1:382:A:ARG:HD2	10	0.11
(1,433)	1:381:A:ASN:HA	1:381:A:ASN:HB3	3	0.11
(1,433)	1:381:A:ASN:HA	1:381:A:ASN:HB3	10	0.11
(1,433)	1:381:A:ASN:HA	1:381:A:ASN:HB3	19	0.11
(1,400)	1:377:A:GLY:HA3	1:382:A:ARG:HB3	17	0.11
(1,364)	1:374:A:ARG:HA	1:374:A:ARG:HG3	11	0.11
(1,358)	1:374:A:ARG:HA	1:374:A:ARG:HD2	4	0.11
(1,268)	1:364:A:PHE:HA	1:345:A:LEU:HD23	16	0.11
(1,268)	1:364:A:PHE:HA	1:345:A:LEU:HD22	17	0.11
(1,266)	1:363:A:ILE:HG22	1:406:A:GLU:HG2	5	0.11
(1,259)	1:362:A:LYS:HG2	1:362:A:LYS:HD2	3	0.11
(1,259)	1:362:A:LYS:HG2	1:362:A:LYS:HD2	4	0.11
(1,259)	1:362:A:LYS:HG2	1:362:A:LYS:HD2	5	0.11
(1,259)	1:362:A:LYS:HG2	1:362:A:LYS:HD2	8	0.11
(1,259)	1:362:A:LYS:HG2	1:362:A:LYS:HD2	10	0.11
(1,259)	1:362:A:LYS:HG2	1:362:A:LYS:HD2	12	0.11
(1,259)	1:362:A:LYS:HG2	1:362:A:LYS:HD2	13	0.11
(1,259)	1:362:A:LYS:HG2	1:362:A:LYS:HD2	14	0.11
(1,259)	1:362:A:LYS:HG2	1:362:A:LYS:HD2	18	0.11
(1,232)	1:359:A:LYS:HG2	1:359:A:LYS:HE2	19	0.11
(1,229)	1:356:A:TRP:HD1	1:359:A:LYS:HD3	17	0.11
(1,204)	1:357:A:GLU:HB3	1:412:A:LEU:HD13	7	0.11
(1,138)	1:351:A:GLU:HG3	1:351:A:GLU:HB2	5	0.11
(1,138)	1:351:A:GLU:HG3	1:351:A:GLU:HB2	12	0.11
(1,125)	1:349:A:ARG:HG2	1:349:A:ARG:HD3	13	0.11
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	8	0.11
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	14	0.11
(1,117)	1:348:A:SER:HB2	1:348:A:SER:H	17	0.11
(1,105)	1:365:A:ARG:H	1:345:A:LEU:HD22	19	0.11
(1,104)	1:345:A:LEU:HD23	1:356:A:TRP:HE3	13	0.11
(1,93)	1:345:A:LEU:HA	1:354:A:ILE:HG21	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:345:A:LEU:HA	1:354:A:ILE:HG21	16	0.11
(1,88)	1:346:A:SER:HB2	1:346:A:SER:HA	1	0.11
(1,88)	1:346:A:SER:HB2	1:346:A:SER:HA	3	0.11
(1,85)	1:344:A:LEU:HD21	1:350:A:TYR:HD1	8	0.11
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	9	0.11
(1,61)	1:390:A:MET:HB2	1:390:A:MET:H	19	0.11
(1,58)	1:343:A:GLN:HG2	1:343:A:GLN:HB3	10	0.11
(1,58)	1:343:A:GLN:HG3	1:343:A:GLN:HB2	11	0.11
(1,37)	1:341:A:VAL:HG11	1:341:A:VAL:HG22	4	0.11
(1,27)	1:341:A:VAL:HA	1:372:A:LEU:HD11	12	0.11
(1,15)	1:339:A:ASP:HB2	1:336:A:LEU:HB2	2	0.11
(1,15)	1:339:A:ASP:HB3	1:336:A:LEU:HB2	8	0.11
(1,15)	1:339:A:ASP:HB3	1:336:A:LEU:HB2	9	0.11
(1,5)	1:337:A:LEU:HD22	1:390:A:MET:HG3	11	0.11
(1,2967)	1:444:A:GLN:H	1:444:A:GLN:HB3	2	0.1
(1,2931)	1:420:A:ASP:H	1:421:A:GLU:HG3	18	0.1
(1,2867)	1:372:A:LEU:HD11	1:340:A:TYR:HE2	18	0.1
(1,2836)	1:404:A:ARG:HG3	1:405:A:LYS:H	19	0.1
(1,2812)	1:421:A:GLU:HB3	1:421:A:GLU:HA	10	0.1
(1,2812)	1:375:A:LEU:HB3	1:375:A:LEU:HA	19	0.1
(1,2811)	1:428:A:ASP:HA	1:431:A:GLU:HB2	19	0.1
(1,2798)	1:412:A:LEU:HD22	1:410:A:ARG:HD3	1	0.1
(1,2798)	1:412:A:LEU:HD21	1:410:A:ARG:HD2	18	0.1
(1,2774)	1:443:A:TYR:HD1	1:445:A:GLU:HB2	2	0.1
(1,2763)	1:398:A:TYR:HD1	1:398:A:TYR:HE1	1	0.1
(1,2763)	1:398:A:TYR:HD1	1:398:A:TYR:HE1	2	0.1
(1,2763)	1:398:A:TYR:HD1	1:398:A:TYR:HE1	3	0.1
(1,2763)	1:398:A:TYR:HD1	1:398:A:TYR:HE1	5	0.1
(1,2763)	1:398:A:TYR:HD1	1:398:A:TYR:HE1	7	0.1
(1,2763)	1:398:A:TYR:HD1	1:398:A:TYR:HE1	8	0.1
(1,2763)	1:398:A:TYR:HD1	1:398:A:TYR:HE1	9	0.1
(1,2763)	1:398:A:TYR:HD1	1:398:A:TYR:HE1	10	0.1
(1,2763)	1:398:A:TYR:HD1	1:398:A:TYR:HE1	12	0.1
(1,2763)	1:398:A:TYR:HD1	1:398:A:TYR:HE1	13	0.1
(1,2763)	1:398:A:TYR:HD1	1:398:A:TYR:HE1	16	0.1
(1,2763)	1:398:A:TYR:HD1	1:398:A:TYR:HE1	17	0.1
(1,2763)	1:398:A:TYR:HD1	1:398:A:TYR:HE1	18	0.1
(1,2763)	1:398:A:TYR:HD1	1:398:A:TYR:HE1	19	0.1
(1,2739)	1:362:A:LYS:HB2	1:356:A:TRP:HZ3	12	0.1
(1,2721)	1:354:A:ILE:HD11	1:372:A:LEU:HD23	10	0.1
(1,2719)	1:372:A:LEU:HD13	1:340:A:TYR:HD2	1	0.1
(1,2717)	1:372:A:LEU:HB3	1:372:A:LEU:HD13	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2682)	1:418:A:THR:HG23	1:419:A:PRO:HD2	17	0.1
(1,2667)	1:414:A:ARG:HA	1:414:A:ARG:HD2	8	0.1
(1,2655)	1:410:A:ARG:HB2	1:410:A:ARG:HD3	19	0.1
(1,2599)	1:363:A:ILE:HG21	1:363:A:ILE:HB	18	0.1
(1,2596)	1:363:A:ILE:HG23	1:364:A:PHE:HA	6	0.1
(1,2596)	1:363:A:ILE:HG22	1:364:A:PHE:HA	15	0.1
(1,2567)	1:345:A:LEU:HD22	1:355:A:ARG:HA	3	0.1
(1,2567)	1:345:A:LEU:HD21	1:355:A:ARG:HA	8	0.1
(1,2529)	1:373:A:ALA:H	1:373:A:ALA:HB3	13	0.1
(1,2529)	1:373:A:ALA:H	1:373:A:ALA:HB3	16	0.1
(1,2516)	1:342:A:TYR:H	1:341:A:VAL:HG22	1	0.1
(1,2516)	1:342:A:TYR:H	1:341:A:VAL:HG21	7	0.1
(1,2493)	1:440:A:GLU:H	1:439:A:ASP:HB3	15	0.1
(1,2473)	1:409:A:GLN:HE21	1:412:A:LEU:HD13	6	0.1
(1,2470)	1:410:A:ARG:HE	1:409:A:GLN:HB3	19	0.1
(1,2419)	1:443:A:TYR:H	1:442:A:THR:HA	10	0.1
(1,2364)	1:380:A:LYS:H	1:377:A:GLY:HA3	9	0.1
(1,2295)	1:356:A:TRP:HE1	1:345:A:LEU:HG	6	0.1
(1,2295)	1:356:A:TRP:HE1	1:345:A:LEU:HG	16	0.1
(1,2276)	1:410:A:ARG:HE	1:365:A:ARG:HE	14	0.1
(1,2257)	1:450:A:ILE:H	1:450:A:ILE:HB	18	0.1
(1,2199)	1:412:A:LEU:H	1:412:A:LEU:HD11	17	0.1
(1,2191)	1:403:A:ILE:H	1:397:A:TYR:HB2	5	0.1
(1,2141)	1:385:A:MET:H	1:384:A:ASN:H	1	0.1
(1,2115)	1:377:A:GLY:H	1:385:A:MET:HB2	19	0.1
(1,2025)	1:381:A:ASN:H	1:381:A:ASN:HB3	17	0.1
(1,2009)	1:355:A:ARG:H	1:354:A:ILE:HD12	6	0.1
(1,1931)	1:335:A:ARG:H	1:336:A:LEU:HB2	11	0.1
(1,1891)	1:394:A:LEU:HD21	1:403:A:ILE:HD13	11	0.1
(1,1891)	1:394:A:LEU:HD22	1:403:A:ILE:HD11	12	0.1
(1,1877)	1:388:A:GLU:H	1:388:A:GLU:HG2	1	0.1
(1,1874)	1:382:A:ARG:HD3	1:382:A:ARG:HA	5	0.1
(1,1865)	1:431:A:GLU:HA	1:431:A:GLU:HB2	12	0.1
(1,1865)	1:431:A:GLU:HA	1:431:A:GLU:HB2	15	0.1
(1,1865)	1:431:A:GLU:HA	1:431:A:GLU:HB2	19	0.1
(1,1843)	1:370:A:ASN:HA	1:373:A:ALA:HB2	11	0.1
(1,1828)	1:398:A:TYR:HA	1:399:A:LYS:HD2	12	0.1
(1,1828)	1:398:A:TYR:HA	1:399:A:LYS:HD2	14	0.1
(1,1784)	1:337:A:LEU:HD13	1:340:A:TYR:H	1	0.1
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	10	0.1
(1,1718)	1:342:A:TYR:HB3	1:342:A:TYR:HD1	13	0.1
(1,1667)	1:403:A:ILE:HG12	1:403:A:ILE:H	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1647)	1:404:A:ARG:HB2	1:404:A:ARG:HG2	19	0.1
(1,1645)	1:404:A:ARG:HB3	1:404:A:ARG:HG3	7	0.1
(1,1626)	1:406:A:GLU:H	1:406:A:GLU:HG3	17	0.1
(1,1567)	1:422:A:ILE:HD12	1:415:A:PHE:HD1	14	0.1
(1,1461)	1:435:A:SER:H	1:435:A:SER:HB2	11	0.1
(1,1454)	1:438:A:LEU:HD13	1:376:A:TRP:HH2	11	0.1
(1,1444)	1:442:A:THR:HG23	1:443:A:TYR:HA	6	0.1
(1,1444)	1:442:A:THR:HG22	1:443:A:TYR:HA	15	0.1
(1,1407)	1:456:A:TRP:HB3	1:456:A:TRP:HZ3	6	0.1
(1,1403)	1:383:A:THR:HG22	1:382:A:ARG:HD2	10	0.1
(1,1390)	1:387:A:TYR:HE2	1:390:A:MET:HG2	14	0.1
(1,1369)	1:393:A:ALA:H	1:390:A:MET:HA	8	0.1
(1,1352)	1:396:A:HIS:HD2	1:396:A:HIS:HA	17	0.1
(1,1276)	1:382:A:ARG:HG2	1:382:A:ARG:HB2	13	0.1
(1,1270)	1:382:A:ARG:HG3	1:380:A:LYS:H	15	0.1
(1,1265)	1:354:A:ILE:HG23	1:355:A:ARG:H	5	0.1
(1,1236)	1:356:A:TRP:HZ3	1:356:A:TRP:HA	14	0.1
(1,1203)	1:360:A:GLU:H	1:360:A:GLU:HA	2	0.1
(1,1203)	1:360:A:GLU:H	1:360:A:GLU:HA	17	0.1
(1,1180)	1:363:A:ILE:HD13	1:414:A:ARG:HD2	7	0.1
(1,1131)	1:367:A:VAL:HA	1:367:A:VAL:HG12	5	0.1
(1,1123)	1:354:A:ILE:H	1:367:A:VAL:HG22	13	0.1
(1,1118)	1:367:A:VAL:HG21	1:366:A:ILE:HA	2	0.1
(1,1044)	1:349:A:ARG:HB2	1:349:A:ARG:HG3	5	0.1
(1,969)	1:450:A:ILE:HB	1:450:A:ILE:HG23	5	0.1
(1,956)	1:450:A:ILE:H	1:449:A:THR:HB	16	0.1
(1,943)	1:446:A:ASP:HB3	1:446:A:ASP:HA	2	0.1
(1,943)	1:446:A:ASP:HB3	1:446:A:ASP:HA	8	0.1
(1,943)	1:446:A:ASP:HB3	1:446:A:ASP:HA	9	0.1
(1,943)	1:446:A:ASP:HB3	1:446:A:ASP:HA	12	0.1
(1,943)	1:446:A:ASP:HB3	1:446:A:ASP:HA	13	0.1
(1,943)	1:446:A:ASP:HB3	1:446:A:ASP:HA	17	0.1
(1,929)	1:443:A:TYR:H	1:442:A:THR:HB	1	0.1
(1,926)	1:442:A:THR:H	1:441:A:GLN:HG2	7	0.1
(1,903)	1:438:A:LEU:HD22	1:438:A:LEU:HB3	4	0.1
(1,884)	1:437:A:VAL:HG21	1:392:A:ARG:HG3	11	0.1
(1,876)	1:436:A:GLN:HB2	1:437:A:VAL:HG13	16	0.1
(1,868)	1:434:A:GLU:HA	1:393:A:ALA:HB1	3	0.1
(1,848)	1:428:A:ASP:HA	1:431:A:GLU:HB2	8	0.1
(1,845)	1:431:A:GLU:HA	1:431:A:GLU:HG3	17	0.1
(1,842)	1:430:A:LEU:HG	1:430:A:LEU:HD22	3	0.1
(1,842)	1:430:A:LEU:HG	1:430:A:LEU:HD22	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,838)	1:430:A:LEU:HB2	1:430:A:LEU:HD13	1	0.1
(1,813)	1:427:A:THR:HG23	1:425:A:GLY:H	14	0.1
(1,794)	1:423:A:MET:H	1:423:A:MET:HG2	8	0.1
(1,666)	1:352:A:ASN:HA	1:351:A:GLU:HG3	6	0.1
(1,657)	1:406:A:GLU:HB2	1:412:A:LEU:HB2	13	0.1
(1,573)	1:399:A:LYS:HB2	1:396:A:HIS:HA	3	0.1
(1,556)	1:397:A:TYR:HA	1:400:A:LEU:HB3	14	0.1
(1,556)	1:397:A:TYR:HA	1:400:A:LEU:HB3	15	0.1
(1,530)	1:394:A:LEU:HD23	1:397:A:TYR:HB3	3	0.1
(1,528)	1:394:A:LEU:HD22	1:364:A:PHE:HZ	1	0.1
(1,528)	1:394:A:LEU:HD23	1:364:A:PHE:HZ	5	0.1
(1,521)	1:387:A:TYR:HE2	1:394:A:LEU:HD11	5	0.1
(1,520)	1:391:A:SER:HB3	1:394:A:LEU:HD13	5	0.1
(1,498)	1:392:A:ARG:HG2	1:392:A:ARG:HD2	7	0.1
(1,433)	1:381:A:ASN:HA	1:381:A:ASN:HB3	6	0.1
(1,318)	1:367:A:VAL:HA	1:367:A:VAL:HG23	10	0.1
(1,301)	1:366:A:ILE:HG22	1:372:A:LEU:HB3	8	0.1
(1,301)	1:366:A:ILE:HG21	1:372:A:LEU:HB3	17	0.1
(1,268)	1:364:A:PHE:HA	1:345:A:LEU:HD22	7	0.1
(1,259)	1:362:A:LYS:HG2	1:362:A:LYS:HD2	1	0.1
(1,259)	1:362:A:LYS:HG2	1:362:A:LYS:HD2	16	0.1
(1,259)	1:362:A:LYS:HG2	1:362:A:LYS:HD2	19	0.1
(1,215)	1:359:A:LYS:HA	1:359:A:LYS:HG2	17	0.1
(1,174)	1:354:A:ILE:HD13	1:341:A:VAL:HA	10	0.1
(1,144)	1:353:A:PHE:HB3	1:353:A:PHE:HD1	13	0.1
(1,127)	1:349:A:ARG:HD2	1:350:A:TYR:HE1	5	0.1
(1,58)	1:343:A:GLN:HG3	1:343:A:GLN:HB2	12	0.1
(1,27)	1:341:A:VAL:HA	1:372:A:LEU:HD13	16	0.1
(1,25)	1:341:A:VAL:HA	1:344:A:LEU:HD23	11	0.1

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

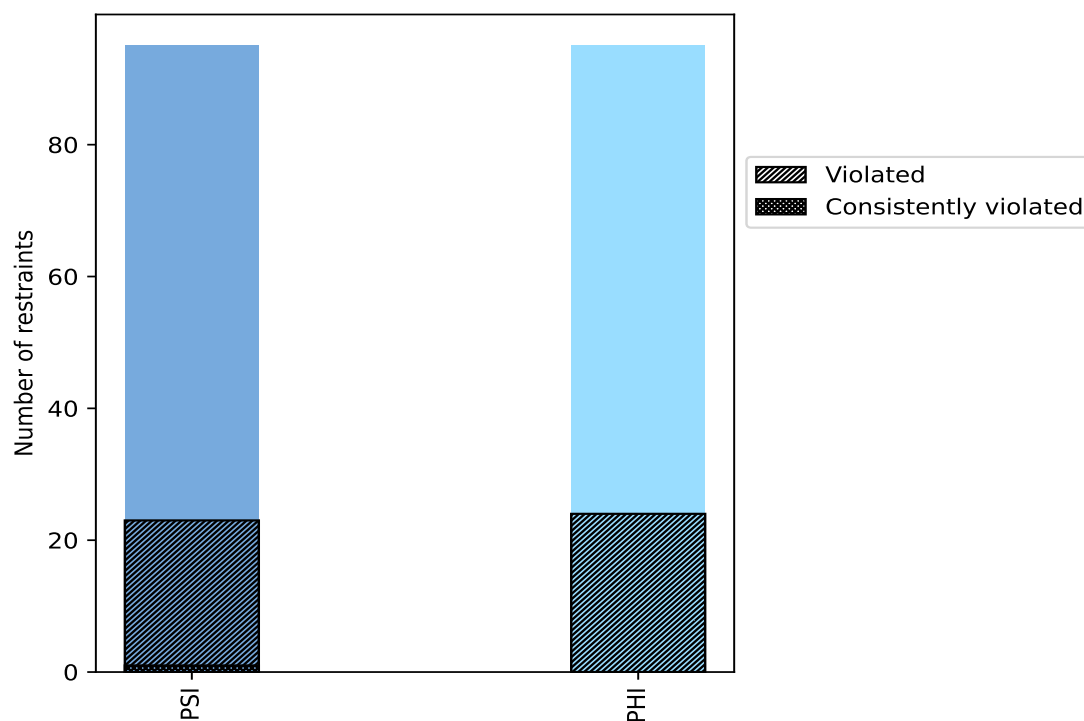
### 10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
PSI	95	50.0	23	24.2	12.1	1	1.1	0.5
PHI	95	50.0	24	25.3	12.6	0	0.0	0.0
Total	190	100.0	47	24.7	24.7	1	0.5	0.5

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

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



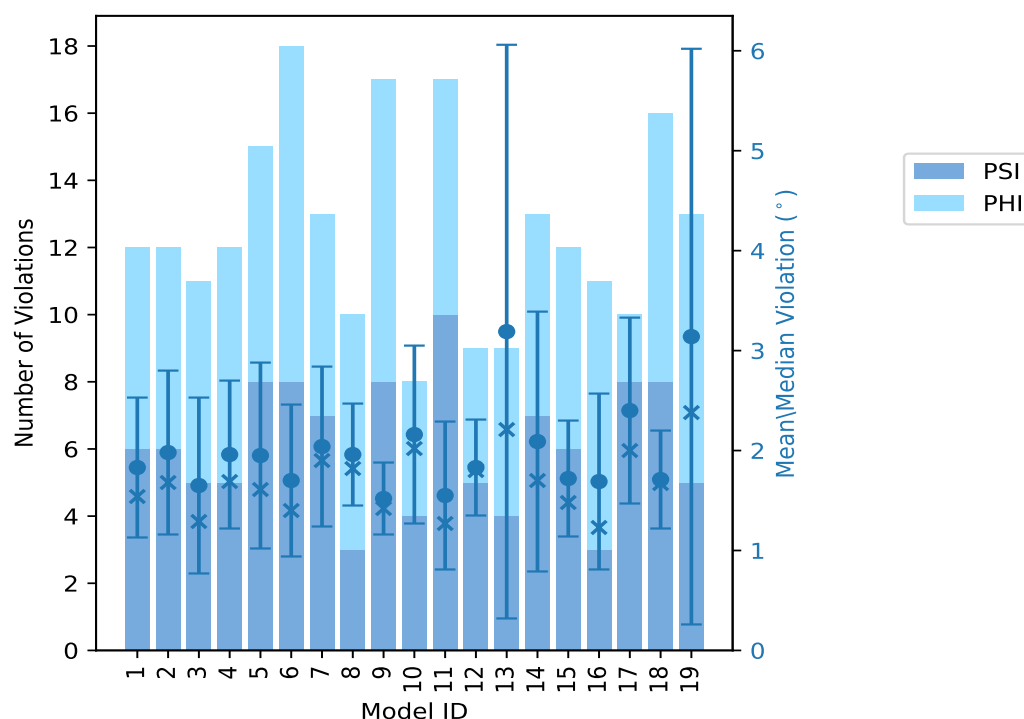
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	6	6	12	1.83	3.04	0.7	1.54
2	6	6	12	1.98	4.06	0.82	1.68
3	5	6	11	1.65	4.35	0.88	1.29
4	5	7	12	1.96	3.23	0.74	1.69
5	8	7	15	1.95	4.71	0.93	1.61
6	8	10	18	1.7	4.09	0.76	1.4
7	7	6	13	2.04	3.58	0.8	1.9
8	3	7	10	1.96	3.11	0.51	1.82
9	8	9	17	1.52	2.14	0.36	1.42
10	4	4	8	2.16	4.04	0.89	2.02
11	10	7	17	1.55	4.04	0.74	1.27
12	5	4	9	1.83	2.95	0.48	1.8
13	4	5	9	3.19	11.12	2.87	2.21
14	7	6	13	2.09	6.38	1.3	1.7
15	6	6	12	1.72	3.12	0.58	1.48
16	3	8	11	1.69	4.14	0.88	1.23
17	8	2	10	2.4	4.09	0.93	2.0
18	8	8	16	1.71	2.47	0.49	1.67
19	5	8	13	3.14	12.33	2.88	2.38

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
5	8	13	1	5.3
6	4	10	2	10.5
1	1	2	3	15.8
1	0	1	4	21.1
3	3	6	5	26.3
2	1	3	6	31.6
1	1	2	7	36.8
1	1	2	8	42.1
0	1	1	9	47.4
0	0	0	10	52.6
0	0	0	11	57.9

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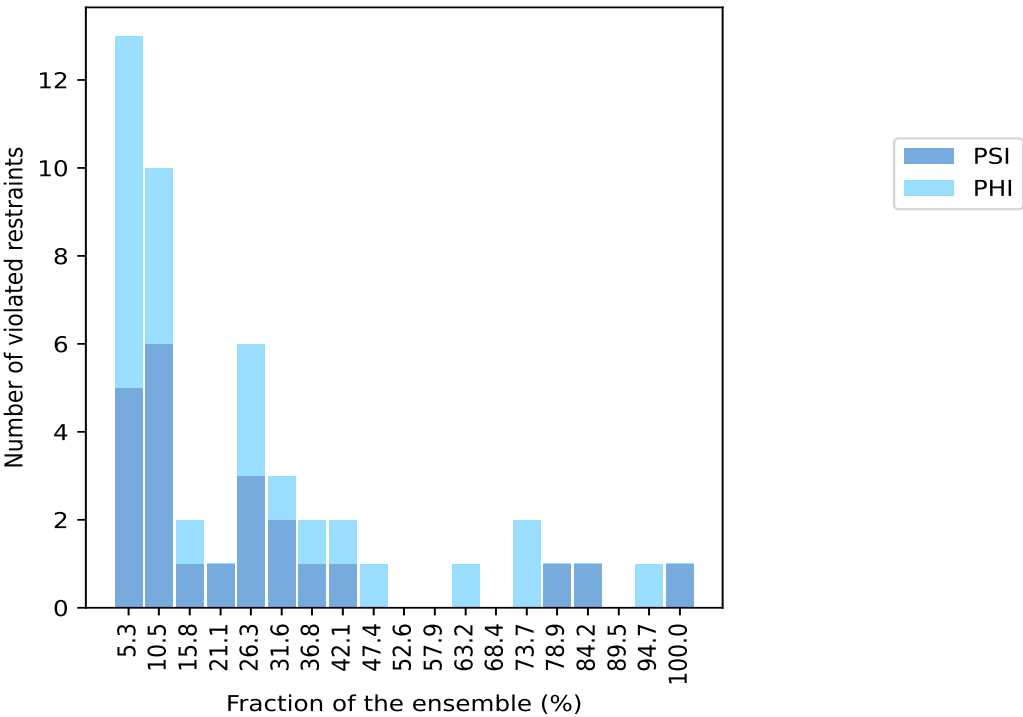


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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
0	1	1	12	63.2
0	0	0	13	68.4
0	2	2	14	73.7
1	0	1	15	78.9
1	0	1	16	84.2
0	0	0	17	89.5
0	1	1	18	94.7
1	0	1	19	100.0

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

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

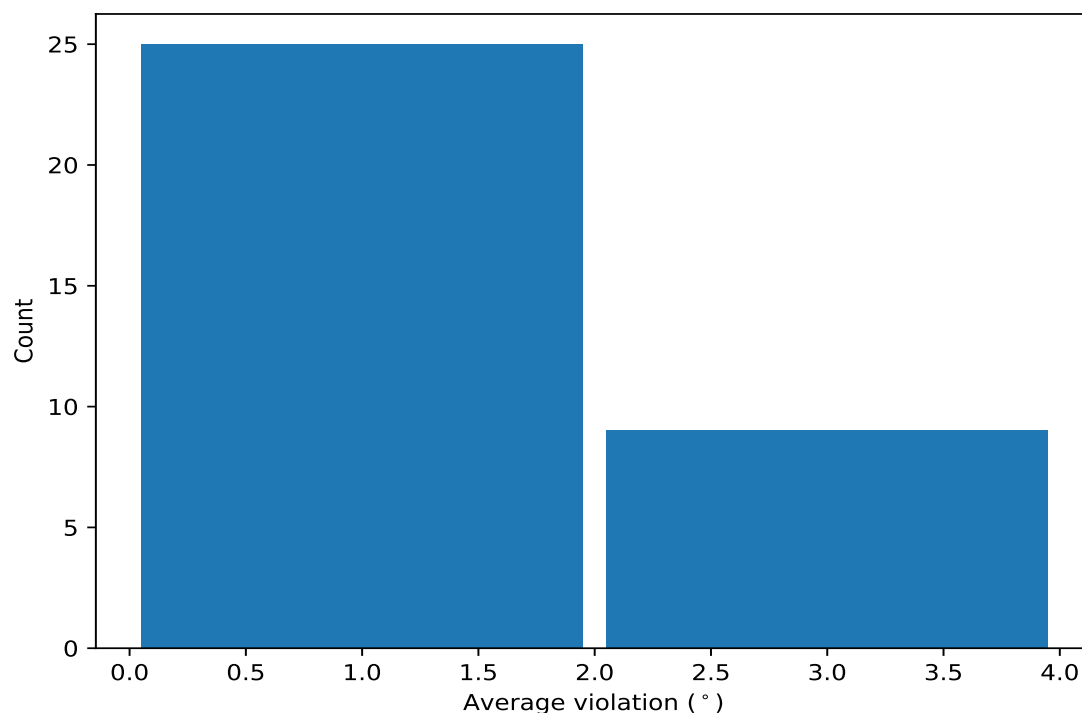


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	19	3.46	0.84	3.12
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	18	1.79	0.41	1.75
(1,145)	1:391:A:SER:N	1:391:A:SER:CA	1:391:A:SER:C	1:392:A:ARG:N	16	1.73	0.42	1.74
(1,97)	1:338:A:TRP:N	1:338:A:TRP:CA	1:338:A:TRP:C	1:339:A:ASP:N	15	1.81	0.39	1.73
(1,90)	1:435:A:SER:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	14	2.14	0.76	2.0
(1,59)	1:399:A:LYS:C	1:400:A:LEU:N	1:400:A:LEU:CA	1:400:A:LEU:C	14	1.88	0.61	1.73
(1,18)	1:354:A:ILE:C	1:355:A:ARG:N	1:355:A:ARG:CA	1:355:A:ARG:C	12	1.58	0.36	1.54
(1,48)	1:388:A:GLU:C	1:389:A:LYS:N	1:389:A:LYS:CA	1:389:A:LYS:C	9	1.88	0.67	1.58
(1,11)	1:347:A:ASP:C	1:348:A:SER:N	1:348:A:SER:CA	1:348:A:SER:C	8	3.95	4.5	1.38
(1,161)	1:407:A:PRO:N	1:407:A:PRO:CA	1:407:A:PRO:C	1:408:A:GLY:N	8	2.24	1.6	1.75
(1,136)	1:380:A:LYS:N	1:380:A:LYS:CA	1:380:A:LYS:C	1:381:A:ASN:N	7	2.19	0.5	2.18
(1,1)	1:336:A:LEU:C	1:337:A:LEU:N	1:337:A:LEU:CA	1:337:A:LEU:C	7	1.53	0.38	1.42
(1,148)	1:394:A:LEU:N	1:394:A:LEU:CA	1:394:A:LEU:C	1:395:A:ARG:N	6	1.52	0.45	1.38
(1,101)	1:342:A:TYR:N	1:342:A:TYR:CA	1:342:A:TYR:C	1:343:A:GLN:N	6	1.3	0.11	1.33
(1,60)	1:400:A:LEU:C	1:401:A:ASN:N	1:401:A:ASN:CA	1:401:A:ASN:C	6	1.24	0.17	1.18
(1,108)	1:350:A:TYR:N	1:350:A:TYR:CA	1:350:A:TYR:C	1:351:A:GLU:N	5	2.6	1.02	2.38
(1,143)	1:389:A:LYS:N	1:389:A:LYS:CA	1:389:A:LYS:C	1:390:A:MET:N	5	1.79	0.43	1.67
(1,89)	1:434:A:GLU:C	1:435:A:SER:N	1:435:A:SER:CA	1:435:A:SER:C	5	1.65	0.21	1.71
(1,84)	1:429:A:ARG:C	1:430:A:LEU:N	1:430:A:LEU:CA	1:430:A:LEU:C	5	1.54	0.34	1.48
(1,86)	1:431:A:GLU:C	1:432:A:HIS:N	1:432:A:HIS:CA	1:432:A:HIS:C	5	1.53	0.42	1.46

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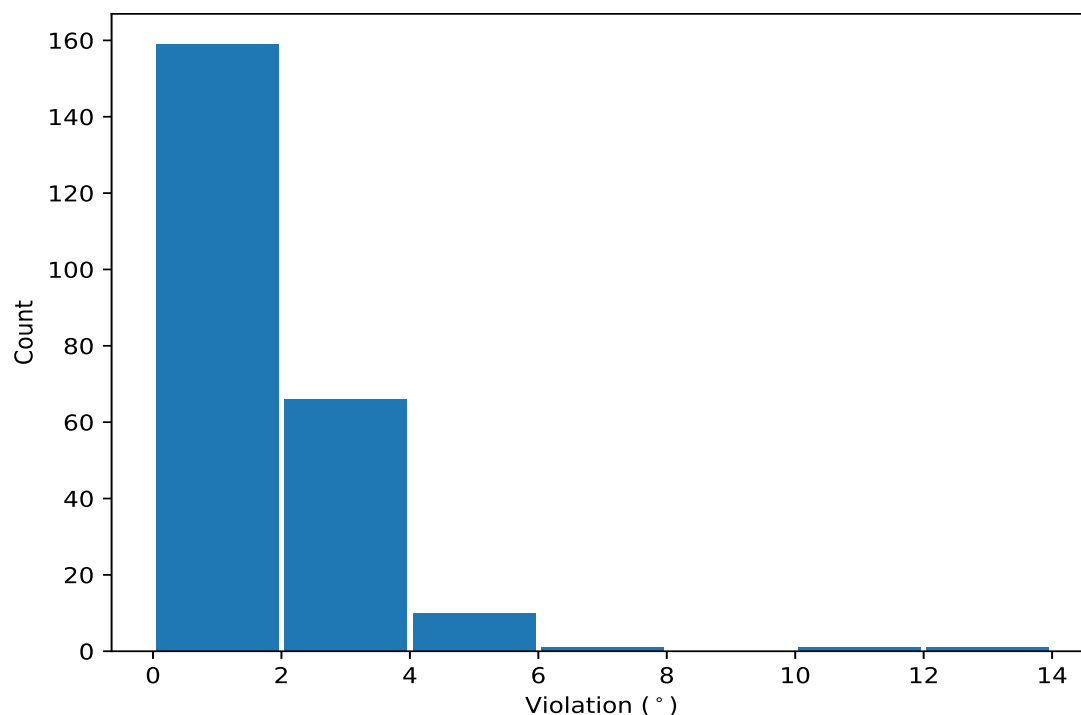
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,118)	1:361:A:SER:N	1:361:A:SER:CA	1:361:A:SER:C	1:362:A:LYS:N	5	1.27	0.23	1.2
(1,110)	1:352:A:ASN:N	1:352:A:ASN:CA	1:352:A:ASN:C	1:353:A:PHE:N	4	1.16	0.11	1.16
(1,81)	1:426:A:ARG:C	1:427:A:THR:N	1:427:A:THR:CA	1:427:A:THR:C	3	2.33	1.68	1.23
(1,119)	1:362:A:LYS:N	1:362:A:LYS:CA	1:362:A:LYS:C	1:363:A:ILE:N	3	1.14	0.07	1.09
(1,106)	1:348:A:SER:N	1:348:A:SER:CA	1:348:A:SER:C	1:349:A:ARG:N	2	2.87	0.13	2.87
(1,184)	1:435:A:SER:N	1:435:A:SER:CA	1:435:A:SER:C	1:436:A:GLN:N	2	2.0	0.77	2.0
(1,116)	1:359:A:LYS:N	1:359:A:LYS:CA	1:359:A:LYS:C	1:360:A:GLU:N	2	1.94	0.37	1.94
(1,78)	1:421:A:GLU:C	1:422:A:ILE:N	1:422:A:ILE:CA	1:422:A:ILE:C	2	1.93	0.57	1.93
(1,146)	1:392:A:ARG:N	1:392:A:ARG:CA	1:392:A:ARG:C	1:393:A:ALA:N	2	1.54	0.28	1.54
(1,3)	1:338:A:TRP:C	1:339:A:ASP:N	1:339:A:ASP:CA	1:339:A:ASP:C	2	1.44	0.06	1.44
(1,168)	1:415:A:PHE:N	1:415:A:PHE:CA	1:415:A:PHE:C	1:416:A:MET:N	2	1.43	0.14	1.43
(1,85)	1:430:A:LEU:C	1:431:A:GLU:N	1:431:A:GLU:CA	1:431:A:GLU:C	2	1.3	0.18	1.3
(1,15)	1:351:A:GLU:C	1:352:A:ASN:N	1:352:A:ASN:CA	1:352:A:ASN:C	2	1.17	0.04	1.17
(1,175)	1:424:A:SER:N	1:424:A:SER:CA	1:424:A:SER:C	1:425:A:GLY:N	2	1.07	0.02	1.07

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

## 10.5 All violated dihedral-angle restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,11)	1:347:A:ASP:C	1:348:A:SER:N	1:348:A:SER:CA	1:348:A:SER:C	19	12.33
(1,11)	1:347:A:ASP:C	1:348:A:SER:N	1:348:A:SER:CA	1:348:A:SER:C	13	11.12
(1,161)	1:407:A:PRO:N	1:407:A:PRO:CA	1:407:A:PRO:C	1:408:A:GLY:N	14	6.38
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	19	5.55
(1,81)	1:426:A:ARG:C	1:427:A:THR:N	1:427:A:THR:CA	1:427:A:THR:C	5	4.71
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	3	4.35
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	16	4.14
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	6	4.09
(1,108)	1:350:A:TYR:N	1:350:A:TYR:CA	1:350:A:TYR:C	1:351:A:GLU:N	17	4.09
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	2	4.06
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	10	4.04
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	11	4.04
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	17	4.0
(1,90)	1:435:A:SER:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	19	3.66
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	7	3.58
(1,108)	1:350:A:TYR:N	1:350:A:TYR:CA	1:350:A:TYR:C	1:351:A:GLU:N	13	3.23
(1,90)	1:435:A:SER:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	4	3.23
(1,136)	1:380:A:LYS:N	1:380:A:LYS:CA	1:380:A:LYS:C	1:381:A:ASN:N	7	3.14
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	15	3.12
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	8	3.11
(1,90)	1:435:A:SER:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	7	3.08
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	4	3.05
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	13	3.05
(1,48)	1:388:A:GLU:C	1:389:A:LYS:N	1:389:A:LYS:CA	1:389:A:LYS:C	1	3.04
(1,106)	1:348:A:SER:N	1:348:A:SER:CA	1:348:A:SER:C	1:349:A:ARG:N	17	3.0
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	5	2.99
(1,48)	1:388:A:GLU:C	1:389:A:LYS:N	1:389:A:LYS:CA	1:389:A:LYS:C	6	2.99
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	12	2.95
(1,59)	1:399:A:LYS:C	1:400:A:LEU:N	1:400:A:LEU:CA	1:400:A:LEU:C	4	2.91
(1,184)	1:435:A:SER:N	1:435:A:SER:CA	1:435:A:SER:C	1:436:A:GLN:N	2	2.78
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	1	2.78
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	1	2.78
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	14	2.74
(1,106)	1:348:A:SER:N	1:348:A:SER:CA	1:348:A:SER:C	1:349:A:ARG:N	10	2.74
(1,90)	1:435:A:SER:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	11	2.73
(1,97)	1:338:A:TRP:N	1:338:A:TRP:CA	1:338:A:TRP:C	1:339:A:ASP:N	2	2.7
(1,12)	1:348:A:SER:C	1:349:A:ARG:N	1:349:A:ARG:CA	1:349:A:ARG:C	19	2.7
(1,18)	1:354:A:ILE:C	1:355:A:ARG:N	1:355:A:ARG:CA	1:355:A:ARG:C	13	2.58
(1,59)	1:399:A:LYS:C	1:400:A:LEU:N	1:400:A:LEU:CA	1:400:A:LEU:C	16	2.53
(1,59)	1:399:A:LYS:C	1:400:A:LEU:N	1:400:A:LEU:CA	1:400:A:LEU:C	19	2.53
(1,145)	1:391:A:SER:N	1:391:A:SER:CA	1:391:A:SER:C	1:392:A:ARG:N	5	2.52
(1,59)	1:399:A:LYS:C	1:400:A:LEU:N	1:400:A:LEU:CA	1:400:A:LEU:C	1	2.51
(1,78)	1:421:A:GLU:C	1:422:A:ILE:N	1:422:A:ILE:CA	1:422:A:ILE:C	10	2.5
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	18	2.47
(1,103)	1:344:A:LEU:N	1:344:A:LEU:CA	1:344:A:LEU:C	1:345:A:LEU:N	19	2.47
(1,148)	1:394:A:LEU:N	1:394:A:LEU:CA	1:394:A:LEU:C	1:395:A:ARG:N	17	2.45
(1,59)	1:399:A:LYS:C	1:400:A:LEU:N	1:400:A:LEU:CA	1:400:A:LEU:C	6	2.44

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,145)	1:391:A:SER:N	1:391:A:SER:CA	1:391:A:SER:C	1:392:A:ARG:N	7	2.41
(1,143)	1:389:A:LYS:N	1:389:A:LYS:CA	1:389:A:LYS:C	1:390:A:MET:N	18	2.41
(1,136)	1:380:A:LYS:N	1:380:A:LYS:CA	1:380:A:LYS:C	1:381:A:ASN:N	4	2.41
(1,97)	1:338:A:TRP:N	1:338:A:TRP:CA	1:338:A:TRP:C	1:339:A:ASP:N	8	2.39
(1,108)	1:350:A:TYR:N	1:350:A:TYR:CA	1:350:A:TYR:C	1:351:A:GLU:N	19	2.38
(1,90)	1:435:A:SER:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	15	2.36
(1,97)	1:338:A:TRP:N	1:338:A:TRP:CA	1:338:A:TRP:C	1:339:A:ASP:N	5	2.34
(1,116)	1:359:A:LYS:N	1:359:A:LYS:CA	1:359:A:LYS:C	1:360:A:GLU:N	2	2.31
(1,86)	1:431:A:GLU:C	1:432:A:HIS:N	1:432:A:HIS:CA	1:432:A:HIS:C	18	2.29
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	8	2.28
(1,161)	1:407:A:PRO:N	1:407:A:PRO:CA	1:407:A:PRO:C	1:408:A:GLY:N	7	2.25
(1,59)	1:399:A:LYS:C	1:400:A:LEU:N	1:400:A:LEU:CA	1:400:A:LEU:C	18	2.25
(1,48)	1:388:A:GLU:C	1:389:A:LYS:N	1:389:A:LYS:CA	1:389:A:LYS:C	7	2.24
(1,108)	1:350:A:TYR:N	1:350:A:TYR:CA	1:350:A:TYR:C	1:351:A:GLU:N	10	2.23
(1,136)	1:380:A:LYS:N	1:380:A:LYS:CA	1:380:A:LYS:C	1:381:A:ASN:N	13	2.21
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	5	2.21
(1,90)	1:435:A:SER:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	18	2.2
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	12	2.2
(1,136)	1:380:A:LYS:N	1:380:A:LYS:CA	1:380:A:LYS:C	1:381:A:ASN:N	15	2.18
(1,182)	1:433:A:LEU:N	1:433:A:LEU:CA	1:433:A:LEU:C	1:434:A:GLU:N	17	2.17
(1,90)	1:435:A:SER:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	8	2.17
(1,1)	1:336:A:LEU:C	1:337:A:LEU:N	1:337:A:LEU:CA	1:337:A:LEU:C	5	2.17
(1,84)	1:429:A:ARG:C	1:430:A:LEU:N	1:430:A:LEU:CA	1:430:A:LEU:C	4	2.16
(1,145)	1:391:A:SER:N	1:391:A:SER:CA	1:391:A:SER:C	1:392:A:ARG:N	9	2.14
(1,143)	1:389:A:LYS:N	1:389:A:LYS:CA	1:389:A:LYS:C	1:390:A:MET:N	14	2.14
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	9	2.09
(1,145)	1:391:A:SER:N	1:391:A:SER:CA	1:391:A:SER:C	1:392:A:ARG:N	19	2.08
(1,145)	1:391:A:SER:N	1:391:A:SER:CA	1:391:A:SER:C	1:392:A:ARG:N	14	2.06
(1,136)	1:380:A:LYS:N	1:380:A:LYS:CA	1:380:A:LYS:C	1:381:A:ASN:N	9	2.06
(1,158)	1:404:A:ARG:N	1:404:A:ARG:CA	1:404:A:ARG:C	1:405:A:LYS:N	8	2.01
(1,136)	1:380:A:LYS:N	1:380:A:LYS:CA	1:380:A:LYS:C	1:381:A:ASN:N	5	2.01
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	2	2.01
(1,1)	1:336:A:LEU:C	1:337:A:LEU:N	1:337:A:LEU:CA	1:337:A:LEU:C	6	1.99
(1,97)	1:338:A:TRP:N	1:338:A:TRP:CA	1:338:A:TRP:C	1:339:A:ASP:N	15	1.97
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	18	1.97
(1,97)	1:338:A:TRP:N	1:338:A:TRP:CA	1:338:A:TRP:C	1:339:A:ASP:N	16	1.9
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	7	1.9
(1,89)	1:434:A:GLU:C	1:435:A:SER:N	1:435:A:SER:CA	1:435:A:SER:C	9	1.89
(1,11)	1:347:A:ASP:C	1:348:A:SER:N	1:348:A:SER:CA	1:348:A:SER:C	4	1.88
(1,145)	1:391:A:SER:N	1:391:A:SER:CA	1:391:A:SER:C	1:392:A:ARG:N	12	1.84
(1,97)	1:338:A:TRP:N	1:338:A:TRP:CA	1:338:A:TRP:C	1:339:A:ASP:N	6	1.84
(1,90)	1:435:A:SER:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	12	1.84
(1,18)	1:354:A:ILE:C	1:355:A:ARG:N	1:355:A:ARG:CA	1:355:A:ARG:C	17	1.84
(1,146)	1:392:A:ARG:N	1:392:A:ARG:CA	1:392:A:ARG:C	1:393:A:ALA:N	17	1.82
(1,89)	1:434:A:GLU:C	1:435:A:SER:N	1:435:A:SER:CA	1:435:A:SER:C	10	1.82
(1,161)	1:407:A:PRO:N	1:407:A:PRO:CA	1:407:A:PRO:C	1:408:A:GLY:N	18	1.81
(1,18)	1:354:A:ILE:C	1:355:A:ARG:N	1:355:A:ARG:CA	1:355:A:ARG:C	12	1.8
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	6	1.8
(1,161)	1:407:A:PRO:N	1:407:A:PRO:CA	1:407:A:PRO:C	1:408:A:GLY:N	15	1.78
(1,145)	1:391:A:SER:N	1:391:A:SER:CA	1:391:A:SER:C	1:392:A:ARG:N	2	1.78
(1,145)	1:391:A:SER:N	1:391:A:SER:CA	1:391:A:SER:C	1:392:A:ARG:N	18	1.77

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,59)	1:399:A:LYS:C	1:400:A:LEU:N	1:400:A:LEU:CA	1:400:A:LEU:C	3	1.75
(1,97)	1:338:A:TRP:N	1:338:A:TRP:CA	1:338:A:TRP:C	1:339:A:ASP:N	14	1.74
(1,97)	1:338:A:TRP:N	1:338:A:TRP:CA	1:338:A:TRP:C	1:339:A:ASP:N	1	1.73
(1,164)	1:411:A:LEU:N	1:411:A:LEU:CA	1:411:A:LEU:C	1:412:A:LEU:N	9	1.72
(1,161)	1:407:A:PRO:N	1:407:A:PRO:CA	1:407:A:PRO:C	1:408:A:GLY:N	11	1.72
(1,145)	1:391:A:SER:N	1:391:A:SER:CA	1:391:A:SER:C	1:392:A:ARG:N	17	1.71
(1,89)	1:434:A:GLU:C	1:435:A:SER:N	1:435:A:SER:CA	1:435:A:SER:C	3	1.71
(1,59)	1:399:A:LYS:C	1:400:A:LEU:N	1:400:A:LEU:CA	1:400:A:LEU:C	9	1.71
(1,118)	1:361:A:SER:N	1:361:A:SER:CA	1:361:A:SER:C	1:362:A:LYS:N	13	1.7
(1,67)	1:407:A:PRO:C	1:408:A:GLY:N	1:408:A:GLY:CA	1:408:A:GLY:C	14	1.7
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	14	1.7
(1,90)	1:435:A:SER:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	14	1.69
(1,143)	1:389:A:LYS:N	1:389:A:LYS:CA	1:389:A:LYS:C	1:390:A:MET:N	11	1.67
(1,97)	1:338:A:TRP:N	1:338:A:TRP:CA	1:338:A:TRP:C	1:339:A:ASP:N	7	1.66
(1,97)	1:338:A:TRP:N	1:338:A:TRP:CA	1:338:A:TRP:C	1:339:A:ASP:N	11	1.66
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	13	1.66
(1,18)	1:354:A:ILE:C	1:355:A:ARG:N	1:355:A:ARG:CA	1:355:A:ARG:C	8	1.64
(1,90)	1:435:A:SER:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	13	1.63
(1,48)	1:388:A:GLU:C	1:389:A:LYS:N	1:389:A:LYS:CA	1:389:A:LYS:C	16	1.62
(1,148)	1:394:A:LEU:N	1:394:A:LEU:CA	1:394:A:LEU:C	1:395:A:ARG:N	5	1.61
(1,145)	1:391:A:SER:N	1:391:A:SER:CA	1:391:A:SER:C	1:392:A:ARG:N	3	1.61
(1,97)	1:338:A:TRP:N	1:338:A:TRP:CA	1:338:A:TRP:C	1:339:A:ASP:N	12	1.59
(1,161)	1:407:A:PRO:N	1:407:A:PRO:CA	1:407:A:PRO:C	1:408:A:GLY:N	12	1.58
(1,59)	1:399:A:LYS:C	1:400:A:LEU:N	1:400:A:LEU:CA	1:400:A:LEU:C	8	1.58
(1,48)	1:388:A:GLU:C	1:389:A:LYS:N	1:389:A:LYS:CA	1:389:A:LYS:C	14	1.58
(1,168)	1:415:A:PHE:N	1:415:A:PHE:CA	1:415:A:PHE:C	1:416:A:MET:N	5	1.57
(1,116)	1:359:A:LYS:N	1:359:A:LYS:CA	1:359:A:LYS:C	1:360:A:GLU:N	14	1.57
(1,84)	1:429:A:ARG:C	1:430:A:LEU:N	1:430:A:LEU:CA	1:430:A:LEU:C	2	1.57
(1,60)	1:400:A:LEU:C	1:401:A:ASN:N	1:401:A:ASN:CA	1:401:A:ASN:C	18	1.57
(1,145)	1:391:A:SER:N	1:391:A:SER:CA	1:391:A:SER:C	1:392:A:ARG:N	1	1.55
(1,86)	1:431:A:GLU:C	1:432:A:HIS:N	1:432:A:HIS:CA	1:432:A:HIS:C	15	1.55
(1,18)	1:354:A:ILE:C	1:355:A:ARG:N	1:355:A:ARG:CA	1:355:A:ARG:C	19	1.55
(1,48)	1:388:A:GLU:C	1:389:A:LYS:N	1:389:A:LYS:CA	1:389:A:LYS:C	9	1.54
(1,18)	1:354:A:ILE:C	1:355:A:ARG:N	1:355:A:ARG:CA	1:355:A:ARG:C	3	1.54
(1,18)	1:354:A:ILE:C	1:355:A:ARG:N	1:355:A:ARG:CA	1:355:A:ARG:C	9	1.54
(1,1)	1:336:A:LEU:C	1:337:A:LEU:N	1:337:A:LEU:CA	1:337:A:LEU:C	1	1.54
(1,148)	1:394:A:LEU:N	1:394:A:LEU:CA	1:394:A:LEU:C	1:395:A:ARG:N	2	1.51
(1,97)	1:338:A:TRP:N	1:338:A:TRP:CA	1:338:A:TRP:C	1:339:A:ASP:N	4	1.51
(1,97)	1:338:A:TRP:N	1:338:A:TRP:CA	1:338:A:TRP:C	1:339:A:ASP:N	17	1.51
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	11	1.51
(1,89)	1:434:A:GLU:C	1:435:A:SER:N	1:435:A:SER:CA	1:435:A:SER:C	11	1.5
(1,3)	1:338:A:TRP:C	1:339:A:ASP:N	1:339:A:ASP:CA	1:339:A:ASP:C	13	1.5
(1,90)	1:435:A:SER:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	6	1.48
(1,85)	1:430:A:LEU:C	1:431:A:GLU:N	1:431:A:GLU:CA	1:431:A:GLU:C	18	1.48
(1,84)	1:429:A:ARG:C	1:430:A:LEU:N	1:430:A:LEU:CA	1:430:A:LEU:C	8	1.48
(1,11)	1:347:A:ASP:C	1:348:A:SER:N	1:348:A:SER:CA	1:348:A:SER:C	8	1.48
(1,48)	1:388:A:GLU:C	1:389:A:LYS:N	1:389:A:LYS:CA	1:389:A:LYS:C	19	1.47
(1,143)	1:389:A:LYS:N	1:389:A:LYS:CA	1:389:A:LYS:C	1:390:A:MET:N	6	1.46
(1,86)	1:431:A:GLU:C	1:432:A:HIS:N	1:432:A:HIS:CA	1:432:A:HIS:C	8	1.46
(1,97)	1:338:A:TRP:N	1:338:A:TRP:CA	1:338:A:TRP:C	1:339:A:ASP:N	19	1.44
(1,59)	1:399:A:LYS:C	1:400:A:LEU:N	1:400:A:LEU:CA	1:400:A:LEU:C	17	1.44

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,24)	1:361:A:SER:C	1:362:A:LYS:N	1:362:A:LYS:CA	1:362:A:LYS:C	14	1.44
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	4	1.43
(1,18)	1:354:A:ILE:C	1:355:A:ARG:N	1:355:A:ARG:CA	1:355:A:ARG:C	6	1.42
(1,18)	1:354:A:ILE:C	1:355:A:ARG:N	1:355:A:ARG:CA	1:355:A:ARG:C	10	1.42
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	15	1.42
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	16	1.42
(1,1)	1:336:A:LEU:C	1:337:A:LEU:N	1:337:A:LEU:CA	1:337:A:LEU:C	9	1.42
(1,101)	1:342:A:TYR:N	1:342:A:TYR:CA	1:342:A:TYR:C	1:343:A:GLN:N	5	1.41
(1,90)	1:435:A:SER:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	9	1.41
(1,145)	1:391:A:SER:N	1:391:A:SER:CA	1:391:A:SER:C	1:392:A:ARG:N	15	1.4
(1,101)	1:342:A:TYR:N	1:342:A:TYR:CA	1:342:A:TYR:C	1:343:A:GLN:N	9	1.4
(1,98)	1:339:A:ASP:N	1:339:A:ASP:CA	1:339:A:ASP:C	1:340:A:TYR:N	9	1.4
(1,3)	1:338:A:TRP:C	1:339:A:ASP:N	1:339:A:ASP:CA	1:339:A:ASP:C	18	1.39
(1,84)	1:429:A:ARG:C	1:430:A:LEU:N	1:430:A:LEU:CA	1:430:A:LEU:C	6	1.38
(1,101)	1:342:A:TYR:N	1:342:A:TYR:CA	1:342:A:TYR:C	1:343:A:GLN:N	12	1.36
(1,78)	1:421:A:GLU:C	1:422:A:ILE:N	1:422:A:ILE:CA	1:422:A:ILE:C	7	1.36
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	10	1.36
(1,86)	1:431:A:GLU:C	1:432:A:HIS:N	1:432:A:HIS:CA	1:432:A:HIS:C	6	1.35
(1,60)	1:400:A:LEU:C	1:401:A:ASN:N	1:401:A:ASN:CA	1:401:A:ASN:C	19	1.33
(1,136)	1:380:A:LYS:N	1:380:A:LYS:CA	1:380:A:LYS:C	1:381:A:ASN:N	14	1.32
(1,89)	1:434:A:GLU:C	1:435:A:SER:N	1:435:A:SER:CA	1:435:A:SER:C	18	1.32
(1,18)	1:354:A:ILE:C	1:355:A:ARG:N	1:355:A:ARG:CA	1:355:A:ARG:C	15	1.32
(1,145)	1:391:A:SER:N	1:391:A:SER:CA	1:391:A:SER:C	1:392:A:ARG:N	4	1.31
(1,1)	1:336:A:LEU:C	1:337:A:LEU:N	1:337:A:LEU:CA	1:337:A:LEU:C	15	1.31
(1,110)	1:352:A:ASN:N	1:352:A:ASN:CA	1:352:A:ASN:C	1:353:A:PHE:N	5	1.3
(1,101)	1:342:A:TYR:N	1:342:A:TYR:CA	1:342:A:TYR:C	1:343:A:GLN:N	7	1.3
(1,168)	1:415:A:PHE:N	1:415:A:PHE:CA	1:415:A:PHE:C	1:416:A:MET:N	1	1.29
(1,145)	1:391:A:SER:N	1:391:A:SER:CA	1:391:A:SER:C	1:392:A:ARG:N	6	1.29
(1,52)	1:392:A:ARG:C	1:393:A:ALA:N	1:393:A:ALA:CA	1:393:A:ALA:C	2	1.29
(1,49)	1:389:A:LYS:C	1:390:A:MET:N	1:390:A:MET:CA	1:390:A:MET:C	3	1.29
(1,47)	1:387:A:TYR:C	1:388:A:GLU:N	1:388:A:GLU:CA	1:388:A:GLU:C	11	1.29
(1,1)	1:336:A:LEU:C	1:337:A:LEU:N	1:337:A:LEU:CA	1:337:A:LEU:C	2	1.29
(1,59)	1:399:A:LYS:C	1:400:A:LEU:N	1:400:A:LEU:CA	1:400:A:LEU:C	2	1.28
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	3	1.28
(1,17)	1:353:A:PHE:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	19	1.28
(1,11)	1:347:A:ASP:C	1:348:A:SER:N	1:348:A:SER:CA	1:348:A:SER:C	12	1.28
(1,146)	1:392:A:ARG:N	1:392:A:ARG:CA	1:392:A:ARG:C	1:393:A:ALA:N	6	1.27
(1,118)	1:361:A:SER:N	1:361:A:SER:CA	1:361:A:SER:C	1:362:A:LYS:N	11	1.27
(1,148)	1:394:A:LEU:N	1:394:A:LEU:CA	1:394:A:LEU:C	1:395:A:ARG:N	3	1.26
(1,148)	1:394:A:LEU:N	1:394:A:LEU:CA	1:394:A:LEU:C	1:395:A:ARG:N	7	1.26
(1,11)	1:347:A:ASP:C	1:348:A:SER:N	1:348:A:SER:CA	1:348:A:SER:C	3	1.26
(1,161)	1:407:A:PRO:N	1:407:A:PRO:CA	1:407:A:PRO:C	1:408:A:GLY:N	4	1.25
(1,143)	1:389:A:LYS:N	1:389:A:LYS:CA	1:389:A:LYS:C	1:390:A:MET:N	1	1.25
(1,48)	1:388:A:GLU:C	1:389:A:LYS:N	1:389:A:LYS:CA	1:389:A:LYS:C	4	1.25
(1,119)	1:362:A:LYS:N	1:362:A:LYS:CA	1:362:A:LYS:C	1:363:A:ILE:N	11	1.24
(1,101)	1:342:A:TYR:N	1:342:A:TYR:CA	1:342:A:TYR:C	1:343:A:GLN:N	11	1.24
(1,184)	1:435:A:SER:N	1:435:A:SER:CA	1:435:A:SER:C	1:436:A:GLN:N	6	1.23
(1,81)	1:426:A:ARG:C	1:427:A:THR:N	1:427:A:THR:CA	1:427:A:THR:C	16	1.23
(1,59)	1:399:A:LYS:C	1:400:A:LEU:N	1:400:A:LEU:CA	1:400:A:LEU:C	7	1.23
(1,110)	1:352:A:ASN:N	1:352:A:ASN:CA	1:352:A:ASN:C	1:353:A:PHE:N	18	1.22
(1,90)	1:435:A:SER:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	2	1.22

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,90)	1:435:A:SER:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	5	1.21
(1,15)	1:351:A:GLU:C	1:352:A:ASN:N	1:352:A:ASN:CA	1:352:A:ASN:C	16	1.21
(1,118)	1:361:A:SER:N	1:361:A:SER:CA	1:361:A:SER:C	1:362:A:LYS:N	6	1.2
(1,60)	1:400:A:LEU:C	1:401:A:ASN:N	1:401:A:ASN:CA	1:401:A:ASN:C	11	1.2
(1,48)	1:388:A:GLU:C	1:389:A:LYS:N	1:389:A:LYS:CA	1:389:A:LYS:C	15	1.19
(1,18)	1:354:A:ILE:C	1:355:A:ARG:N	1:355:A:ARG:CA	1:355:A:ARG:C	11	1.18
(1,161)	1:407:A:PRO:N	1:407:A:PRO:CA	1:407:A:PRO:C	1:408:A:GLY:N	1	1.17
(1,60)	1:400:A:LEU:C	1:401:A:ASN:N	1:401:A:ASN:CA	1:401:A:ASN:C	16	1.17
(1,145)	1:391:A:SER:N	1:391:A:SER:CA	1:391:A:SER:C	1:392:A:ARG:N	16	1.16
(1,97)	1:338:A:TRP:N	1:338:A:TRP:CA	1:338:A:TRP:C	1:339:A:ASP:N	10	1.16
(1,77)	1:420:A:ASP:C	1:421:A:GLU:N	1:421:A:GLU:CA	1:421:A:GLU:C	1	1.16
(1,18)	1:354:A:ILE:C	1:355:A:ARG:N	1:355:A:ARG:CA	1:355:A:ARG:C	1	1.15
(1,11)	1:347:A:ASP:C	1:348:A:SER:N	1:348:A:SER:CA	1:348:A:SER:C	16	1.15
(1,60)	1:400:A:LEU:C	1:401:A:ASN:N	1:401:A:ASN:CA	1:401:A:ASN:C	6	1.14
(1,84)	1:429:A:ARG:C	1:430:A:LEU:N	1:430:A:LEU:CA	1:430:A:LEU:C	5	1.13
(1,15)	1:351:A:GLU:C	1:352:A:ASN:N	1:352:A:ASN:CA	1:352:A:ASN:C	9	1.13
(1,11)	1:347:A:ASP:C	1:348:A:SER:N	1:348:A:SER:CA	1:348:A:SER:C	14	1.12
(1,85)	1:430:A:LEU:C	1:431:A:GLU:N	1:431:A:GLU:CA	1:431:A:GLU:C	4	1.11
(1,59)	1:399:A:LYS:C	1:400:A:LEU:N	1:400:A:LEU:CA	1:400:A:LEU:C	5	1.11
(1,118)	1:361:A:SER:N	1:361:A:SER:CA	1:361:A:SER:C	1:362:A:LYS:N	9	1.1
(1,175)	1:424:A:SER:N	1:424:A:SER:CA	1:424:A:SER:C	1:425:A:GLY:N	6	1.09
(1,119)	1:362:A:LYS:N	1:362:A:LYS:CA	1:362:A:LYS:C	1:363:A:ILE:N	18	1.09
(1,110)	1:352:A:ASN:N	1:352:A:ASN:CA	1:352:A:ASN:C	1:353:A:PHE:N	9	1.09
(1,4)	1:339:A:ASP:C	1:340:A:TYR:N	1:340:A:TYR:CA	1:340:A:TYR:C	9	1.09
(1,119)	1:362:A:LYS:N	1:362:A:LYS:CA	1:362:A:LYS:C	1:363:A:ILE:N	3	1.08
(1,101)	1:342:A:TYR:N	1:342:A:TYR:CA	1:342:A:TYR:C	1:343:A:GLN:N	18	1.08
(1,180)	1:431:A:GLU:N	1:431:A:GLU:CA	1:431:A:GLU:C	1:432:A:HIS:N	11	1.07
(1,118)	1:361:A:SER:N	1:361:A:SER:CA	1:361:A:SER:C	1:362:A:LYS:N	18	1.06
(1,81)	1:426:A:ARG:C	1:427:A:THR:N	1:427:A:THR:CA	1:427:A:THR:C	6	1.06
(1,175)	1:424:A:SER:N	1:424:A:SER:CA	1:424:A:SER:C	1:425:A:GLY:N	3	1.05
(1,108)	1:350:A:TYR:N	1:350:A:TYR:CA	1:350:A:TYR:C	1:351:A:GLU:N	9	1.05
(1,60)	1:400:A:LEU:C	1:401:A:ASN:N	1:401:A:ASN:CA	1:401:A:ASN:C	7	1.05
(1,148)	1:394:A:LEU:N	1:394:A:LEU:CA	1:394:A:LEU:C	1:395:A:ARG:N	11	1.04
(1,145)	1:391:A:SER:N	1:391:A:SER:CA	1:391:A:SER:C	1:392:A:ARG:N	11	1.03
(1,110)	1:352:A:ASN:N	1:352:A:ASN:CA	1:352:A:ASN:C	1:353:A:PHE:N	15	1.02
(1,86)	1:431:A:GLU:C	1:432:A:HIS:N	1:432:A:HIS:CA	1:432:A:HIS:C	5	1.02
(1,59)	1:399:A:LYS:C	1:400:A:LEU:N	1:400:A:LEU:CA	1:400:A:LEU:C	11	1.02
(1,1)	1:336:A:LEU:C	1:337:A:LEU:N	1:337:A:LEU:CA	1:337:A:LEU:C	16	1.01