Full wwPDB NMR Structure Validation Report ⓘ

Jun 18, 2024 – 12:19 PM JST

PDB ID	:	8K2R
BMRB ID	:	36580
Title	:	The structure of HtpG M domain in complex with unstructured D131D binding site b
Authors	:	Qu, X.; Huang, C.
Deposited on	:	2023-07-13

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

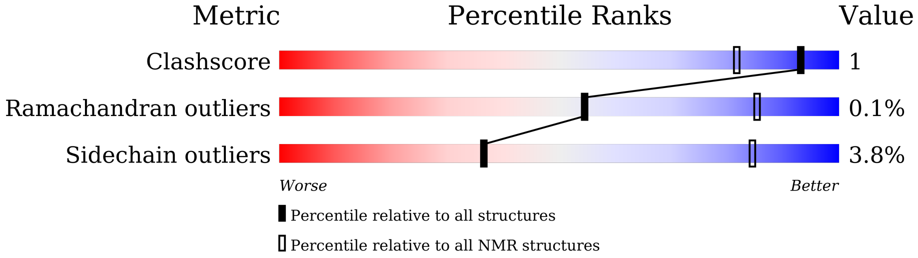
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

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

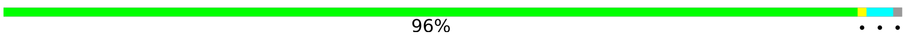
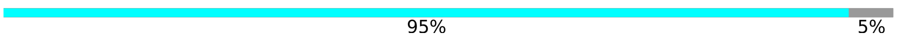
The overall completeness of chemical shifts assignment is 25%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	268	
2	B	75	

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:232-A:489 (258)	1.16	17

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 4 clusters. No single-model clusters were found.

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

3 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 5513 atoms, of which 2743 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Molecular chaperone HtpG (Fragment).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	265	4332	1390	2146	371	418	7	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	GLY	-	expression tag	UNP A0A7A6VTW3
A	228	HIS	-	expression tag	UNP A0A7A6VTW3
A	229	MET	-	expression tag	UNP A0A7A6VTW3

- Molecule 2 is a protein called Disordered protein(D131D).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	71	1181	370	597	107	106	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	597	LEU	-	expression tag	UNP P00644
B	598	GLU	-	expression tag	UNP P00644
B	599	HIS	-	expression tag	UNP P00644
B	600	MET	-	expression tag	UNP P00644

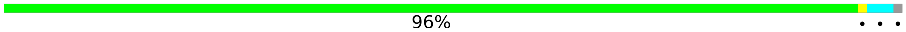
4 Residue-property plots ⓘ

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.

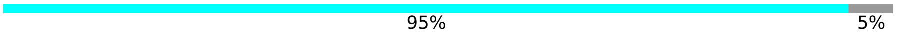
- Molecule 1: Molecular chaperone HtpG (Fragment)

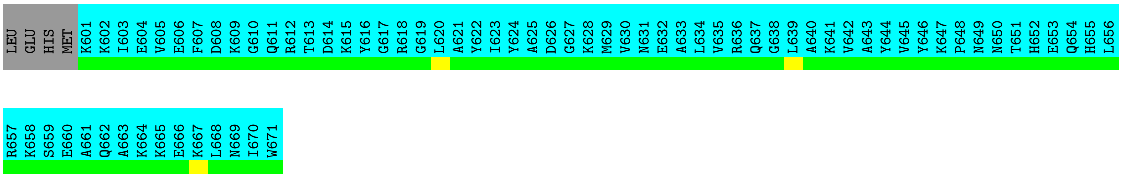
Chain A:



- Molecule 2: Disordered protein(D131D)

Chain B:





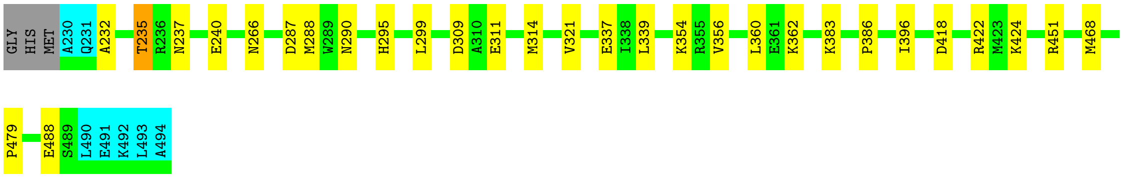
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

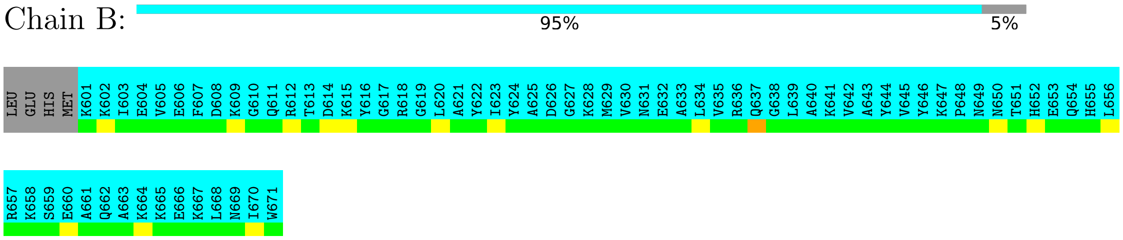
4.2.1 Score per residue for model 1

- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A:

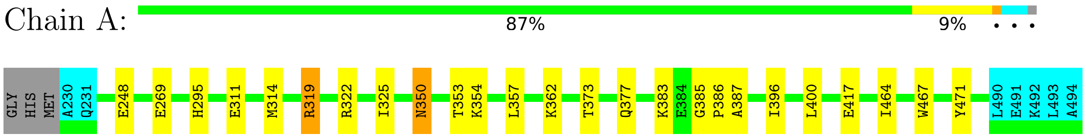


- Molecule 2: Disordered protein(D131D)

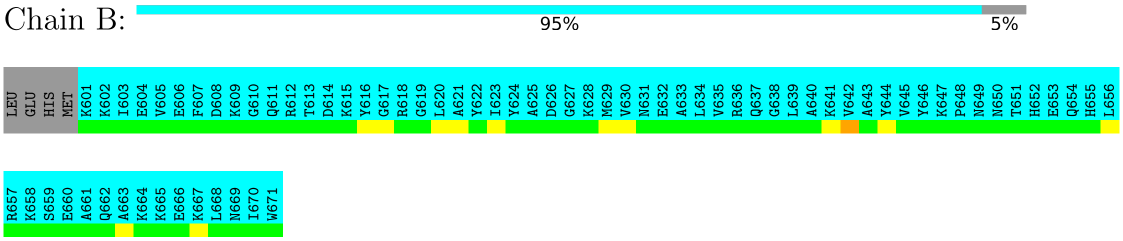


4.2.2 Score per residue for model 2

- Molecule 1: Molecular chaperone HtpG (Fragment)

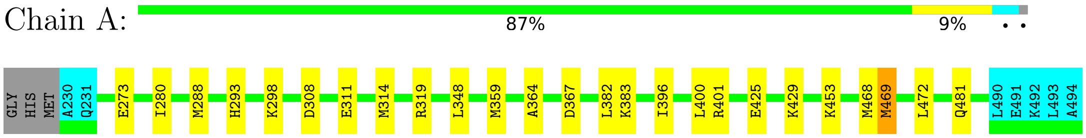


- Molecule 2: Disordered protein(D131D)

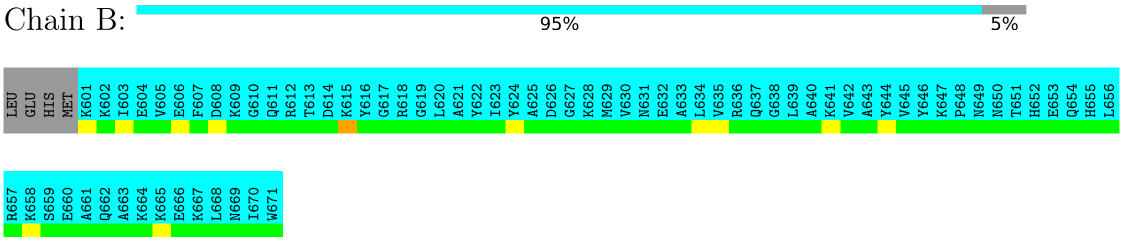


4.2.3 Score per residue for model 3

- Molecule 1: Molecular chaperone HtpG (Fragment)



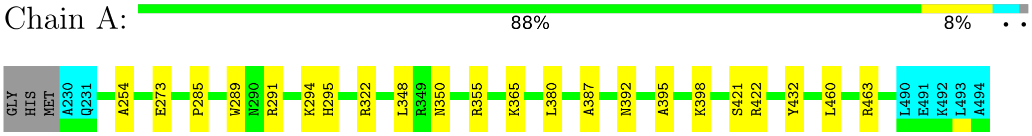
- Molecule 2: Disordered protein(D131D)



4.2.4 Score per residue for model 4

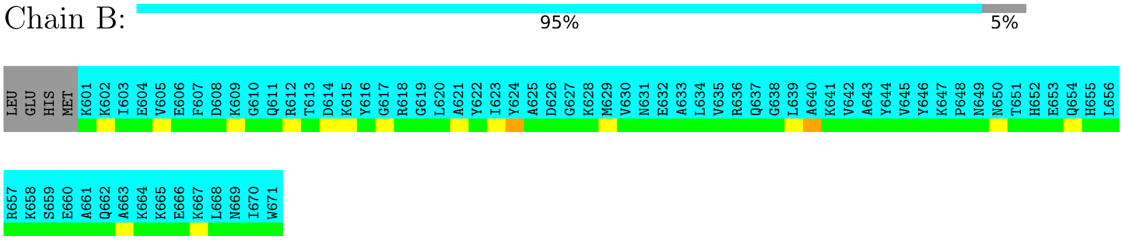
- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A:



- Molecule 2: Disordered protein(D131D)

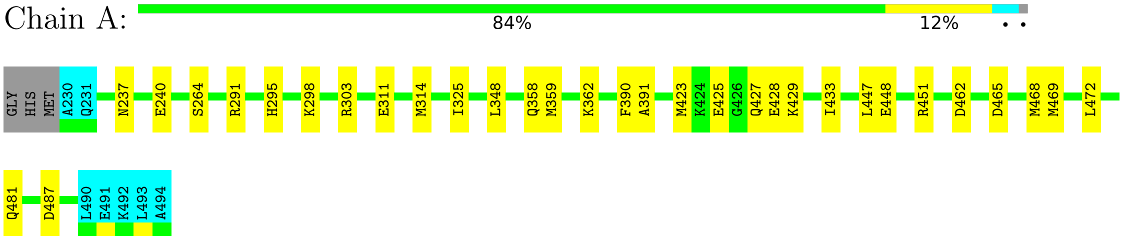
Chain B:



4.2.5 Score per residue for model 5

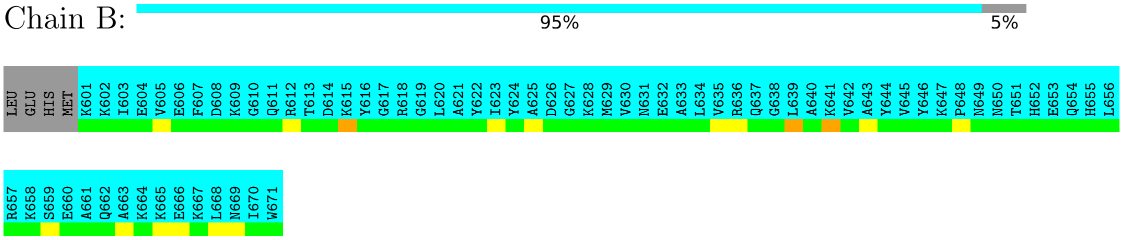
- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A:



- Molecule 2: Disordered protein(D131D)

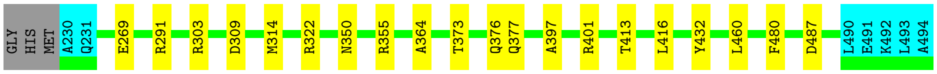
Chain B:



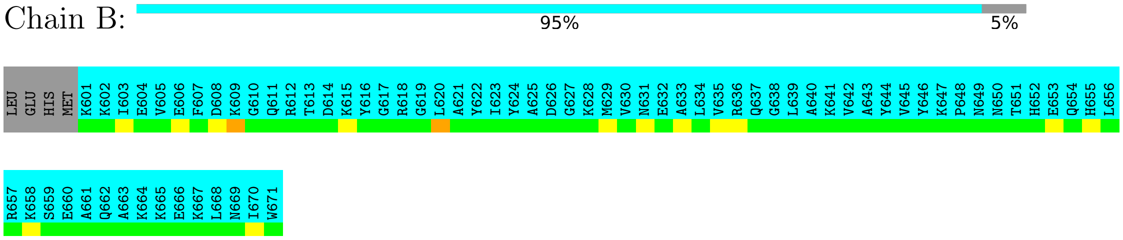
4.2.6 Score per residue for model 6

- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A:

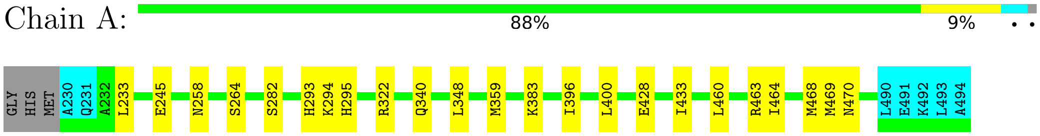


- Molecule 2: Disordered protein(D131D)

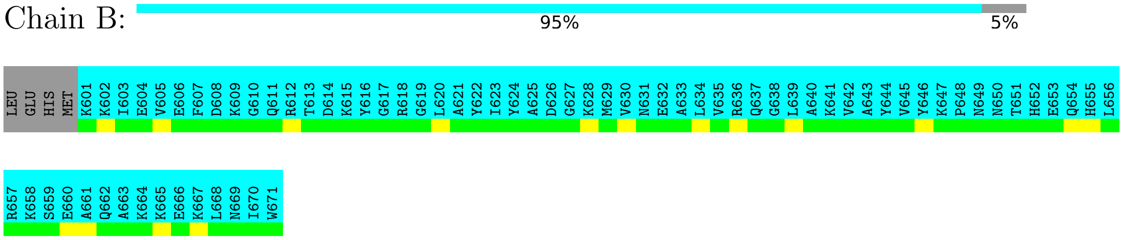


4.2.7 Score per residue for model 7

- Molecule 1: Molecular chaperone HtpG (Fragment)

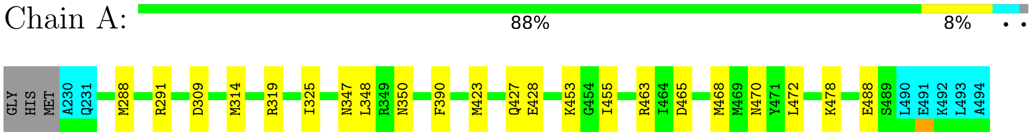


- Molecule 2: Disordered protein(D131D)

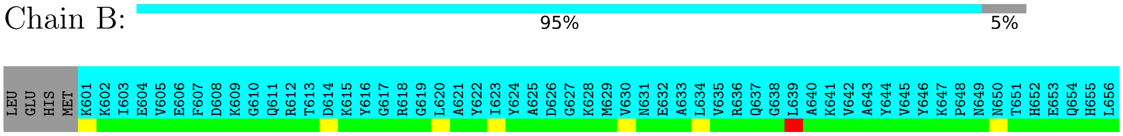


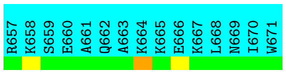
4.2.8 Score per residue for model 8

- Molecule 1: Molecular chaperone HtpG (Fragment)



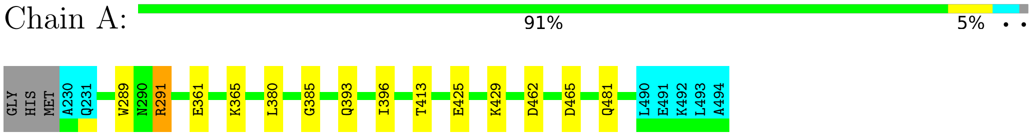
- Molecule 2: Disordered protein(D131D)



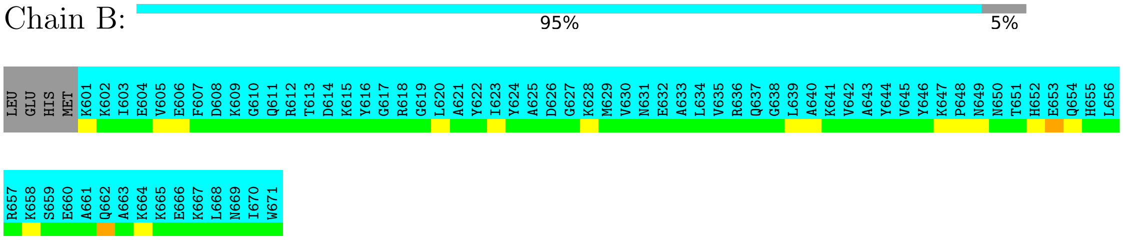


4.2.9 Score per residue for model 9

- Molecule 1: Molecular chaperone HtpG (Fragment)

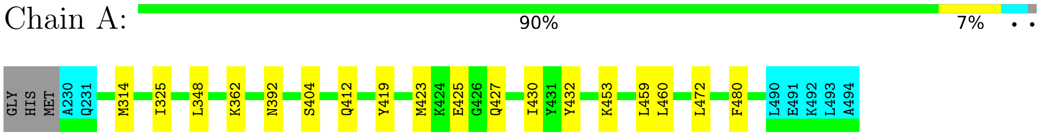


- Molecule 2: Disordered protein(D131D)

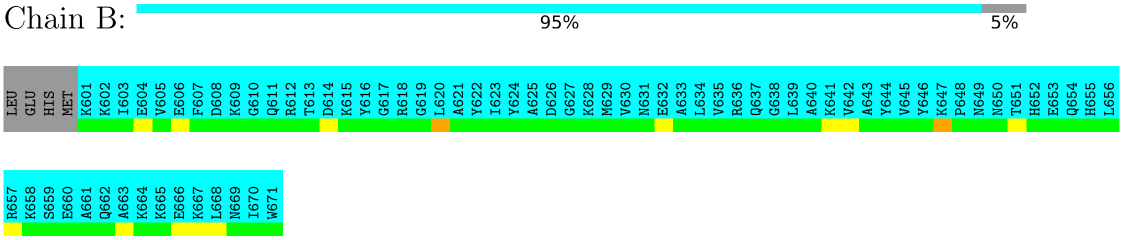


4.2.10 Score per residue for model 10

- Molecule 1: Molecular chaperone HtpG (Fragment)

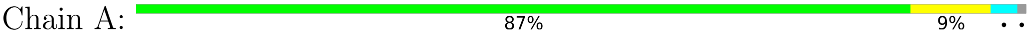


- Molecule 2: Disordered protein(D131D)

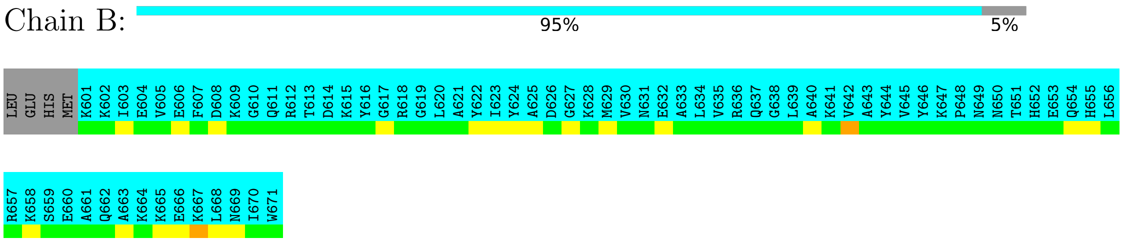


4.2.11 Score per residue for model 11

- Molecule 1: Molecular chaperone HtpG (Fragment)

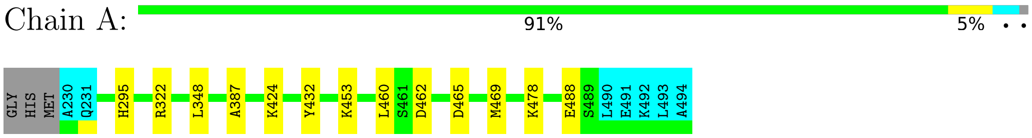


- Molecule 2: Disordered protein(D131D)

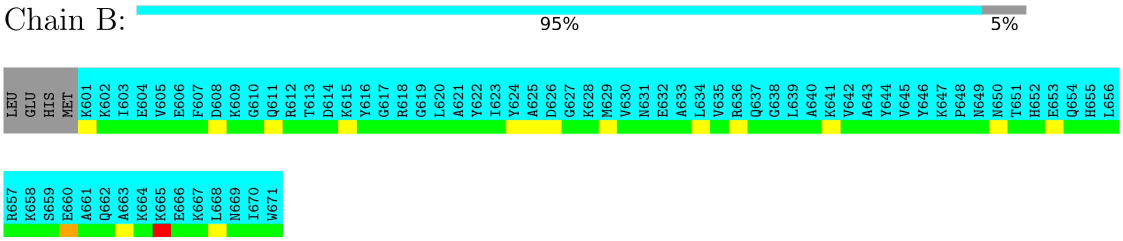


4.2.12 Score per residue for model 12

- Molecule 1: Molecular chaperone HtpG (Fragment)

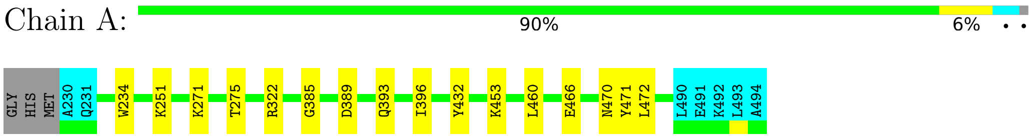


- Molecule 2: Disordered protein(D131D)

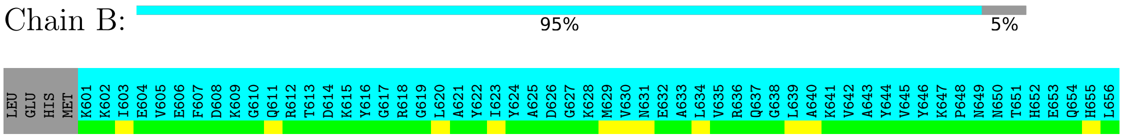


4.2.13 Score per residue for model 13

- Molecule 1: Molecular chaperone HtpG (Fragment)



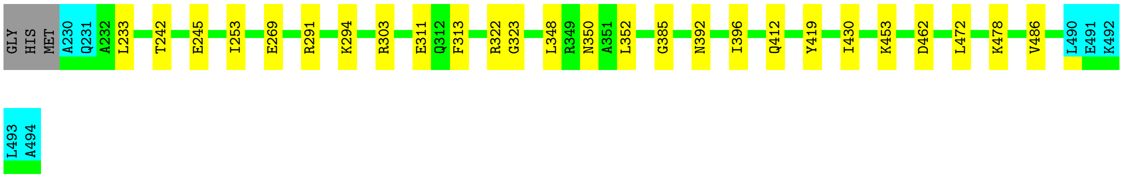
- Molecule 2: Disordered protein(D131D)



4.2.14 Score per residue for model 14

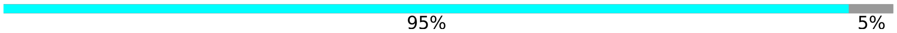
- Molecule 1: Molecular chaperone HtpG (Fragment)

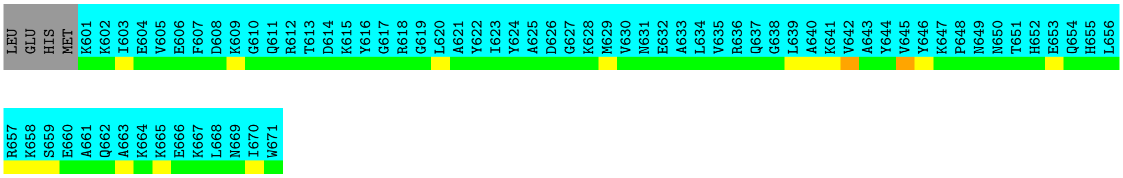
Chain A:



- Molecule 2: Disordered protein(D131D)

Chain B:

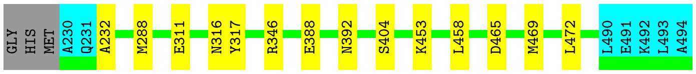




4.2.15 Score per residue for model 15

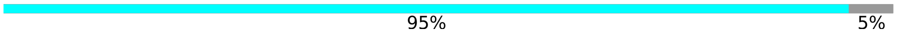
- Molecule 1: Molecular chaperone HtpG (Fragment)

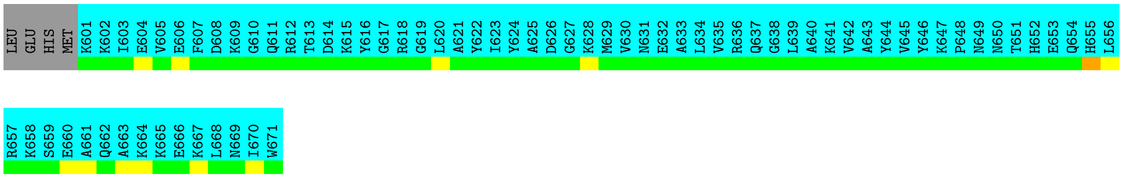
Chain A:



- Molecule 2: Disordered protein(D131D)

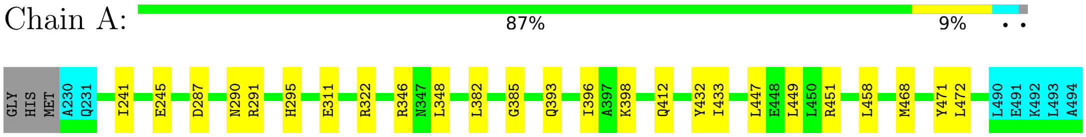
Chain B:



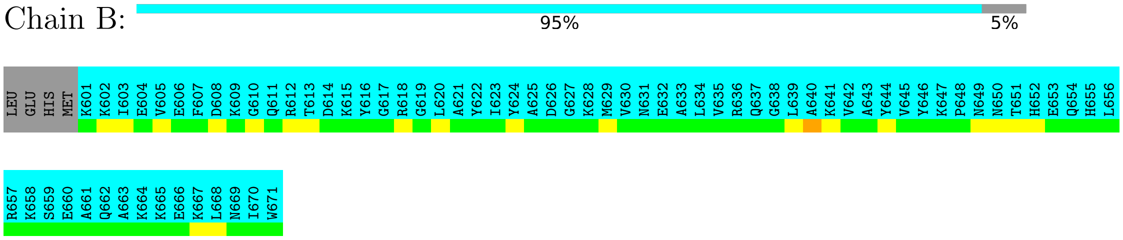


4.2.16 Score per residue for model 16

- Molecule 1: Molecular chaperone HtpG (Fragment)

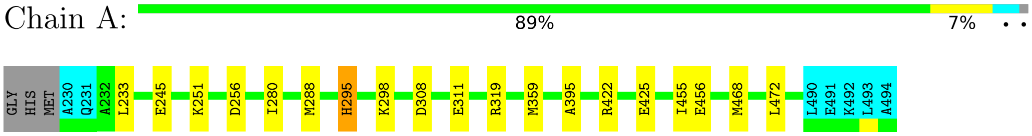


- Molecule 2: Disordered protein(D131D)

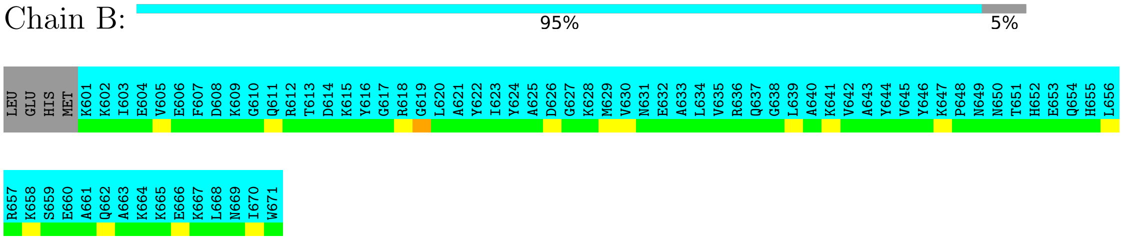


4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Molecular chaperone HtpG (Fragment)

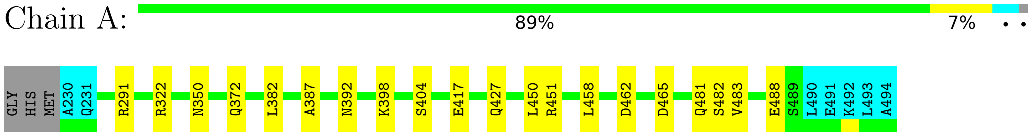


- Molecule 2: Disordered protein(D131D)

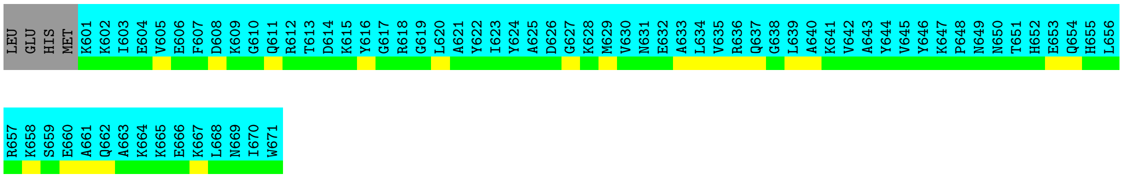


4.2.18 Score per residue for model 18

- Molecule 1: Molecular chaperone HtpG (Fragment)



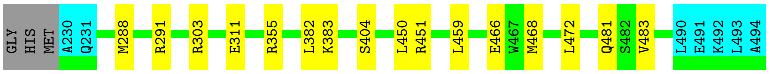
- Molecule 2: Disordered protein(D131D)



4.2.19 Score per residue for model 19

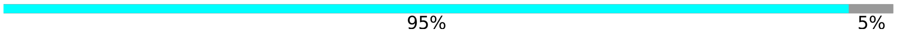
- Molecule 1: Molecular chaperone HtpG (Fragment)

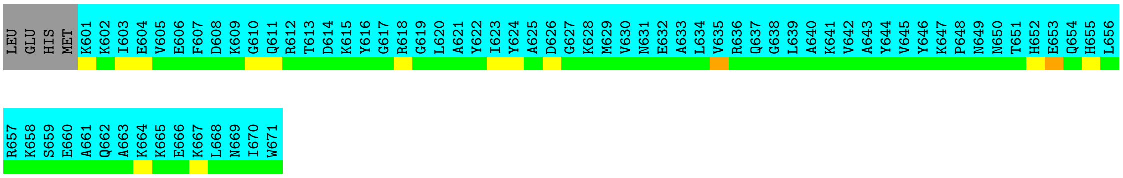
Chain A:



- Molecule 2: Disordered protein(D131D)

Chain B:





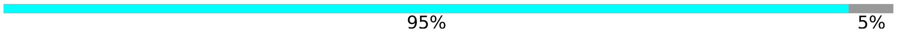
4.2.20 Score per residue for model 20

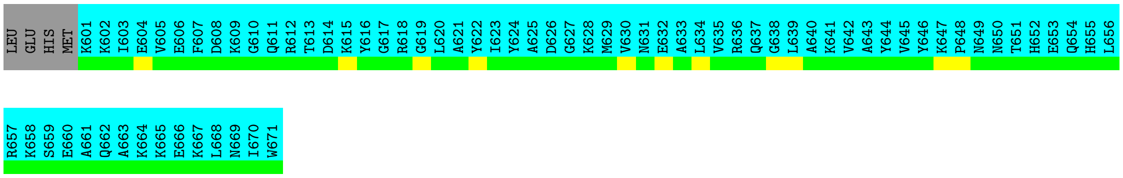
- Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A:

- Molecule 2: Disordered protein(D131D)

Chain B:





5 Refinement protocol and experimental data overview (i)

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

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

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

Software name	**Classification**	**Version**
CNS	refinement	
CYANA	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	955
Number of shifts mapped to atoms	955
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	25%

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	2133	2087	2080	5±2
2	B	0	0	0	0±0
All	All	42660	41740	41600	107

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:285:PRO:HG3	1:A:322:ARG:HH22	0.62	1.54	4	1
1:A:288:MET:SD	1:A:319:ARG:HG3	0.60	2.37	3	2
1:A:404:SER:HB3	1:A:458:LEU:HD23	0.57	1.76	15	2
1:A:434:THR:HB	1:A:466:GLU:HG2	0.57	1.76	11	1
1:A:468:MET:SD	1:A:472:LEU:HD12	0.55	2.41	17	5
1:A:237:ASN:HB2	1:A:240:GLU:HG2	0.54	1.78	1	1
1:A:314:MET:SD	1:A:321:VAL:HB	0.53	2.44	1	1
1:A:385:GLY:HA3	1:A:396:ILE:HG21	0.52	1.80	13	5
1:A:427:GLN:HE21	1:A:455:ILE:HG23	0.51	1.66	8	1
1:A:423:MET:SD	1:A:478:LYS:HG2	0.51	2.46	8	1
1:A:233:LEU:HD11	1:A:245:GLU:HB3	0.50	1.82	17	3
1:A:317:TYR:HB2	1:A:388:GLU:HG3	0.50	1.82	15	1
1:A:462:ASP:HB3	1:A:465:ASP:HB3	0.49	1.83	5	1

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Atom-1	**Atom-2**	**Clash(Å)**	**Distance(Å)**	**Models**	
				Worst	Total
1:A:462:ASP:HB3	1:A:465:ASP:HB2	0.49	1.83	18	1
1:A:404:SER:HB3	1:A:458:LEU:HD13	0.49	1.85	18	1
1:A:287:ASP:HB2	1:A:294:LYS:HG2	0.49	1.84	20	1
1:A:423:MET:HA	1:A:427:GLN:NE2	0.49	2.21	5	1
1:A:295:HIS:HB3	1:A:319:ARG:HG3	0.49	1.83	17	1
1:A:432:TYR:HD1	1:A:460:LEU:HD11	0.48	1.68	4	2
1:A:383:LYS:HG3	1:A:468:MET:SD	0.48	2.48	7	1
1:A:460:LEU:HD21	1:A:469:MET:HG3	0.48	1.85	7	1
1:A:390:PHE:HA	1:A:393:GLN:HB2	0.48	1.85	11	1
1:A:450:LEU:HD11	1:A:483:VAL:HG11	0.47	1.85	19	2
1:A:383:LYS:HD2	1:A:464:ILE:HG23	0.47	1.87	2	2
1:A:254:ALA:HB1	1:A:322:ARG:HH11	0.47	1.69	4	1
1:A:462:ASP:HB2	1:A:465:ASP:HB3	0.46	1.86	12	2
1:A:280:ILE:HG13	1:A:359:MET:SD	0.46	2.50	17	1
1:A:433:ILE:HG21	1:A:447:LEU:HD23	0.46	1.86	16	1
1:A:241:ILE:HG23	1:A:245:GLU:HG2	0.46	1.86	16	1
1:A:234:TRP:O	1:A:275:THR:HG21	0.46	2.12	13	1
1:A:287:ASP:HA	1:A:290:ASN:HB2	0.45	1.88	16	2
1:A:299:LEU:HD22	1:A:339:LEU:HD11	0.45	1.87	1	1
1:A:264:SER:HB2	1:A:359:MET:SD	0.45	2.52	7	2
1:A:383:LYS:HB3	1:A:468:MET:SD	0.45	2.52	1	1
1:A:432:TYR:CD2	1:A:460:LEU:HD11	0.45	2.47	12	2
1:A:469:MET:SD	1:A:472:LEU:HD12	0.45	2.52	15	1
1:A:422:ARG:HB3	1:A:456:GLU:HG2	0.45	1.87	17	1
1:A:472:LEU:HB3	1:A:480:PHE:CE1	0.45	2.47	10	1
1:A:295:HIS:HB2	1:A:319:ARG:O	0.45	2.12	20	2
1:A:242:THR:HG22	1:A:245:GLU:HG2	0.45	1.88	14	1
1:A:289:TRP:CH2	1:A:380:LEU:HB2	0.44	2.47	4	2
1:A:298:LYS:HA	1:A:308:ASP:HA	0.44	1.89	3	2
1:A:432:TYR:HE1	1:A:480:PHE:HB3	0.44	1.72	6	1
1:A:463:ARG:H	1:A:463:ARG:HD2	0.44	1.72	8	1
1:A:237:ASN:HB3	1:A:240:GLU:HG2	0.44	1.89	5	1
1:A:347:ASN:HA	1:A:350:ASN:ND2	0.43	2.27	8	1
1:A:386:PRO:HD3	1:A:396:ILE:HG21	0.43	1.89	1	1
1:A:291:ARG:HD2	1:A:291:ARG:H	0.43	1.74	14	1
1:A:419:TYR:CD2	1:A:430:ILE:HG23	0.43	2.48	10	1
1:A:313:PHE:HB3	1:A:352:LEU:HD12	0.43	1.91	14	1
1:A:258:ASN:HB3	1:A:282:SER:OG	0.43	2.13	7	1
1:A:291:ARG:H	1:A:291:ARG:HD3	0.43	1.73	9	1
1:A:396:ILE:O	1:A:400:LEU:HG	0.43	2.14	7	2
1:A:373:THR:O	1:A:377:GLN:HG2	0.42	2.15	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:361:GLU:O	1:A:365:LYS:HG2	0.42	2.13	9	1
1:A:442:LYS:HA	1:A:447:LEU:HD21	0.42	1.90	11	1
1:A:432:TYR:HD1	1:A:458:LEU:HB3	0.42	1.74	16	1
1:A:432:TYR:HB2	1:A:460:LEU:HD13	0.42	1.90	6	1
1:A:429:LYS:NZ	1:A:481:GLN:HB2	0.42	2.30	9	1
1:A:404:SER:HA	1:A:459:LEU:HG	0.42	1.90	19	2
1:A:429:LYS:HD3	1:A:481:GLN:HB2	0.42	1.92	5	1
1:A:307:MET:SD	1:A:336:ARG:HB2	0.41	2.55	11	1
1:A:356:VAL:O	1:A:360:LEU:HG	0.41	2.15	1	1
1:A:317:TYR:HB3	1:A:384:GLU:HB2	0.41	1.92	11	1
1:A:280:ILE:HG12	1:A:359:MET:SD	0.41	2.55	3	1
1:A:364:ALA:HB1	1:A:401:ARG:NH2	0.41	2.30	6	2
1:A:232:ALA:O	1:A:235:THR:HG22	0.41	2.16	1	1
1:A:251:LYS:HA	1:A:256:ASP:O	0.41	2.16	17	1
1:A:395:ALA:HA	1:A:398:LYS:HD3	0.41	1.93	4	1
1:A:386:PRO:HG2	1:A:400:LEU:HD11	0.40	1.92	2	1
1:A:468:MET:SD	1:A:469:MET:HE2	0.40	2.56	5	1
1:A:419:TYR:CE2	1:A:430:ILE:HG23	0.40	2.51	14	1
1:A:429:LYS:HZ2	1:A:429:LYS:HB3	0.40	1.76	3	1
1:A:423:MET:SD	1:A:427:GLN:CB	0.40	3.09	10	1
1:A:432:TYR:CE1	1:A:480:PHE:HB3	0.40	2.51	11	1
1:A:350:ASN:O	1:A:354:LYS:HD3	0.40	2.15	2	1
1:A:383:LYS:HA	1:A:468:MET:SD	0.40	2.56	3	1
1:A:288:MET:HE1	1:A:320:PHE:HB3	0.40	1.92	11	1
1:A:397:ALA:HB1	1:A:416:LEU:HD12	0.40	1.93	6	1
1:A:465:ASP:O	1:A:469:MET:HG2	0.40	2.17	15	1
1:A:253:ILE:HD13	1:A:323:GLY:HA2	0.40	1.94	14	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	258/268 (96%)	250±2 (97±1%)	8±2 (3±1%)	0±0 (0±0%)	54	85
2	B	0	-	-	-	-	

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5160/6860 (75%)	4990 (97%)	167 (3%)	3 (0%)	54	85

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	232	ALA	2
1	A	487	ASP	1

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	233/240 (97%)	224±3 (96±1%)	9±3 (4±1%)	36	84
2	B	0	-	-	-	
All	All	4660/6060 (77%)	4485 (96%)	175 (4%)	36	84

All 60 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	311	GLU	10
1	A	348	LEU	10
1	A	295	HIS	8
1	A	322	ARG	8
1	A	291	ARG	8
1	A	314	MET	7
1	A	453	LYS	7
1	A	451	ARG	6
1	A	425	GLU	6
1	A	325	ILE	5
1	A	382	LEU	5
1	A	288	MET	4
1	A	362	LYS	4
1	A	488	GLU	4
1	A	269	GLU	4
1	A	472	LEU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	303	ARG	4
1	A	393	GLN	4
1	A	309	ASP	3
1	A	350	ASN	3
1	A	293	HIS	3
1	A	294	LYS	3
1	A	355	ARG	3
1	A	412	GLN	3
1	A	337	GLU	2
1	A	422	ARG	2
1	A	424	LYS	2
1	A	248	GLU	2
1	A	417	GLU	2
1	A	471	TYR	2
1	A	273	GLU	2
1	A	463	ARG	2
1	A	433	ILE	2
1	A	376	GLN	2
1	A	478	LYS	2
1	A	466	GLU	2
1	A	346	ARG	2
1	A	235	THR	1
1	A	266	ASN	1
1	A	418	ASP	1
1	A	319	ARG	1
1	A	469	MET	1
1	A	365	LYS	1
1	A	298	LYS	1
1	A	358	GLN	1
1	A	447	LEU	1
1	A	448	GLU	1
1	A	487	ASP	1
1	A	340	GLN	1
1	A	465	ASP	1
1	A	429	LYS	1
1	A	251	LYS	1
1	A	271	LYS	1
1	A	470	ASN	1
1	A	462	ASP	1
1	A	316	ASN	1
1	A	372	GLN	1
1	A	398	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	383	LYS	1
1	A	369	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 25% for the well-defined parts and 20% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_0*

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	955
Number of shifts mapped to atoms	955
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	255	-0.01 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	246	0.94 ± 0.09	Should be checked
$^{13}C'$	0	—	None (insufficient data)
^{15}N	227	-0.03 ± 0.26	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 25%, i.e. 927 atoms were assigned a chemical shift out of a possible 3647. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	688/1282 (54%)	220/516 (43%)	248/516 (48%)	220/250 (88%)
Sidechain	239/2019 (12%)	0/1302 (0%)	239/633 (38%)	0/84 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/346 (0%)	0/167 (0%)	0/159 (0%)	0/20 (0%)
Overall	927/3647 (25%)	220/1985 (11%)	487/1308 (37%)	220/354 (62%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 20%, i.e. 955 atoms were assigned a chemical shift out of a possible 4767. 0 out of 53 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	709/1675 (42%)	227/676 (34%)	255/672 (38%)	227/327 (69%)
Sidechain	246/2663 (9%)	0/1715 (0%)	246/831 (30%)	0/117 (0%)
Aromatic	0/429 (0%)	0/206 (0%)	0/198 (0%)	0/25 (0%)
Overall	955/4767 (20%)	227/2597 (9%)	501/1701 (29%)	227/469 (48%)

7.1.4 Statistically unusual chemical shifts ⓘ

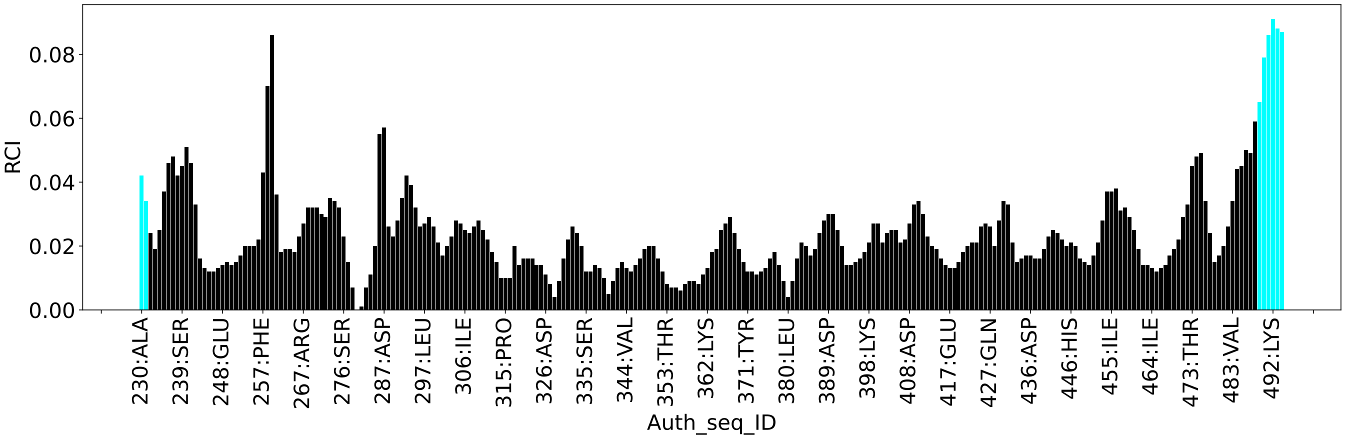
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	279	TYR	H	117.59	4.70 – 11.88	152.2
1	A	328	SER	H	31.14	5.45 – 11.10	40.5
1	A	340	GLN	H	29.41	5.39 – 11.05	37.5
1	A	279	TYR	N	9.63	100.12 – 140.79	-27.2
1	A	380	LEU	CB	57.53	33.11 – 51.34	8.4
1	A	335	SER	CB	51.64	56.28 – 71.32	-8.1
1	A	462	ASP	CB	53.22	32.98 – 48.76	7.8
1	A	380	LEU	CA	40.90	45.17 – 66.21	-7.0
1	A	360	LEU	CB	30.11	33.11 – 51.34	-6.7
1	A	353	THR	CB	58.99	61.12 – 78.27	-6.2

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:


RCI
0.00
0.02
0.04
0.06
0.08
230:ALA
239:SER
248:GLU
257:PHE
267:ARG
276:SER
287:ASP
297:LEU
306:ILE
315:PRO
326:ASP
335:SER
344:VAL
353:THR
362:LYS
371:TYR
380:LEU
389:ASP
398:LYS
408:ASP
417:GLU
427:GLN
436:ASP
446:HIS
455:ILE
464:ILE
473:THR
483:VAL
492:LYS
Auth_seq_ID

8 NMR restraints analysis ⓘ

8.1 Conformationally restricting restraints ⓘ

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

Description	Value
Total distance restraints	3999
Intra-residue (|i-j|=0)	0
Sequential (|i-j|=1)	840
Medium range (|i-j|>1 and |i-j|<5)	1269
Long range (|i-j|≥5)	1872
Inter-chain	18
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	10.9
Number of long range restraints per residue[1]	5.1

---

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

8.2 Residual restraint violations ⓘ

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

8.2.1 Average number of distance violations per model ⓘ

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	42.2	0.2
0.2-0.5 (Medium)	97.3	0.5
>0.5 (Large)	53.4	6.06

8.2.2 Average number of dihedral-angle violations per model ⓘ

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

9 Distance violation analysis ⓘ

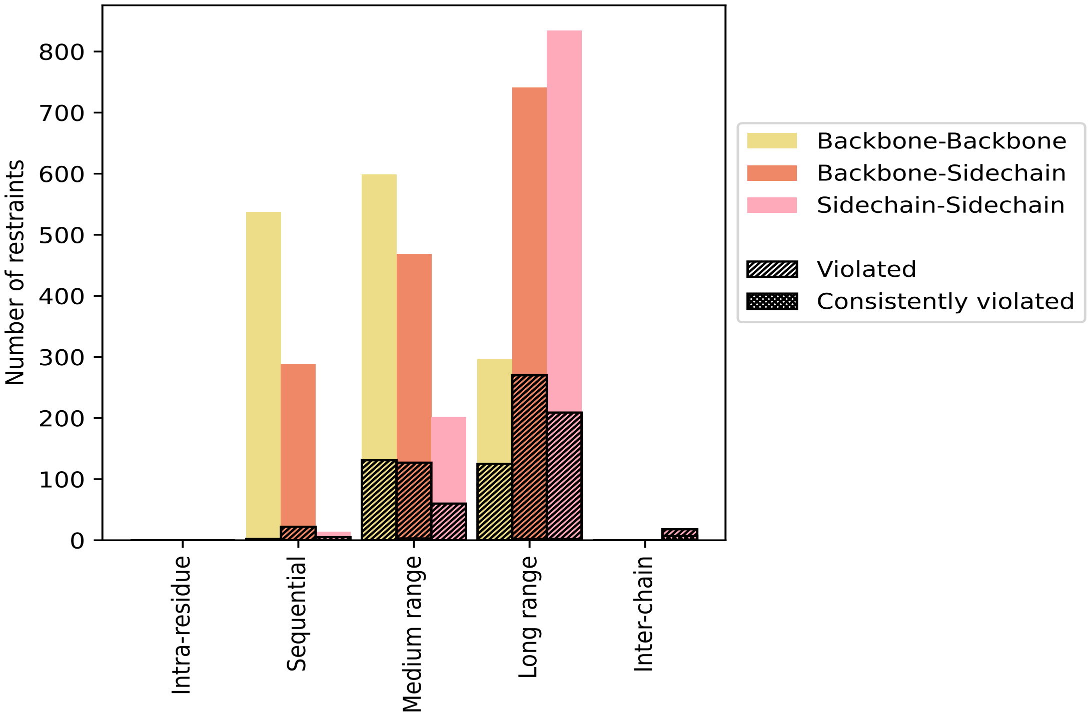
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	840	21.0	29	3.5	0.7	0	0.0	0.0
Backbone-Backbone	537	13.4	2	0.4	0.1	0	0.0	0.0
Backbone-Sidechain	289	7.2	22	7.6	0.6	0	0.0	0.0
Sidechain-Sidechain	14	0.4	5	35.7	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	1269	31.7	318	25.1	8.0	3	0.2	0.1
Backbone-Backbone	599	15.0	131	21.9	3.3	0	0.0	0.0
Backbone-Sidechain	469	11.7	127	27.1	3.2	3	0.6	0.1
Sidechain-Sidechain	201	5.0	60	29.9	1.5	0	0.0	0.0
Long range (|i-j|≥5)	1872	46.8	604	32.3	15.1	4	0.2	0.1
Backbone-Backbone	297	7.4	125	42.1	3.1	0	0.0	0.0
Backbone-Sidechain	741	18.5	270	36.4	6.8	2	0.3	0.1
Sidechain-Sidechain	834	20.9	209	25.1	5.2	2	0.2	0.1
Inter-chain	18	0.5	18	100.0	0.5	7	38.9	0.2
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	18	0.5	18	100.0	0.5	7	38.9	0.2
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3999	100.0	969	24.2	24.2	14	0.4	0.4
Backbone-Backbone	1433	35.8	258	18.0	6.5	0	0.0	0.0
Backbone-Sidechain	1499	37.5	419	28.0	10.5	5	0.3	0.1
Sidechain-Sidechain	1067	26.7	292	27.4	7.3	9	0.8	0.2

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

9.1.1 Bar chart : Distribution of distance restraints and violations ⓘ



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

9.2 Distance violation statistics for each model ⓘ

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	4	63	108	14	189	0.45	2.78	0.38	0.37
2	0	9	71	103	12	195	0.46	6.06	0.57	0.36
3	0	6	56	129	12	203	0.45	3.55	0.46	0.34
4	0	9	71	114	16	210	0.47	3.84	0.49	0.36
5	0	5	65	99	17	186	0.56	5.92	0.82	0.37
6	0	5	55	93	13	166	0.48	3.3	0.59	0.3
7	0	8	54	135	15	212	0.49	4.59	0.56	0.36
8	0	11	66	104	14	195	0.49	4.07	0.6	0.36
9	0	7	58	106	15	186	0.52	5.13	0.73	0.39
10	0	7	66	110	17	200	0.51	4.51	0.6	0.36

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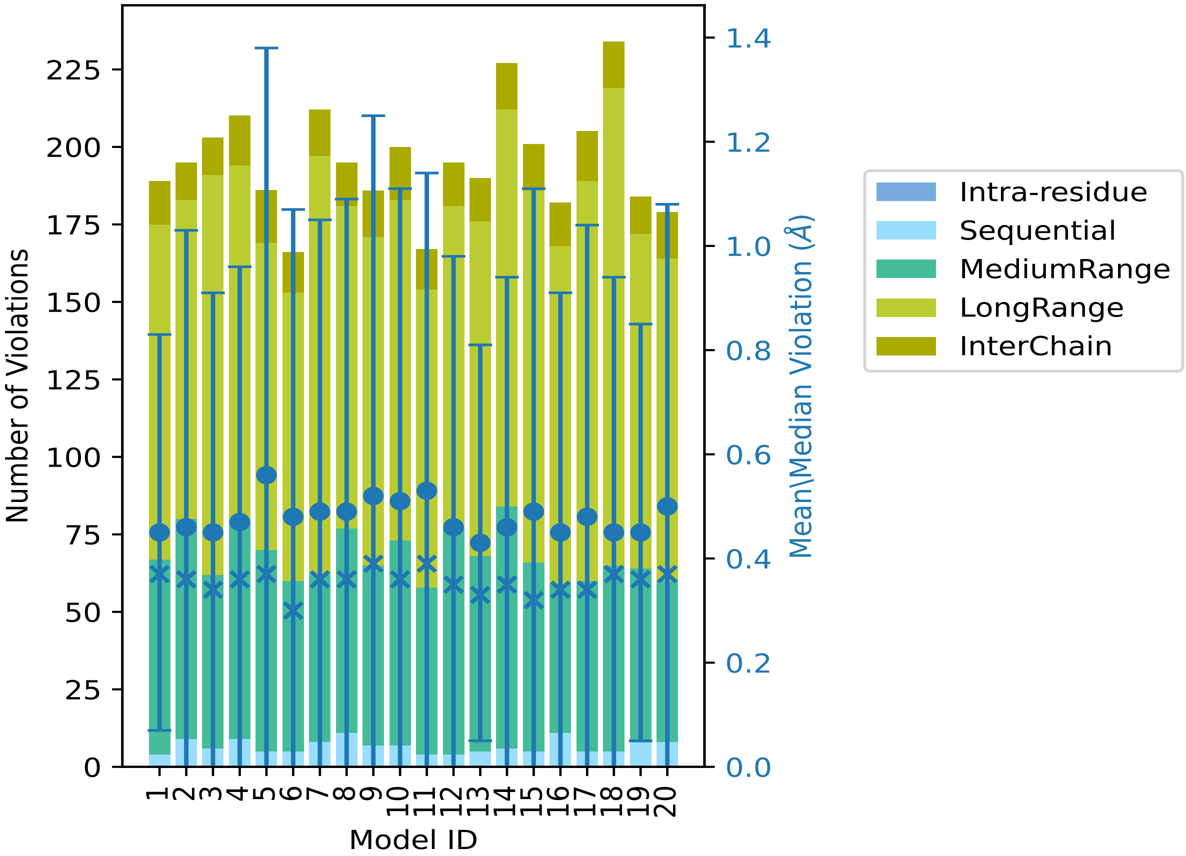
Model ID	Number of violations						Mean (Å)	Max (Å)	SD^6 (Å)	Median (Å)
	IR^1	SQ^2	MR^3	LR^4	IC^5	Total				
11	0	4	54	96	13	167	0.53	3.54	0.61	0.39
12	0	4	73	104	14	195	0.46	3.64	0.52	0.35
13	0	5	63	108	14	190	0.43	3.2	0.38	0.33
14	0	6	78	128	15	227	0.46	4.41	0.48	0.35
15	0	5	61	120	15	201	0.49	4.54	0.62	0.32
16	0	11	48	109	14	182	0.45	3.98	0.46	0.34
17	0	5	55	129	16	205	0.48	3.36	0.56	0.34
18	0	5	60	154	15	234	0.45	3.71	0.49	0.37
19	0	8	56	108	12	184	0.45	2.58	0.4	0.36
20	0	8	52	104	15	179	0.5	4.18	0.58	0.37

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

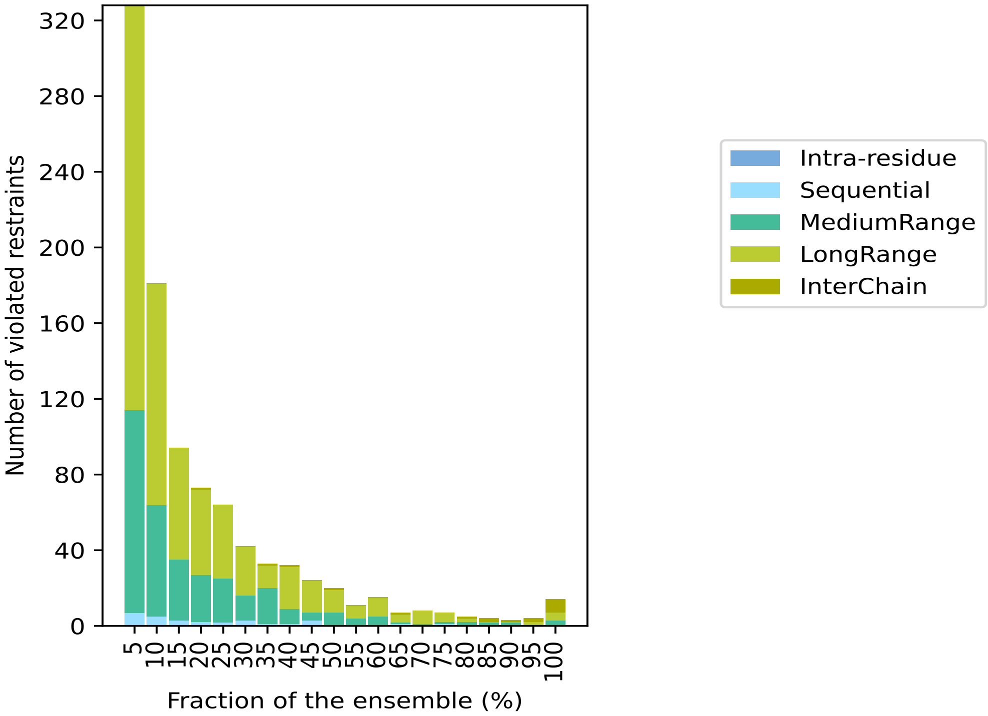
9.3 Distance violation statistics for the ensemble

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, 3030(IR:0, SQ:811, MR:951, LR:1268, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	7	107	214	0	328	1	5.0
0	5	59	117	0	181	2	10.0
0	3	32	59	0	94	3	15.0
0	2	25	45	1	73	4	20.0
0	2	23	39	0	64	5	25.0
0	3	13	26	0	42	6	30.0
0	1	19	12	1	33	7	35.0
0	1	8	22	1	32	8	40.0
0	3	4	17	0	24	9	45.0
0	0	7	12	1	20	10	50.0
0	0	4	7	0	11	11	55.0
0	0	5	10	0	15	12	60.0
0	1	1	4	1	7	13	65.0
0	0	1	7	0	8	14	70.0
0	1	1	5	0	7	15	75.0
0	0	2	2	1	5	16	80.0
0	0	2	0	2	4	17	85.0
0	0	2	0	1	3	18	90.0
0	0	0	2	2	4	19	95.0
0	0	3	4	7	14	20	100.0

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

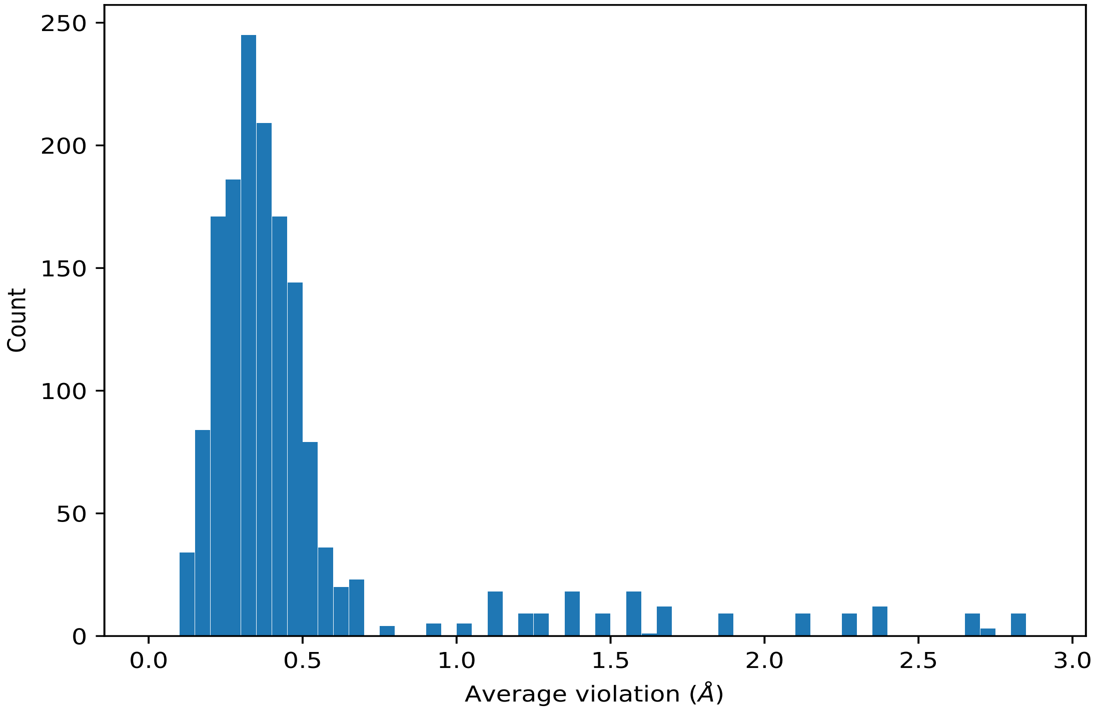
9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ



9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	20	2.81	1.33	2.57
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	20	2.81	1.33	2.57
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	20	2.81	1.33	2.57
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	20	2.81	1.33	2.57
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	20	2.81	1.33	2.57
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	20	2.81	1.33	2.57
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	20	2.81	1.33	2.57
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	20	2.81	1.33	2.57
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	20	2.81	1.33	2.57
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	20	2.66	1.09	2.76
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	20	2.66	1.09	2.76
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	20	2.66	1.09	2.76
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	20	2.66	1.09	2.76
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	20	2.66	1.09	2.76
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	20	2.66	1.09	2.76
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	20	2.66	1.09	2.76

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	20	2.66	1.09	2.76
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	20	2.66	1.09	2.76
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	20	2.39	0.91	2.56
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	20	2.39	0.91	2.56
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	20	2.39	0.91	2.56
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	20	2.39	0.91	2.56
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	20	2.39	0.91	2.56
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	20	2.39	0.91	2.56
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	20	2.39	0.91	2.56
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	20	2.39	0.91	2.56
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	20	2.39	0.91	2.56
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	20	2.38	1.22	2.13
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	20	2.38	1.22	2.13
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	20	2.38	1.22	2.13
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	20	2.11	0.68	2.3
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	20	2.11	0.68	2.3
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	20	2.11	0.68	2.3
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	20	2.11	0.68	2.3
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	20	2.11	0.68	2.3
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	20	2.11	0.68	2.3
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	20	2.11	0.68	2.3
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	20	2.11	0.68	2.3
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	20	2.11	0.68	2.3
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	20	1.89	1.02	1.85
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	20	1.89	1.02	1.85
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	20	1.89	1.02	1.85
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	20	1.89	1.02	1.85
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	20	1.89	1.02	1.85
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	20	1.89	1.02	1.85
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	20	1.89	1.02	1.85
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	20	1.89	1.02	1.85
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	20	1.89	1.02	1.85
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	20	1.57	0.89	1.56
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	20	1.57	0.89	1.56
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	20	1.57	0.89	1.56
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	20	1.57	0.89	1.56
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	20	1.57	0.89	1.56
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	20	1.57	0.89	1.56
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	20	1.57	0.89	1.56
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	20	1.57	0.89	1.56
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	20	1.57	0.89	1.56
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	20	0.67	0.1	0.69

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	20	0.67	0.14	0.67
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	20	0.67	0.14	0.67
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	20	0.67	0.14	0.67
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	20	0.67	0.14	0.67
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	20	0.67	0.14	0.67
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	20	0.67	0.14	0.67
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	20	0.67	0.14	0.67
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	20	0.67	0.14	0.67
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	20	0.67	0.14	0.67
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	20	0.59	0.09	0.62
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	20	0.59	0.09	0.62
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	20	0.59	0.09	0.62
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	20	0.53	0.12	0.56
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	20	0.46	0.14	0.53
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	20	0.36	0.06	0.37
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	20	0.34	0.12	0.36
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	19	2.25	0.62	2.1
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	19	2.25	0.62	2.1
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	19	2.25	0.62	2.1
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	19	2.25	0.62	2.1
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	19	2.25	0.62	2.1
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	19	2.25	0.62	2.1
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	19	2.25	0.62	2.1
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	19	2.25	0.62	2.1
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	19	2.25	0.62	2.1
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	19	1.25	0.73	0.99
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	19	1.25	0.73	0.99
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	19	1.25	0.73	0.99
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	19	1.25	0.73	0.99
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	19	1.25	0.73	0.99
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	19	1.25	0.73	0.99
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	19	1.25	0.73	0.99
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	19	1.25	0.73	0.99
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	19	1.25	0.73	0.99
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	19	0.6	0.08	0.6
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	19	0.6	0.08	0.6
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	19	0.6	0.08	0.6
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	19	0.6	0.08	0.6
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	19	0.6	0.08	0.6
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	19	0.6	0.08	0.6
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	19	0.6	0.08	0.6
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	19	0.6	0.08	0.6

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	19	0.6	0.08	0.6
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	19	0.52	0.15	0.57
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	18	1.58	0.81	1.56
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	18	1.58	0.81	1.56
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	18	1.58	0.81	1.56
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	18	1.58	0.81	1.56
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	18	1.58	0.81	1.56
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	18	1.58	0.81	1.56
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	18	1.58	0.81	1.56
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	18	1.58	0.81	1.56
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	18	1.58	0.81	1.56
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	18	0.46	0.12	0.48
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	18	0.42	0.08	0.44
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	17	1.69	1.03	2.06
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	17	1.69	1.03	2.06
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	17	1.69	1.03	2.06
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	17	1.69	1.03	2.06
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	17	1.69	1.03	2.06
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	17	1.69	1.03	2.06
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	17	1.69	1.03	2.06
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	17	1.69	1.03	2.06
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	17	1.69	1.03	2.06
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	17	1.49	1.51	0.8
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	17	1.49	1.51	0.8
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	17	1.49	1.51	0.8
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	17	1.49	1.51	0.8
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	17	1.49	1.51	0.8
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	17	1.49	1.51	0.8
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	17	1.49	1.51	0.8
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	17	1.49	1.51	0.8
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	17	1.49	1.51	0.8
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	17	0.33	0.11	0.35
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	17	0.33	0.11	0.35
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	17	0.33	0.11	0.35
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	17	0.3	0.14	0.3
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG11	16	1.37	0.98	1.18
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG12	16	1.37	0.98	1.18
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG13	16	1.37	0.98	1.18
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG11	16	1.37	0.98	1.18
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG12	16	1.37	0.98	1.18
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG13	16	1.37	0.98	1.18
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG11	16	1.37	0.98	1.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG12	16	1.37	0.98	1.18
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG13	16	1.37	0.98	1.18
(1,2938)	1:414:A:VAL:HG21	1:418:A:ASP:H	16	0.66	0.07	0.64
(1,2938)	1:414:A:VAL:HG22	1:418:A:ASP:H	16	0.66	0.07	0.64
(1,2938)	1:414:A:VAL:HG23	1:418:A:ASP:H	16	0.66	0.07	0.64
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD2	16	0.58	0.16	0.62
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD3	16	0.58	0.16	0.62
(1,3848)	1:481:A:GLN:HG2	1:486:A:VAL:HA	16	0.4	0.13	0.42
(1,3848)	1:481:A:GLN:HG3	1:486:A:VAL:HA	16	0.4	0.13	0.42
(1,3891)	1:486:A:VAL:HG11	1:490:A:LEU:H	16	0.31	0.12	0.26
(1,3891)	1:486:A:VAL:HG12	1:490:A:LEU:H	16	0.31	0.12	0.26
(1,3891)	1:486:A:VAL:HG13	1:490:A:LEU:H	16	0.31	0.12	0.26
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	15	1.63	1.23	1.15
(1,3110)	1:426:A:GLY:HA2	1:492:A:LYS:HD3	15	0.66	0.07	0.65
(1,3110)	1:426:A:GLY:HA3	1:492:A:LYS:HD3	15	0.66	0.07	0.65
(1,3479)	1:446:A:HIS:HD2	1:484:A:SER:H	15	0.57	0.13	0.64
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	15	0.5	0.13	0.54
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	15	0.5	0.13	0.54
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	15	0.45	0.06	0.46
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	15	0.45	0.06	0.46
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	15	0.33	0.09	0.34
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	15	0.33	0.09	0.34
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	15	0.33	0.15	0.43
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	14	0.48	0.16	0.54
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	14	0.48	0.16	0.54
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	14	0.48	0.16	0.54
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	14	0.48	0.16	0.54
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	14	0.45	0.17	0.52
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD21	14	0.42	0.15	0.42
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD22	14	0.42	0.15	0.42
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD21	14	0.42	0.15	0.42
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD22	14	0.42	0.15	0.42
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE1	14	0.39	0.15	0.36
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE2	14	0.39	0.15	0.36
(1,3936)	1:490:A:LEU:HB2	1:494:A:ALA:H	14	0.38	0.09	0.41
(1,3936)	1:490:A:LEU:HB3	1:494:A:ALA:H	14	0.38	0.09	0.41
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB2	14	0.35	0.12	0.34
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB3	14	0.35	0.12	0.34
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	14	0.34	0.13	0.4
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	14	0.34	0.13	0.4
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	14	0.34	0.13	0.4
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	14	0.34	0.13	0.4

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	14	0.27	0.08	0.29
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	14	0.27	0.08	0.29
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB1	13	1.37	0.78	1.51
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB2	13	1.37	0.78	1.51
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB3	13	1.37	0.78	1.51
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB1	13	1.37	0.78	1.51
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB2	13	1.37	0.78	1.51
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB3	13	1.37	0.78	1.51
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB1	13	1.37	0.78	1.51
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB2	13	1.37	0.78	1.51
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB3	13	1.37	0.78	1.51
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD11	13	0.46	0.14	0.51
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD12	13	0.46	0.14	0.51
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD13	13	0.46	0.14	0.51
(1,1044)	1:291:A:ARG:HA	1:293:A:HIS:HA	13	0.42	0.16	0.42
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD11	13	0.34	0.12	0.3
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD12	13	0.34	0.12	0.3
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD13	13	0.34	0.12	0.3
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	13	0.33	0.11	0.32
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	13	0.33	0.11	0.32
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	13	0.33	0.11	0.32
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	13	0.31	0.11	0.36
(1,2042)	1:357:A:LEU:HD21	1:396:A:ILE:HA	13	0.3	0.05	0.31
(1,2042)	1:357:A:LEU:HD22	1:396:A:ILE:HA	13	0.3	0.05	0.31
(1,2042)	1:357:A:LEU:HD23	1:396:A:ILE:HA	13	0.3	0.05	0.31
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG2	12	0.49	0.19	0.5
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG3	12	0.49	0.19	0.5
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG2	12	0.49	0.19	0.5
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG3	12	0.49	0.19	0.5
(1,1726)	1:331:A:PRO:HB2	1:338:A:ILE:HB	12	0.46	0.11	0.43
(1,1726)	1:331:A:PRO:HB3	1:338:A:ILE:HB	12	0.46	0.11	0.43
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	12	0.45	0.15	0.46
(1,2045)	1:357:A:LEU:HD21	1:395:A:ALA:H	12	0.42	0.16	0.38
(1,2045)	1:357:A:LEU:HD22	1:395:A:ALA:H	12	0.42	0.16	0.38
(1,2045)	1:357:A:LEU:HD23	1:395:A:ALA:H	12	0.42	0.16	0.38
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	12	0.41	0.15	0.42
(1,2984)	1:417:A:GLU:HA	1:421:A:SER:H	12	0.4	0.12	0.4
(1,3170)	1:430:A:ILE:H	1:481:A:GLN:H	12	0.39	0.1	0.43
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG11	12	0.39	0.18	0.38
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG12	12	0.39	0.18	0.38
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG13	12	0.39	0.18	0.38
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	12	0.36	0.1	0.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	12	0.34	0.11	0.34
(1,3938)	1:490:A:LEU:HA	1:493:A:LEU:H	12	0.32	0.08	0.32
(1,3207)	1:431:A:TYR:HA	1:482:A:SER:HA	12	0.28	0.14	0.26
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	12	0.28	0.14	0.25
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	12	0.23	0.09	0.2
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	12	0.23	0.06	0.22
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	12	0.23	0.06	0.22
(1,2889)	1:408:A:ASP:HB3	1:451:A:ARG:HH22	11	0.58	0.09	0.6
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	11	0.51	0.1	0.52
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	11	0.51	0.1	0.52
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	11	0.51	0.1	0.52
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	11	0.51	0.1	0.52
(1,1072)	1:295:A:HIS:HE1	1:311:A:GLU:HA	11	0.45	0.18	0.51
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	11	0.43	0.19	0.47
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	11	0.4	0.18	0.39
(1,3772)	1:472:A:LEU:HD21	1:474:A:GLU:HA	11	0.38	0.12	0.36
(1,3772)	1:472:A:LEU:HD22	1:474:A:GLU:HA	11	0.38	0.12	0.36
(1,3772)	1:472:A:LEU:HD23	1:474:A:GLU:HA	11	0.38	0.12	0.36
(1,3674)	1:462:A:ASP:HB2	1:464:A:ILE:H	11	0.36	0.11	0.37
(1,3674)	1:462:A:ASP:HB3	1:464:A:ILE:H	11	0.36	0.11	0.37
(1,3235)	1:432:A:TYR:H	1:482:A:SER:HA	11	0.32	0.07	0.31
(1,2041)	1:357:A:LEU:HD21	1:396:A:ILE:H	11	0.28	0.11	0.27
(1,2041)	1:357:A:LEU:HD22	1:396:A:ILE:H	11	0.28	0.11	0.27
(1,2041)	1:357:A:LEU:HD23	1:396:A:ILE:H	11	0.28	0.11	0.27
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE21	11	0.27	0.1	0.34
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE22	11	0.27	0.1	0.34
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	11	0.25	0.09	0.2
(1,3972)	1:318:A:LEU:HD11	2:622:B:TYR:HE1	10	1.67	1.29	1.36
(1,3972)	1:318:A:LEU:HD12	2:622:B:TYR:HE1	10	1.67	1.29	1.36
(1,3972)	1:318:A:LEU:HD13	2:622:B:TYR:HE1	10	1.67	1.29	1.36
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	10	0.55	0.2	0.6
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	10	0.55	0.2	0.6
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	10	0.55	0.2	0.6
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	10	0.55	0.2	0.6
(1,2122)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	10	0.55	0.2	0.61
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD21	10	0.47	0.19	0.55
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD22	10	0.47	0.19	0.55
(1,3245)	1:432:A:TYR:HB2	1:458:A:LEU:H	10	0.46	0.06	0.45
(1,3245)	1:432:A:TYR:HB3	1:458:A:LEU:H	10	0.46	0.06	0.45
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG21	10	0.45	0.2	0.5
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG22	10	0.45	0.2	0.5
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG23	10	0.45	0.2	0.5

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG21	10	0.45	0.2	0.5
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG22	10	0.45	0.2	0.5
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG23	10	0.45	0.2	0.5
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG21	10	0.45	0.2	0.5
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG22	10	0.45	0.2	0.5
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG23	10	0.45	0.2	0.5
(1,1452)	1:313:A:PHE:HZ	1:345:A:THR:HA	10	0.43	0.22	0.56
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA2	10	0.43	0.17	0.39
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA3	10	0.43	0.17	0.39
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB2	10	0.42	0.16	0.5
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB3	10	0.42	0.16	0.5
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	10	0.41	0.07	0.39
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	10	0.41	0.07	0.39
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	10	0.41	0.07	0.39
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	10	0.41	0.07	0.39
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	10	0.41	0.07	0.39
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	10	0.41	0.07	0.39
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG2	10	0.39	0.16	0.44
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG3	10	0.39	0.16	0.44
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG2	10	0.39	0.16	0.44
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG3	10	0.39	0.16	0.44
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG11	10	0.35	0.15	0.36
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG12	10	0.35	0.15	0.36
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG13	10	0.35	0.15	0.36
(1,2982)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	10	0.35	0.07	0.34
(1,2982)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	10	0.35	0.07	0.34
(1,3567)	1:450:A:LEU:HA	1:454:A:GLY:H	10	0.34	0.13	0.36
(1,3135)	1:428:A:GLU:HA	1:478:A:LYS:HA	10	0.34	0.16	0.29
(1,1037)	1:290:A:ASN:HB2	1:292:A:ASP:H	10	0.29	0.08	0.34
(1,1037)	1:290:A:ASN:HB3	1:292:A:ASP:H	10	0.29	0.08	0.34
(1,2824)	1:404:A:SER:H	1:414:A:VAL:HB	10	0.26	0.13	0.23
(1,1937)	1:350:A:ASN:HA	1:353:A:THR:H	10	0.26	0.09	0.26
(1,2989)	1:417:A:GLU:HA	1:420:A:VAL:HB	10	0.25	0.08	0.23
(1,376)	1:251:A:LYS:HG2	1:257:A:PHE:HA	10	0.23	0.05	0.23
(1,376)	1:251:A:LYS:HG3	1:257:A:PHE:HA	10	0.23	0.05	0.23
(1,3635)	1:458:A:LEU:HD11	1:480:A:PHE:HD1	9	1.0	0.56	0.81
(1,3635)	1:458:A:LEU:HD12	1:480:A:PHE:HE1	9	1.0	0.56	0.81
(1,3635)	1:458:A:LEU:HD13	1:480:A:PHE:HE1	9	1.0	0.56	0.81
(1,3635)	1:458:A:LEU:HD13	1:480:A:PHE:HE2	9	1.0	0.56	0.81
(1,3635)	1:458:A:LEU:HD11	1:480:A:PHE:HE2	9	1.0	0.56	0.81
(1,2565)	1:387:A:ALA:HB1	1:471:A:TYR:HD1	9	0.9	0.42	1.0
(1,2565)	1:387:A:ALA:HB3	1:471:A:TYR:HD1	9	0.9	0.42	1.0

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2565)	1:387:A:ALA:HB2	1:471:A:TYR:HD1	9	0.9	0.42	1.0
(1,2565)	1:387:A:ALA:HB1	1:471:A:TYR:HD2	9	0.9	0.42	1.0
(1,2565)	1:387:A:ALA:HB2	1:471:A:TYR:HD2	9	0.9	0.42	1.0
(1,3882)	1:485:A:LYS:HB2	1:487:A:ASP:HB3	9	0.53	0.12	0.57
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	9	0.52	0.13	0.56
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	9	0.52	0.13	0.56
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB1	9	0.5	0.18	0.5
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB2	9	0.5	0.18	0.5
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB3	9	0.5	0.18	0.5
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB1	9	0.5	0.18	0.5
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB2	9	0.5	0.18	0.5
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB3	9	0.5	0.18	0.5
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD2	9	0.43	0.14	0.43
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD3	9	0.43	0.14	0.43
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB2	9	0.42	0.14	0.39
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB3	9	0.42	0.14	0.39
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB2	9	0.42	0.14	0.39
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB3	9	0.42	0.14	0.39
(1,1367)	1:307:A:MET:HE1	1:339:A:LEU:H	9	0.41	0.17	0.34
(1,1367)	1:307:A:MET:HE2	1:339:A:LEU:H	9	0.41	0.17	0.34
(1,1367)	1:307:A:MET:HE3	1:339:A:LEU:H	9	0.41	0.17	0.34
(1,3144)	1:429:A:LYS:HD2	1:489:A:SER:HA	9	0.37	0.09	0.35
(1,3144)	1:429:A:LYS:HD3	1:489:A:SER:HA	9	0.37	0.09	0.35
(1,3329)	1:435:A:ALA:H	1:461:A:SER:HA	9	0.37	0.07	0.38
(1,1321)	1:302:A:GLN:HA	1:328:A:SER:HA	9	0.37	0.09	0.38
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE1	9	0.34	0.14	0.37
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE2	9	0.34	0.14	0.37
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE3	9	0.34	0.14	0.37
(1,2575)	1:388:A:GLU:HA	1:390:A:PHE:H	9	0.34	0.1	0.3
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD2	9	0.34	0.2	0.31
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD3	9	0.34	0.2	0.31
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD2	9	0.34	0.2	0.31
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD3	9	0.34	0.2	0.31
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD2	9	0.34	0.2	0.31
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD3	9	0.34	0.2	0.31
(1,1933)	1:350:A:ASN:HA	1:354:A:LYS:H	9	0.33	0.16	0.33
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB2	9	0.32	0.13	0.24
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB3	9	0.32	0.13	0.24
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD21	9	0.31	0.15	0.28
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD22	9	0.31	0.15	0.28
(1,3476)	1:445:A:PRO:HG2	1:446:A:HIS:H	9	0.31	0.08	0.31
(1,3476)	1:445:A:PRO:HG3	1:446:A:HIS:H	9	0.31	0.08	0.31

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3143)	1:429:A:LYS:HD2	1:489:A:SER:H	9	0.31	0.17	0.22
(1,3143)	1:429:A:LYS:HD3	1:489:A:SER:H	9	0.31	0.17	0.22
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD2	9	0.31	0.09	0.29
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD3	9	0.31	0.09	0.29
(1,1024)	1:289:A:TRP:HH2	1:381:A:VAL:HA	9	0.31	0.1	0.32
(1,1023)	1:289:A:TRP:HZ2	1:381:A:VAL:H	9	0.29	0.13	0.32
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG11	9	0.21	0.07	0.23
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG12	9	0.21	0.07	0.23
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG13	9	0.21	0.07	0.23
(1,1843)	1:342:A:SER:HB2	1:343:A:THR:H	9	0.15	0.03	0.14
(1,1843)	1:342:A:SER:HB3	1:343:A:THR:H	9	0.15	0.03	0.14
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG11	8	1.11	0.7	0.86
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG12	8	1.11	0.7	0.86
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG13	8	1.11	0.7	0.86
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG11	8	1.11	0.7	0.86
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG12	8	1.11	0.7	0.86
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG13	8	1.11	0.7	0.86
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG11	8	1.11	0.7	0.86
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG12	8	1.11	0.7	0.86
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG13	8	1.11	0.7	0.86
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG21	8	1.11	0.7	0.86
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG22	8	1.11	0.7	0.86
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG23	8	1.11	0.7	0.86
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG21	8	1.11	0.7	0.86
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG22	8	1.11	0.7	0.86
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG23	8	1.11	0.7	0.86
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG21	8	1.11	0.7	0.86
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG22	8	1.11	0.7	0.86
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG23	8	1.11	0.7	0.86
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB2	8	0.67	0.1	0.7
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB3	8	0.67	0.1	0.7
(1,3315)	1:434:A:THR:HA	1:461:A:SER:HA	8	0.6	0.13	0.62
(1,102)	1:234:A:TRP:HE1	1:235:A:THR:HB	8	0.55	0.03	0.55
(1,3178)	1:430:A:ILE:HD11	1:479:A:PRO:HA	8	0.52	0.13	0.55
(1,3178)	1:430:A:ILE:HD12	1:479:A:PRO:HA	8	0.52	0.13	0.55
(1,3178)	1:430:A:ILE:HD13	1:479:A:PRO:HA	8	0.52	0.13	0.55
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB2	8	0.5	0.11	0.46
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB3	8	0.5	0.11	0.46
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB2	8	0.5	0.11	0.46
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB3	8	0.5	0.11	0.46
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB2	8	0.5	0.11	0.46
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB3	8	0.5	0.11	0.46

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	8	0.49	0.21	0.61
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE1	8	0.49	0.07	0.51
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE2	8	0.49	0.07	0.51
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE3	8	0.49	0.07	0.51
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE1	8	0.49	0.07	0.51
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE2	8	0.49	0.07	0.51
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE3	8	0.49	0.07	0.51
(1,2427)	1:380:A:LEU:HD11	1:463:A:ARG:H	8	0.45	0.23	0.59
(1,2427)	1:380:A:LEU:HD12	1:463:A:ARG:H	8	0.45	0.23	0.59
(1,2427)	1:380:A:LEU:HD13	1:463:A:ARG:H	8	0.45	0.23	0.59
(1,2755)	1:402:A:PHE:HD2	1:460:A:LEU:HD13	8	0.44	0.3	0.31
(1,2755)	1:402:A:PHE:HD1	1:460:A:LEU:HD13	8	0.44	0.3	0.31
(1,2755)	1:402:A:PHE:HD1	1:460:A:LEU:HD12	8	0.44	0.3	0.31
(1,2755)	1:402:A:PHE:HD2	1:460:A:LEU:HD11	8	0.44	0.3	0.31
(1,2755)	1:402:A:PHE:HD2	1:460:A:LEU:HD12	8	0.44	0.3	0.31
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE2	8	0.43	0.1	0.45
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE3	8	0.43	0.1	0.45
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE2	8	0.43	0.1	0.45
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE3	8	0.43	0.1	0.45
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD11	8	0.42	0.06	0.44
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD12	8	0.42	0.06	0.44
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD13	8	0.42	0.06	0.44
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD11	8	0.42	0.1	0.4
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD12	8	0.42	0.1	0.4
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD13	8	0.42	0.1	0.4
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD11	8	0.42	0.1	0.4
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD12	8	0.42	0.1	0.4
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD13	8	0.42	0.1	0.4
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	8	0.4	0.12	0.42
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB2	8	0.4	0.1	0.38
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB3	8	0.4	0.1	0.38
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB2	8	0.4	0.1	0.38
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB3	8	0.4	0.1	0.38
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	8	0.39	0.15	0.35
(1,3536)	1:449:A:LEU:HA	1:453:A:LYS:H	8	0.37	0.17	0.38
(1,2317)	1:374:A:PHE:HZ	1:382:A:LEU:H	8	0.35	0.16	0.34
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE21	8	0.35	0.09	0.39
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE22	8	0.35	0.09	0.39
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG2	8	0.35	0.21	0.24
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG3	8	0.35	0.21	0.24
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG2	8	0.35	0.21	0.24
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG3	8	0.35	0.21	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1140)	1:297:A:LEU:HA	1:309:A:ASP:HA	8	0.34	0.1	0.36
(1,1318)	1:302:A:GLN:H	1:329:A:ASP:H	8	0.31	0.09	0.29
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	8	0.28	0.12	0.28
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD11	8	0.28	0.12	0.24
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD12	8	0.28	0.12	0.24
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD13	8	0.28	0.12	0.24
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD1	8	0.27	0.11	0.24
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD2	8	0.27	0.11	0.24
(1,3214)	1:431:A:TYR:H	1:458:A:LEU:H	8	0.24	0.1	0.22
(1,1219)	1:299:A:LEU:H	1:306:A:ILE:H	8	0.23	0.12	0.19
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	8	0.21	0.09	0.17
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	8	0.21	0.09	0.17
(1,3248)	1:432:A:TYR:HA	1:457:A:VAL:HA	8	0.21	0.09	0.19
(1,764)	1:276:A:SER:HB2	1:326:A:ASP:H	8	0.2	0.11	0.14
(1,764)	1:276:A:SER:HB3	1:326:A:ASP:H	8	0.2	0.11	0.14
(1,2574)	1:388:A:GLU:H	1:390:A:PHE:H	8	0.17	0.04	0.16
(1,763)	1:276:A:SER:HA	1:326:A:ASP:H	8	0.14	0.03	0.14
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG11	7	2.74	1.73	2.43
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG12	7	2.74	1.73	2.43
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG13	7	2.74	1.73	2.43
(1,2595)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	7	0.65	0.07	0.65
(1,2595)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	7	0.65	0.07	0.65
(1,2595)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	7	0.65	0.07	0.65
(1,2595)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	7	0.65	0.07	0.65
(1,2997)	1:418:A:ASP:HA	1:422:A:ARG:HG2	7	0.63	0.21	0.68
(1,2997)	1:418:A:ASP:HA	1:422:A:ARG:HG3	7	0.63	0.21	0.68
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG21	7	0.61	0.07	0.63
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG22	7	0.61	0.07	0.63
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG23	7	0.61	0.07	0.63
(1,1946)	1:351:A:ALA:HA	1:355:A:ARG:HD2	7	0.56	0.18	0.63
(1,1946)	1:351:A:ALA:HA	1:355:A:ARG:HD3	7	0.56	0.18	0.63
(1,2426)	1:380:A:LEU:HD22	1:464:A:ILE:H	7	0.52	0.14	0.58
(2,9)	1:338:A:ILE:HD11	1:342:A:SER:H	7	0.52	0.13	0.52
(2,9)	1:338:A:ILE:HD12	1:342:A:SER:H	7	0.52	0.13	0.52
(2,9)	1:338:A:ILE:HD13	1:342:A:SER:H	7	0.52	0.13	0.52
(1,3007)	1:419:A:TYR:HE2	1:478:A:LYS:HG2	7	0.45	0.22	0.48
(1,3007)	1:419:A:TYR:HE2	1:478:A:LYS:HG3	7	0.45	0.22	0.48
(1,1505)	1:315:A:PRO:HD2	1:350:A:ASN:HA	7	0.44	0.17	0.54
(1,1505)	1:315:A:PRO:HD3	1:350:A:ASN:HA	7	0.44	0.17	0.54
(1,1886)	1:346:A:ARG:HG2	1:350:A:ASN:HD21	7	0.43	0.15	0.47
(1,1886)	1:346:A:ARG:HG2	1:350:A:ASN:HD22	7	0.43	0.15	0.47
(1,1886)	1:346:A:ARG:HG3	1:350:A:ASN:HD21	7	0.43	0.15	0.47

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1886)	1:346:A:ARG:HG3	1:350:A:ASN:HD22	7	0.43	0.15	0.47
(1,3154)	1:429:A:LYS:HA	1:480:A:PHE:HA	7	0.4	0.16	0.45
(1,3726)	1:468:A:MET:HG2	1:472:A:LEU:HB2	7	0.39	0.1	0.45
(1,3726)	1:468:A:MET:HG2	1:472:A:LEU:HB3	7	0.39	0.1	0.45
(1,3726)	1:468:A:MET:HG3	1:472:A:LEU:HB2	7	0.39	0.1	0.45
(1,3726)	1:468:A:MET:HG3	1:472:A:LEU:HB3	7	0.39	0.1	0.45
(1,2538)	1:386:A:PRO:HA	1:471:A:TYR:HB2	7	0.39	0.16	0.41
(1,2538)	1:386:A:PRO:HA	1:471:A:TYR:HB3	7	0.39	0.16	0.41
(1,2359)	1:375:A:TRP:HH2	1:383:A:LYS:HG2	7	0.38	0.06	0.4
(1,2359)	1:375:A:TRP:HH2	1:383:A:LYS:HG3	7	0.38	0.06	0.4
(1,1674)	1:325:A:ILE:HD11	1:327:A:SER:H	7	0.37	0.16	0.42
(1,1674)	1:325:A:ILE:HD12	1:327:A:SER:H	7	0.37	0.16	0.42
(1,1674)	1:325:A:ILE:HD13	1:327:A:SER:H	7	0.37	0.16	0.42
(1,1060)	1:294:A:LYS:HD2	1:309:A:ASP:HB2	7	0.36	0.19	0.48
(1,1060)	1:294:A:LYS:HD2	1:309:A:ASP:HB3	7	0.36	0.19	0.48
(1,1060)	1:294:A:LYS:HD3	1:309:A:ASP:HB2	7	0.36	0.19	0.48
(1,1060)	1:294:A:LYS:HD3	1:309:A:ASP:HB3	7	0.36	0.19	0.48
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HA	7	0.36	0.11	0.29
(1,2196)	1:365:A:LYS:HE2	1:398:A:LYS:HE2	7	0.34	0.2	0.21
(1,2196)	1:365:A:LYS:HE2	1:398:A:LYS:HE3	7	0.34	0.2	0.21
(1,2196)	1:365:A:LYS:HE3	1:398:A:LYS:HE2	7	0.34	0.2	0.21
(1,2196)	1:365:A:LYS:HE3	1:398:A:LYS:HE3	7	0.34	0.2	0.21
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD21	7	0.34	0.1	0.4
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD22	7	0.34	0.1	0.4
(1,2632)	1:393:A:GLN:HA	1:396:A:ILE:HB	7	0.33	0.17	0.26
(1,3353)	1:436:A:ASP:HA	1:461:A:SER:HA	7	0.32	0.21	0.25
(1,2290)	1:372:A:GLN:HG2	1:376:A:GLN:HE21	7	0.31	0.13	0.33
(1,2290)	1:372:A:GLN:HG2	1:376:A:GLN:HE22	7	0.31	0.13	0.33
(1,2290)	1:372:A:GLN:HG3	1:376:A:GLN:HE21	7	0.31	0.13	0.33
(1,2290)	1:372:A:GLN:HG3	1:376:A:GLN:HE22	7	0.31	0.13	0.33
(1,1790)	1:337:A:GLU:HG2	1:341:A:ASP:HB2	7	0.28	0.15	0.35
(1,1790)	1:337:A:GLU:HG2	1:341:A:ASP:HB3	7	0.28	0.15	0.35
(1,1790)	1:337:A:GLU:HG3	1:341:A:ASP:HB2	7	0.28	0.15	0.35
(1,1790)	1:337:A:GLU:HG3	1:341:A:ASP:HB3	7	0.28	0.15	0.35
(1,1762)	1:335:A:SER:H	1:339:A:LEU:H	7	0.27	0.15	0.21
(1,3155)	1:429:A:LYS:HB2	1:480:A:PHE:HA	7	0.27	0.16	0.23
(1,3155)	1:429:A:LYS:HB3	1:480:A:PHE:HA	7	0.27	0.16	0.23
(1,293)	1:248:A:GLU:HA	1:251:A:LYS:H	7	0.26	0.06	0.27
(1,382)	1:251:A:LYS:HA	1:255:A:HIS:HA	7	0.25	0.08	0.24
(1,1938)	1:350:A:ASN:HA	1:353:A:THR:HB	7	0.23	0.08	0.22
(1,1053)	1:293:A:HIS:HB2	1:295:A:HIS:H	7	0.22	0.1	0.18
(1,1053)	1:293:A:HIS:HB3	1:295:A:HIS:H	7	0.22	0.1	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2181)	1:364:A:ALA:HA	1:371:A:TYR:HD1	7	0.21	0.08	0.18
(1,2181)	1:364:A:ALA:HA	1:371:A:TYR:HD2	7	0.21	0.08	0.18
(1,3935)	1:490:A:LEU:HA	1:494:A:ALA:H	7	0.21	0.06	0.2
(1,2940)	1:414:A:VAL:HG21	1:418:A:ASP:HB2	7	0.17	0.06	0.14
(1,2940)	1:414:A:VAL:HG21	1:418:A:ASP:HB3	7	0.17	0.06	0.14
(1,2940)	1:414:A:VAL:HG22	1:418:A:ASP:HB2	7	0.17	0.06	0.14
(1,2940)	1:414:A:VAL:HG22	1:418:A:ASP:HB3	7	0.17	0.06	0.14
(1,2940)	1:414:A:VAL:HG23	1:418:A:ASP:HB2	7	0.17	0.06	0.14
(1,2940)	1:414:A:VAL:HG23	1:418:A:ASP:HB3	7	0.17	0.06	0.14
(1,1882)	1:345:A:THR:HB	1:346:A:ARG:H	7	0.17	0.03	0.16
(1,988)	1:287:A:ASP:HB2	1:293:A:HIS:HA	6	0.58	0.19	0.66
(1,988)	1:287:A:ASP:HB3	1:293:A:HIS:HA	6	0.58	0.19	0.66
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD11	6	0.53	0.06	0.54
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD12	6	0.53	0.06	0.54
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD13	6	0.53	0.06	0.54
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD11	6	0.53	0.06	0.54
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD12	6	0.53	0.06	0.54
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD13	6	0.53	0.06	0.54
(1,1511)	1:315:A:PRO:HG2	1:319:A:ARG:H	6	0.52	0.16	0.56
(1,1511)	1:315:A:PRO:HG3	1:319:A:ARG:H	6	0.52	0.16	0.56
(1,2875)	1:406:A:HIS:HB2	1:414:A:VAL:HB	6	0.5	0.13	0.52
(1,2875)	1:406:A:HIS:HB3	1:414:A:VAL:HB	6	0.5	0.13	0.52
(1,447)	1:256:A:ASP:HA	1:258:A:ASN:HD21	6	0.5	0.24	0.42
(1,447)	1:256:A:ASP:HA	1:258:A:ASN:HD22	6	0.5	0.24	0.42
(1,684)	1:272:A:GLN:HE21	1:351:A:ALA:H	6	0.49	0.21	0.47
(1,684)	1:272:A:GLN:HE22	1:351:A:ALA:H	6	0.49	0.21	0.47
(1,2288)	1:372:A:GLN:HE21	1:376:A:GLN:H	6	0.47	0.12	0.48
(1,2288)	1:372:A:GLN:HE22	1:376:A:GLN:H	6	0.47	0.12	0.48
(1,2699)	1:398:A:LYS:HE2	1:417:A:GLU:HG2	6	0.46	0.19	0.48
(1,2699)	1:398:A:LYS:HE2	1:417:A:GLU:HG3	6	0.46	0.19	0.48
(1,2699)	1:398:A:LYS:HE3	1:417:A:GLU:HG2	6	0.46	0.19	0.48
(1,2699)	1:398:A:LYS:HE3	1:417:A:GLU:HG3	6	0.46	0.19	0.48
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG21	6	0.44	0.11	0.45
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG22	6	0.44	0.11	0.45
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG23	6	0.44	0.11	0.45
(1,2425)	1:380:A:LEU:HB2	1:464:A:ILE:H	6	0.42	0.15	0.42
(1,2425)	1:380:A:LEU:HB3	1:464:A:ILE:H	6	0.42	0.15	0.42
(1,1658)	1:322:A:ARG:HD2	1:323:A:GLY:H	6	0.4	0.1	0.38
(1,1658)	1:322:A:ARG:HD3	1:323:A:GLY:H	6	0.4	0.1	0.38
(1,574)	1:264:A:SER:HB2	1:358:A:GLN:HB2	6	0.38	0.1	0.36
(1,574)	1:264:A:SER:HB2	1:358:A:GLN:HB3	6	0.38	0.1	0.36
(1,574)	1:264:A:SER:HB3	1:358:A:GLN:HB2	6	0.38	0.1	0.36

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,574)	1:264:A:SER:HB3	1:358:A:GLN:HB3	6	0.38	0.1	0.36
(1,2937)	1:414:A:VAL:HG21	1:419:A:TYR:HA	6	0.38	0.12	0.39
(1,2937)	1:414:A:VAL:HG22	1:419:A:TYR:HA	6	0.38	0.12	0.39
(1,2937)	1:414:A:VAL:HG23	1:419:A:TYR:HA	6	0.38	0.12	0.39
(1,3147)	1:429:A:LYS:HD2	1:488:A:GLU:HG2	6	0.38	0.23	0.32
(1,3147)	1:429:A:LYS:HD2	1:488:A:GLU:HG3	6	0.38	0.23	0.32
(1,3147)	1:429:A:LYS:HD3	1:488:A:GLU:HG2	6	0.38	0.23	0.32
(1,3147)	1:429:A:LYS:HD3	1:488:A:GLU:HG3	6	0.38	0.23	0.32
(1,2986)	1:417:A:GLU:HA	1:421:A:SER:HB2	6	0.37	0.19	0.29
(1,2986)	1:417:A:GLU:HA	1:421:A:SER:HB3	6	0.37	0.19	0.29
(1,3538)	1:449:A:LEU:HD11	1:453:A:LYS:HB2	6	0.36	0.15	0.26
(1,3538)	1:449:A:LEU:HD11	1:453:A:LYS:HB3	6	0.36	0.15	0.26
(1,3538)	1:449:A:LEU:HD12	1:453:A:LYS:HB2	6	0.36	0.15	0.26
(1,3538)	1:449:A:LEU:HD12	1:453:A:LYS:HB3	6	0.36	0.15	0.26
(1,3538)	1:449:A:LEU:HD13	1:453:A:LYS:HB2	6	0.36	0.15	0.26
(1,3538)	1:449:A:LEU:HD13	1:453:A:LYS:HB3	6	0.36	0.15	0.26
(1,153)	1:238:A:LYS:HE2	1:264:A:SER:HA	6	0.36	0.15	0.44
(1,153)	1:238:A:LYS:HE3	1:264:A:SER:HA	6	0.36	0.15	0.44
(1,2562)	1:387:A:ALA:HB1	1:471:A:TYR:HD1	6	0.34	0.11	0.38
(1,2562)	1:387:A:ALA:HB1	1:471:A:TYR:HD2	6	0.34	0.11	0.38
(1,2562)	1:387:A:ALA:HB2	1:471:A:TYR:HD1	6	0.34	0.11	0.38
(1,2562)	1:387:A:ALA:HB2	1:471:A:TYR:HD2	6	0.34	0.11	0.38
(1,2562)	1:387:A:ALA:HB3	1:471:A:TYR:HD1	6	0.34	0.11	0.38
(1,2562)	1:387:A:ALA:HB3	1:471:A:TYR:HD2	6	0.34	0.11	0.38
(1,3730)	1:468:A:MET:HA	1:471:A:TYR:HD1	6	0.33	0.15	0.34
(1,3730)	1:468:A:MET:HA	1:471:A:TYR:HD2	6	0.33	0.15	0.34
(1,2337)	1:375:A:TRP:HD1	1:413:A:THR:HA	6	0.32	0.16	0.28
(1,1324)	1:302:A:GLN:H	1:327:A:SER:H	6	0.32	0.13	0.3
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	6	0.31	0.08	0.33
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB2	6	0.3	0.15	0.26
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB3	6	0.3	0.15	0.26
(1,2855)	1:405:A:THR:HB	1:451:A:ARG:HA	6	0.3	0.18	0.26
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD11	6	0.3	0.11	0.32
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD12	6	0.3	0.11	0.32
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD13	6	0.3	0.11	0.32
(1,3222)	1:431:A:TYR:HD1	1:456:A:GLU:H	6	0.29	0.11	0.26
(1,3222)	1:431:A:TYR:HD2	1:456:A:GLU:H	6	0.29	0.11	0.26
(1,2914)	1:410:A:SER:HA	1:438:A:TYR:HE1	6	0.28	0.18	0.22
(1,2914)	1:410:A:SER:HA	1:438:A:TYR:HE2	6	0.28	0.18	0.22
(1,2914)	1:410:A:SER:HA	1:438:A:TYR:HD1	6	0.28	0.18	0.22
(1,2914)	1:410:A:SER:HA	1:438:A:TYR:HD2	6	0.28	0.18	0.22
(1,1334)	1:303:A:ARG:H	1:327:A:SER:H	6	0.27	0.14	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1159)	1:298:A:LYS:H	1:322:A:ARG:HD2	6	0.27	0.08	0.24
(1,1159)	1:298:A:LYS:H	1:322:A:ARG:HD3	6	0.27	0.08	0.24
(1,2133)	1:361:A:GLU:HA	1:365:A:LYS:H	6	0.27	0.15	0.24
(1,3492)	1:447:A:LEU:HA	1:483:A:VAL:HB	6	0.25	0.1	0.25
(1,848)	1:279:A:TYR:H	1:322:A:ARG:H	6	0.23	0.12	0.24
(1,1223)	1:299:A:LEU:H	1:305:A:PHE:HA	6	0.23	0.13	0.18
(1,1167)	1:298:A:LYS:HA	1:309:A:ASP:HA	6	0.22	0.18	0.16
(1,2014)	1:355:A:ARG:HA	1:358:A:GLN:HB2	6	0.22	0.09	0.24
(1,2014)	1:355:A:ARG:HA	1:358:A:GLN:HB3	6	0.22	0.09	0.24
(1,2203)	1:365:A:LYS:HA	1:367:A:ASP:H	6	0.2	0.06	0.22
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD1	6	0.2	0.07	0.18
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD2	6	0.2	0.07	0.18
(1,3807)	1:475:A:PHE:H	1:479:A:PRO:HA	6	0.19	0.06	0.21
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	6	0.18	0.05	0.16
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB2	6	0.17	0.03	0.17
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB3	6	0.17	0.03	0.17
(1,513)	1:261:A:LEU:H	1:281:A:PRO:HA	6	0.16	0.05	0.15
(1,1382)	1:307:A:MET:HB2	1:308:A:ASP:H	6	0.12	0.01	0.12
(1,1382)	1:307:A:MET:HB3	1:308:A:ASP:H	6	0.12	0.01	0.12
(1,1013)	1:288:A:MET:HA	1:294:A:LYS:H	5	0.59	0.16	0.63
(1,986)	1:287:A:ASP:HB2	1:294:A:LYS:H	5	0.59	0.04	0.58
(1,986)	1:287:A:ASP:HB3	1:294:A:LYS:H	5	0.59	0.04	0.58
(1,37)	1:233:A:LEU:HD11	1:249:A:PHE:H	5	0.55	0.12	0.58
(1,37)	1:233:A:LEU:HD12	1:249:A:PHE:H	5	0.55	0.12	0.58
(1,37)	1:233:A:LEU:HD13	1:249:A:PHE:H	5	0.55	0.12	0.58
(1,1935)	1:350:A:ASN:HA	1:354:A:LYS:HG2	5	0.54	0.16	0.64
(1,1935)	1:350:A:ASN:HA	1:354:A:LYS:HG3	5	0.54	0.16	0.64
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD21	5	0.53	0.12	0.52
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD22	5	0.53	0.12	0.52
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD23	5	0.53	0.12	0.52
(1,3360)	1:437:A:SER:HA	1:462:A:ASP:HA	5	0.51	0.19	0.56
(1,2927)	1:412:A:GLN:HA	1:414:A:VAL:HB	5	0.47	0.24	0.54
(1,2915)	1:410:A:SER:HB3	1:438:A:TYR:HD2	5	0.47	0.19	0.39
(1,2915)	1:410:A:SER:HB3	1:438:A:TYR:HD1	5	0.47	0.19	0.39
(1,2915)	1:410:A:SER:HB2	1:438:A:TYR:HD1	5	0.47	0.19	0.39
(1,139)	1:237:A:ASN:HD21	1:239:A:SER:H	5	0.45	0.08	0.42
(1,139)	1:237:A:ASN:HD22	1:239:A:SER:H	5	0.45	0.08	0.42
(1,1989)	1:354:A:LYS:HA	1:392:A:ASN:HD21	5	0.44	0.13	0.44
(1,1989)	1:354:A:LYS:HA	1:392:A:ASN:HD22	5	0.44	0.13	0.44
(1,1029)	1:289:A:TRP:HZ2	1:380:A:LEU:HB2	5	0.44	0.07	0.46
(1,1029)	1:289:A:TRP:HZ2	1:380:A:LEU:HB3	5	0.44	0.07	0.46
(1,2436)	1:380:A:LEU:HA	1:383:A:LYS:HD2	5	0.42	0.17	0.43

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Key	Atom-1	Atom-2	Models^1	Mean (Å)	SD^1 (Å)	Median (Å)
(1,2436)	1:380:A:LEU:HA	1:383:A:LYS:HD3	5	0.42	0.17	0.43
(1,3406)	1:439:A:ALA:HA	1:442:A:LYS:HD2	5	0.42	0.1	0.45
(1,3406)	1:439:A:ALA:HA	1:442:A:LYS:HD3	5	0.42	0.1	0.45
(1,1374)	1:307:A:MET:HE1	1:335:A:SER:HA	5	0.41	0.13	0.47
(1,1374)	1:307:A:MET:HE2	1:335:A:SER:HA	5	0.41	0.13	0.47
(1,1374)	1:307:A:MET:HE3	1:335:A:SER:HA	5	0.41	0.13	0.47
(1,3845)	1:481:A:GLN:HG2	1:487:A:ASP:H	5	0.4	0.11	0.43
(1,3845)	1:481:A:GLN:HG3	1:487:A:ASP:H	5	0.4	0.11	0.43
(1,123)	1:236:A:ARG:HB2	1:240:A:GLU:H	5	0.39	0.15	0.43
(1,123)	1:236:A:ARG:HB3	1:240:A:GLU:H	5	0.39	0.15	0.43
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD11	5	0.39	0.06	0.39
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD12	5	0.39	0.06	0.39
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD13	5	0.39	0.06	0.39
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD11	5	0.39	0.06	0.39
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD12	5	0.39	0.06	0.39
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD13	5	0.39	0.06	0.39
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD11	5	0.39	0.06	0.39
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD12	5	0.39	0.06	0.39
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD13	5	0.39	0.06	0.39
(1,3311)	1:434:A:THR:HB	1:466:A:GLU:HA	5	0.38	0.08	0.43
(1,2887)	1:407:A:THR:HG21	1:408:A:ASP:H	5	0.38	0.09	0.39
(1,2887)	1:407:A:THR:HG22	1:408:A:ASP:H	5	0.38	0.09	0.39
(1,2887)	1:407:A:THR:HG23	1:408:A:ASP:H	5	0.38	0.09	0.39
(1,2487)	1:383:A:LYS:HE2	1:402:A:PHE:HA	5	0.38	0.15	0.36
(1,2487)	1:383:A:LYS:HE3	1:402:A:PHE:HA	5	0.38	0.15	0.36
(1,1776)	1:336:A:ARG:HA	1:340:A:GLN:H	5	0.37	0.13	0.47
(1,1992)	1:354:A:LYS:HG2	1:392:A:ASN:HD21	5	0.37	0.06	0.38
(1,1992)	1:354:A:LYS:HG2	1:392:A:ASN:HD22	5	0.37	0.06	0.38
(1,1992)	1:354:A:LYS:HG3	1:392:A:ASN:HD21	5	0.37	0.06	0.38
(1,1992)	1:354:A:LYS:HG3	1:392:A:ASN:HD22	5	0.37	0.06	0.38
(1,3121)	1:427:A:GLN:HE21	1:455:A:ILE:HA	5	0.36	0.1	0.39
(1,3121)	1:427:A:GLN:HE22	1:455:A:ILE:HA	5	0.36	0.1	0.39
(1,3136)	1:428:A:GLU:HG2	1:478:A:LYS:HA	5	0.36	0.14	0.33
(1,3136)	1:428:A:GLU:HG3	1:478:A:LYS:HA	5	0.36	0.14	0.33
(1,564)	1:263:A:TRP:HE1	1:265:A:HIS:H	5	0.36	0.17	0.34
(1,3084)	1:423:A:MET:HE1	1:427:A:GLN:HG2	5	0.36	0.17	0.36
(1,3084)	1:423:A:MET:HE1	1:427:A:GLN:HG3	5	0.36	0.17	0.36
(1,3084)	1:423:A:MET:HE2	1:427:A:GLN:HG2	5	0.36	0.17	0.36
(1,3084)	1:423:A:MET:HE2	1:427:A:GLN:HG3	5	0.36	0.17	0.36
(1,3084)	1:423:A:MET:HE3	1:427:A:GLN:HG2	5	0.36	0.17	0.36
(1,3084)	1:423:A:MET:HE3	1:427:A:GLN:HG3	5	0.36	0.17	0.36
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG21	5	0.36	0.14	0.35

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG22	5	0.36	0.14	0.35
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG23	5	0.36	0.14	0.35
(1,219)	1:244:A:GLU:HA	1:248:A:GLU:H	5	0.35	0.09	0.39
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD11	5	0.34	0.17	0.28
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD12	5	0.34	0.17	0.28
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD13	5	0.34	0.17	0.28
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD11	5	0.34	0.04	0.31
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD12	5	0.34	0.04	0.31
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD13	5	0.34	0.04	0.31
(1,3896)	1:486:A:VAL:HA	1:489:A:SER:HB2	5	0.33	0.16	0.35
(1,3896)	1:486:A:VAL:HA	1:489:A:SER:HB3	5	0.33	0.16	0.35
(1,2123)	1:361:A:GLU:HA	1:399:A:LEU:HA	5	0.32	0.13	0.28
(1,2861)	1:405:A:THR:HA	1:408:A:ASP:HA	5	0.32	0.08	0.34
(1,1022)	1:289:A:TRP:HH2	1:381:A:VAL:H	5	0.31	0.1	0.27
(1,2380)	1:376:A:GLN:HE21	1:412:A:GLN:H	5	0.31	0.14	0.26
(1,2380)	1:376:A:GLN:HE22	1:412:A:GLN:H	5	0.31	0.14	0.26
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD11	5	0.3	0.09	0.34
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD12	5	0.3	0.09	0.34
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD13	5	0.3	0.09	0.34
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD11	5	0.3	0.09	0.34
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD12	5	0.3	0.09	0.34
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD13	5	0.3	0.09	0.34
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD11	5	0.3	0.09	0.34
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD12	5	0.3	0.09	0.34
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD13	5	0.3	0.09	0.34
(1,2344)	1:375:A:TRP:HZ2	1:402:A:PHE:HA	5	0.29	0.15	0.32
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB2	5	0.28	0.12	0.25
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB3	5	0.28	0.12	0.25
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB2	5	0.28	0.12	0.25
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB3	5	0.28	0.12	0.25
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB2	5	0.28	0.12	0.25
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB3	5	0.28	0.12	0.25
(1,3943)	1:490:A:LEU:HA	1:492:A:LYS:H	5	0.28	0.11	0.32
(1,2827)	1:404:A:SER:H	1:413:A:THR:H	5	0.27	0.12	0.31
(1,1090)	1:296:A:GLY:H	1:311:A:GLU:HA	5	0.26	0.14	0.21
(1,2353)	1:375:A:TRP:HZ3	1:400:A:LEU:HA	5	0.26	0.11	0.3
(1,2318)	1:374:A:PHE:HZ	1:382:A:LEU:HB2	5	0.25	0.09	0.3
(1,2318)	1:374:A:PHE:HZ	1:382:A:LEU:HB3	5	0.25	0.09	0.3
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG11	5	0.25	0.11	0.29
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG12	5	0.25	0.11	0.29
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG13	5	0.25	0.11	0.29
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG11	5	0.25	0.11	0.29

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Key	Atom-1	Atom-2	Models^1	Mean (Å)	SD^1 (Å)	Median (Å)
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG12	5	0.25	0.11	0.29
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG13	5	0.25	0.11	0.29
(1,3208)	1:431:A:TYR:HB2	1:482:A:SER:HA	5	0.24	0.13	0.19
(1,3208)	1:431:A:TYR:HB3	1:482:A:SER:HA	5	0.24	0.13	0.19
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD11	5	0.24	0.12	0.2
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD12	5	0.24	0.12	0.2
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD13	5	0.24	0.12	0.2
(1,2566)	1:387:A:ALA:H	1:468:A:MET:HA	5	0.24	0.16	0.18
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD11	5	0.24	0.12	0.18
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD12	5	0.24	0.12	0.18
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD13	5	0.24	0.12	0.18
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD11	5	0.24	0.12	0.18
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD12	5	0.24	0.12	0.18
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD13	5	0.24	0.12	0.18
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD11	5	0.24	0.12	0.18
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD12	5	0.24	0.12	0.18
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD13	5	0.24	0.12	0.18
(1,1139)	1:297:A:LEU:H	1:309:A:ASP:HA	5	0.23	0.05	0.23
(1,3231)	1:432:A:TYR:H	1:483:A:VAL:H	5	0.23	0.08	0.21
(1,95)	1:234:A:TRP:HA	1:246:A:TYR:HE2	5	0.23	0.09	0.22
(1,2398)	1:378:A:PHE:HA	1:382:A:LEU:H	5	0.23	0.08	0.29
(1,2108)	1:360:A:LEU:HD21	1:364:A:ALA:H	5	0.23	0.04	0.21
(1,2108)	1:360:A:LEU:HD22	1:364:A:ALA:H	5	0.23	0.04	0.21
(1,2108)	1:360:A:LEU:HD23	1:364:A:ALA:H	5	0.23	0.04	0.21
(1,2985)	1:417:A:GLU:HB2	1:421:A:SER:H	5	0.23	0.09	0.18
(1,2985)	1:417:A:GLU:HB3	1:421:A:SER:H	5	0.23	0.09	0.18
(1,3749)	1:469:A:MET:HA	1:471:A:TYR:H	5	0.22	0.1	0.17
(1,3857)	1:481:A:GLN:HE21	1:482:A:SER:H	5	0.21	0.05	0.21
(1,3857)	1:481:A:GLN:HE22	1:482:A:SER:H	5	0.21	0.05	0.21
(1,1626)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	5	0.21	0.1	0.21
(1,2107)	1:360:A:LEU:HA	1:364:A:ALA:H	5	0.2	0.08	0.17
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD11	5	0.2	0.05	0.19
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD12	5	0.2	0.05	0.19
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD13	5	0.2	0.05	0.19
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD11	5	0.19	0.06	0.16
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD12	5	0.19	0.06	0.16
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD13	5	0.19	0.06	0.16
(1,3153)	1:429:A:LYS:HA	1:480:A:PHE:H	5	0.19	0.05	0.19
(1,2250)	1:370:A:LYS:HA	1:373:A:THR:HB	5	0.19	0.03	0.19
(1,2968)	1:416:A:LEU:HA	1:420:A:VAL:H	5	0.16	0.07	0.12
(1,111)	1:235:A:THR:H	1:265:A:HIS:HE1	5	0.13	0.03	0.12
(1,3970)	1:357:A:LEU:HD11	2:620:B:LEU:HD21	4	1.24	0.7	1.35

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3970)	1:357:A:LEU:HD11	2:620:B:LEU:HD22	4	1.24	0.7	1.35
(1,3970)	1:357:A:LEU:HD11	2:620:B:LEU:HD23	4	1.24	0.7	1.35
(1,3970)	1:357:A:LEU:HD12	2:620:B:LEU:HD21	4	1.24	0.7	1.35
(1,3970)	1:357:A:LEU:HD12	2:620:B:LEU:HD22	4	1.24	0.7	1.35
(1,3970)	1:357:A:LEU:HD12	2:620:B:LEU:HD23	4	1.24	0.7	1.35
(1,3970)	1:357:A:LEU:HD13	2:620:B:LEU:HD21	4	1.24	0.7	1.35
(1,3970)	1:357:A:LEU:HD13	2:620:B:LEU:HD22	4	1.24	0.7	1.35
(1,3970)	1:357:A:LEU:HD13	2:620:B:LEU:HD23	4	1.24	0.7	1.35
(2,5)	1:290:A:ASN:HB2	1:293:A:HIS:HA	4	0.62	0.14	0.68
(2,5)	1:290:A:ASN:HB3	1:293:A:HIS:HA	4	0.62	0.14	0.68
(1,1745)	1:333:A:ASN:HD21	1:338:A:ILE:HD11	4	0.55	0.04	0.56
(1,1745)	1:333:A:ASN:HD21	1:338:A:ILE:HD12	4	0.55	0.04	0.56
(1,1745)	1:333:A:ASN:HD21	1:338:A:ILE:HD13	4	0.55	0.04	0.56
(1,1745)	1:333:A:ASN:HD22	1:338:A:ILE:HD11	4	0.55	0.04	0.56
(1,1745)	1:333:A:ASN:HD22	1:338:A:ILE:HD12	4	0.55	0.04	0.56
(1,1745)	1:333:A:ASN:HD22	1:338:A:ILE:HD13	4	0.55	0.04	0.56
(1,2135)	1:361:A:GLU:HG2	1:365:A:LYS:HG2	4	0.54	0.07	0.52
(1,2135)	1:361:A:GLU:HG2	1:365:A:LYS:HG3	4	0.54	0.07	0.52
(1,2135)	1:361:A:GLU:HG3	1:365:A:LYS:HG2	4	0.54	0.07	0.52
(1,2135)	1:361:A:GLU:HG3	1:365:A:LYS:HG3	4	0.54	0.07	0.52
(1,352)	1:250:A:TYR:HE1	1:256:A:ASP:H	4	0.51	0.1	0.54
(1,352)	1:250:A:TYR:HE2	1:256:A:ASP:H	4	0.51	0.1	0.54
(1,2563)	1:387:A:ALA:HA	1:471:A:TYR:HE1	4	0.5	0.06	0.5
(1,2563)	1:387:A:ALA:HA	1:471:A:TYR:HE2	4	0.5	0.06	0.5
(1,1020)	1:289:A:TRP:HH2	1:384:A:GLU:HG2	4	0.49	0.08	0.5
(1,1020)	1:289:A:TRP:HH2	1:384:A:GLU:HG3	4	0.49	0.08	0.5
(1,2382)	1:376:A:GLN:HG2	1:412:A:GLN:HE21	4	0.48	0.16	0.56
(1,2382)	1:376:A:GLN:HG2	1:412:A:GLN:HE22	4	0.48	0.16	0.56
(1,2382)	1:376:A:GLN:HG3	1:412:A:GLN:HE21	4	0.48	0.16	0.56
(1,2382)	1:376:A:GLN:HG3	1:412:A:GLN:HE22	4	0.48	0.16	0.56
(1,3634)	1:458:A:LEU:HD11	1:480:A:PHE:HE1	4	0.48	0.16	0.48
(1,3634)	1:458:A:LEU:HD11	1:480:A:PHE:HE2	4	0.48	0.16	0.48
(1,3634)	1:458:A:LEU:HD12	1:480:A:PHE:HE1	4	0.48	0.16	0.48
(1,3634)	1:458:A:LEU:HD12	1:480:A:PHE:HE2	4	0.48	0.16	0.48
(1,3634)	1:458:A:LEU:HD13	1:480:A:PHE:HE1	4	0.48	0.16	0.48
(1,3634)	1:458:A:LEU:HD13	1:480:A:PHE:HE2	4	0.48	0.16	0.48
(1,3081)	1:423:A:MET:HE1	1:427:A:GLN:HB2	4	0.47	0.12	0.5
(1,3081)	1:423:A:MET:HE1	1:427:A:GLN:HB3	4	0.47	0.12	0.5
(1,3081)	1:423:A:MET:HE2	1:427:A:GLN:HB2	4	0.47	0.12	0.5
(1,3081)	1:423:A:MET:HE2	1:427:A:GLN:HB3	4	0.47	0.12	0.5
(1,3081)	1:423:A:MET:HE3	1:427:A:GLN:HB2	4	0.47	0.12	0.5
(1,3081)	1:423:A:MET:HE3	1:427:A:GLN:HB3	4	0.47	0.12	0.5

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1422)	1:312:A:GLN:HE21	1:340:A:GLN:HA	4	0.46	0.04	0.48
(1,1422)	1:312:A:GLN:HE22	1:340:A:GLN:HA	4	0.46	0.04	0.48
(1,2873)	1:406:A:HIS:HA	1:422:A:ARG:HD2	4	0.46	0.22	0.46
(1,2873)	1:406:A:HIS:HA	1:422:A:ARG:HD3	4	0.46	0.22	0.46
(1,2619)	1:393:A:GLN:HE21	1:474:A:GLU:H	4	0.45	0.14	0.52
(1,2619)	1:393:A:GLN:HE22	1:474:A:GLU:H	4	0.45	0.14	0.52
(1,2694)	1:398:A:LYS:HA	1:475:A:PHE:HZ	4	0.45	0.11	0.44
(1,1486)	1:314:A:MET:HB2	1:319:A:ARG:H	4	0.44	0.16	0.46
(1,1486)	1:314:A:MET:HB3	1:319:A:ARG:H	4	0.44	0.16	0.46
(1,2379)	1:376:A:GLN:HE21	1:413:A:THR:HG21	4	0.44	0.19	0.5
(1,2379)	1:376:A:GLN:HE21	1:413:A:THR:HG22	4	0.44	0.19	0.5
(1,2379)	1:376:A:GLN:HE21	1:413:A:THR:HG23	4	0.44	0.19	0.5
(1,2379)	1:376:A:GLN:HE22	1:413:A:THR:HG21	4	0.44	0.19	0.5
(1,2379)	1:376:A:GLN:HE22	1:413:A:THR:HG22	4	0.44	0.19	0.5
(1,2379)	1:376:A:GLN:HE22	1:413:A:THR:HG23	4	0.44	0.19	0.5
(1,1951)	1:351:A:ALA:HA	1:354:A:LYS:HD2	4	0.43	0.13	0.43
(1,1951)	1:351:A:ALA:HA	1:354:A:LYS:HD3	4	0.43	0.13	0.43
(1,3187)	1:430:A:ILE:HD11	1:474:A:GLU:HA	4	0.42	0.06	0.42
(1,3187)	1:430:A:ILE:HD12	1:474:A:GLU:HA	4	0.42	0.06	0.42
(1,3187)	1:430:A:ILE:HD13	1:474:A:GLU:HA	4	0.42	0.06	0.42
(1,1490)	1:314:A:MET:HB2	1:318:A:LEU:H	4	0.42	0.09	0.46
(1,1490)	1:314:A:MET:HB3	1:318:A:LEU:H	4	0.42	0.09	0.46
(1,2335)	1:375:A:TRP:HH2	1:468:A:MET:HE1	4	0.42	0.17	0.45
(1,2335)	1:375:A:TRP:HH2	1:468:A:MET:HE2	4	0.42	0.17	0.45
(1,2335)	1:375:A:TRP:HH2	1:468:A:MET:HE3	4	0.42	0.17	0.45
(1,2764)	1:402:A:PHE:H	1:414:A:VAL:HB	4	0.42	0.15	0.42
(1,1859)	1:344:A:VAL:HB	1:348:A:LEU:H	4	0.41	0.15	0.46
(1,719)	1:274:A:TYR:HD1	1:348:A:LEU:HD21	4	0.41	0.12	0.4
(1,719)	1:274:A:TYR:HD2	1:348:A:LEU:HD22	4	0.41	0.12	0.4
(1,719)	1:274:A:TYR:HD2	1:348:A:LEU:HD23	4	0.41	0.12	0.4
(1,3165)	1:429:A:LYS:HB2	1:431:A:TYR:HE1	4	0.4	0.23	0.29
(1,3165)	1:429:A:LYS:HB2	1:431:A:TYR:HE2	4	0.4	0.23	0.29
(1,3165)	1:429:A:LYS:HB3	1:431:A:TYR:HE2	4	0.4	0.23	0.29
(1,454)	1:257:A:PHE:H	1:258:A:ASN:HD21	4	0.4	0.05	0.4
(1,454)	1:257:A:PHE:H	1:258:A:ASN:HD22	4	0.4	0.05	0.4
(1,3128)	1:427:A:GLN:HG2	1:429:A:LYS:H	4	0.39	0.09	0.41
(1,3128)	1:427:A:GLN:HG3	1:429:A:LYS:H	4	0.39	0.09	0.41
(1,3846)	1:481:A:GLN:HE21	1:486:A:VAL:H	4	0.38	0.1	0.38
(1,3846)	1:481:A:GLN:HE22	1:486:A:VAL:H	4	0.38	0.1	0.38
(1,3137)	1:428:A:GLU:HA	1:478:A:LYS:HG2	4	0.38	0.11	0.4
(1,3137)	1:428:A:GLU:HA	1:478:A:LYS:HG3	4	0.38	0.11	0.4
(1,3561)	1:450:A:LEU:HD11	1:456:A:GLU:H	4	0.37	0.14	0.4

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3561)	1:450:A:LEU:HD12	1:456:A:GLU:H	4	0.37	0.14	0.4
(1,3561)	1:450:A:LEU:HD13	1:456:A:GLU:H	4	0.37	0.14	0.4
(1,1487)	1:314:A:MET:HB2	1:319:A:ARG:HA	4	0.36	0.1	0.36
(1,1487)	1:314:A:MET:HB3	1:319:A:ARG:HA	4	0.36	0.1	0.36
(1,2790)	1:403:A:ALA:HA	1:414:A:VAL:HB	4	0.36	0.14	0.4
(1,2621)	1:393:A:GLN:HE21	1:473:A:THR:H	4	0.35	0.12	0.39
(1,2621)	1:393:A:GLN:HE22	1:473:A:THR:H	4	0.35	0.12	0.39
(1,1416)	1:312:A:GLN:HB2	1:349:A:ARG:HD2	4	0.34	0.06	0.34
(1,1416)	1:312:A:GLN:HB2	1:349:A:ARG:HD3	4	0.34	0.06	0.34
(1,1416)	1:312:A:GLN:HB3	1:349:A:ARG:HD2	4	0.34	0.06	0.34
(1,1416)	1:312:A:GLN:HB3	1:349:A:ARG:HD3	4	0.34	0.06	0.34
(1,3740)	1:469:A:MET:HE1	1:473:A:THR:H	4	0.33	0.13	0.34
(1,3740)	1:469:A:MET:HE2	1:473:A:THR:H	4	0.33	0.13	0.34
(1,3740)	1:469:A:MET:HE3	1:473:A:THR:H	4	0.33	0.13	0.34
(1,3767)	1:472:A:LEU:HD23	1:480:A:PHE:HE2	4	0.32	0.12	0.38
(1,3767)	1:472:A:LEU:HD21	1:480:A:PHE:HE1	4	0.32	0.12	0.38
(1,3767)	1:472:A:LEU:HD22	1:480:A:PHE:HE2	4	0.32	0.12	0.38
(1,2488)	1:383:A:LYS:HE2	1:402:A:PHE:HZ	4	0.32	0.15	0.3
(1,2488)	1:383:A:LYS:HE3	1:402:A:PHE:HZ	4	0.32	0.15	0.3
(1,3082)	1:423:A:MET:HA	1:427:A:GLN:HE21	4	0.32	0.12	0.38
(1,3082)	1:423:A:MET:HA	1:427:A:GLN:HE22	4	0.32	0.12	0.38
(2,14)	1:442:A:LYS:H	1:461:A:SER:HB2	4	0.32	0.16	0.26
(2,14)	1:442:A:LYS:H	1:461:A:SER:HB3	4	0.32	0.16	0.26
(1,1858)	1:344:A:VAL:HA	1:348:A:LEU:H	4	0.32	0.16	0.29
(1,550)	1:263:A:TRP:HA	1:359:A:MET:HG2	4	0.32	0.1	0.36
(1,550)	1:263:A:TRP:HA	1:359:A:MET:HG3	4	0.32	0.1	0.36
(1,2166)	1:363:A:LEU:HA	1:367:A:ASP:HB2	4	0.31	0.13	0.3
(1,2166)	1:363:A:LEU:HA	1:367:A:ASP:HB3	4	0.31	0.13	0.3
(1,2871)	1:406:A:HIS:HA	1:456:A:GLU:HG2	4	0.31	0.16	0.22
(1,2871)	1:406:A:HIS:HA	1:456:A:GLU:HG3	4	0.31	0.16	0.22
(1,2828)	1:404:A:SER:H	1:412:A:GLN:HA	4	0.3	0.09	0.3
(1,1051)	1:293:A:HIS:HE1	1:309:A:ASP:HB2	4	0.29	0.18	0.26
(1,1051)	1:293:A:HIS:HE1	1:309:A:ASP:HB3	4	0.29	0.18	0.26
(1,3309)	1:434:A:THR:HB	1:466:A:GLU:H	4	0.29	0.16	0.3
(1,960)	1:285:A:PRO:HB2	1:294:A:LYS:HB2	4	0.28	0.14	0.3
(1,960)	1:285:A:PRO:HB2	1:294:A:LYS:HB3	4	0.28	0.14	0.3
(1,960)	1:285:A:PRO:HB3	1:294:A:LYS:HB2	4	0.28	0.14	0.3
(1,960)	1:285:A:PRO:HB3	1:294:A:LYS:HB3	4	0.28	0.14	0.3
(1,2736)	1:401:A:ARG:HD2	1:414:A:VAL:H	4	0.28	0.07	0.27
(1,2736)	1:401:A:ARG:HD3	1:414:A:VAL:H	4	0.28	0.07	0.27
(1,1354)	1:305:A:PHE:HE2	1:307:A:MET:HA	4	0.27	0.11	0.24
(1,2980)	1:417:A:GLU:H	1:475:A:PHE:HZ	4	0.27	0.09	0.23

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1889)	1:346:A:ARG:HA	1:349:A:ARG:HG2	4	0.26	0.1	0.26
(1,1994)	1:354:A:LYS:HA	1:358:A:GLN:H	4	0.26	0.1	0.24
(1,3164)	1:429:A:LYS:HB2	1:431:A:TYR:HE1	4	0.26	0.21	0.15
(1,3164)	1:429:A:LYS:HB2	1:431:A:TYR:HE2	4	0.26	0.21	0.15
(1,3164)	1:429:A:LYS:HB3	1:431:A:TYR:HE1	4	0.26	0.21	0.15
(1,3164)	1:429:A:LYS:HB3	1:431:A:TYR:HE2	4	0.26	0.21	0.15
(1,700)	1:273:A:GLU:HB2	1:329:A:ASP:H	4	0.25	0.2	0.15
(1,700)	1:273:A:GLU:HB3	1:329:A:ASP:H	4	0.25	0.2	0.15
(1,2848)	1:405:A:THR:H	1:457:A:VAL:HB	4	0.25	0.08	0.26
(1,2445)	1:381:A:VAL:HA	1:385:A:GLY:H	4	0.24	0.15	0.18
(1,1768)	1:335:A:SER:H	1:338:A:ILE:HD11	4	0.24	0.13	0.2
(1,1768)	1:335:A:SER:H	1:338:A:ILE:HD12	4	0.24	0.13	0.2
(1,1768)	1:335:A:SER:H	1:338:A:ILE:HD13	4	0.24	0.13	0.2
(1,3133)	1:428:A:GLU:HG2	1:479:A:PRO:HD2	4	0.23	0.06	0.25
(1,3133)	1:428:A:GLU:HG2	1:479:A:PRO:HD3	4	0.23	0.06	0.25
(1,3133)	1:428:A:GLU:HG3	1:479:A:PRO:HD2	4	0.23	0.06	0.25
(1,3133)	1:428:A:GLU:HG3	1:479:A:PRO:HD3	4	0.23	0.06	0.25
(1,2912)	1:410:A:SER:HB2	1:438:A:TYR:HD1	4	0.23	0.1	0.2
(1,2912)	1:410:A:SER:HB2	1:438:A:TYR:HD2	4	0.23	0.1	0.2
(1,2912)	1:410:A:SER:HB3	1:438:A:TYR:HD1	4	0.23	0.1	0.2
(1,2912)	1:410:A:SER:HB3	1:438:A:TYR:HD2	4	0.23	0.1	0.2
(1,2200)	1:365:A:LYS:HA	1:368:A:ALA:HA	4	0.22	0.11	0.22
(1,3076)	1:423:A:MET:HE1	1:429:A:LYS:H	4	0.22	0.05	0.24
(1,3076)	1:423:A:MET:HE2	1:429:A:LYS:H	4	0.22	0.05	0.24
(1,3076)	1:423:A:MET:HE3	1:429:A:LYS:H	4	0.22	0.05	0.24
(1,2524)	1:385:A:GLY:HA2	1:389:A:ASP:H	4	0.21	0.05	0.23
(1,2524)	1:385:A:GLY:HA3	1:389:A:ASP:H	4	0.21	0.05	0.23
(1,879)	1:280:A:ILE:HA	1:321:A:VAL:HA	4	0.21	0.1	0.2
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD11	4	0.21	0.06	0.22
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD12	4	0.21	0.06	0.22
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD13	4	0.21	0.06	0.22
(1,3174)	1:430:A:ILE:H	1:480:A:PHE:HA	4	0.21	0.06	0.24
(1,174)	1:240:A:GLU:HA	1:242:A:THR:H	4	0.21	0.04	0.2
(1,1349)	1:305:A:PHE:HZ	1:308:A:ASP:HA	4	0.2	0.06	0.21
(1,680)	1:271:A:LYS:HA	1:273:A:GLU:H	4	0.18	0.06	0.18
(1,2013)	1:355:A:ARG:HA	1:358:A:GLN:H	4	0.18	0.11	0.14
(1,218)	1:243:A:ASP:HB2	1:244:A:GLU:H	4	0.18	0.05	0.18
(1,218)	1:243:A:ASP:HB3	1:244:A:GLU:H	4	0.18	0.05	0.18
(1,3218)	1:431:A:TYR:H	1:457:A:VAL:HA	4	0.16	0.02	0.16
(1,1810)	1:339:A:LEU:HA	1:345:A:THR:H	4	0.16	0.04	0.15
(1,251)	1:246:A:TYR:HE1	1:263:A:TRP:HE1	4	0.15	0.03	0.16
(1,251)	1:246:A:TYR:HE2	1:263:A:TRP:HE1	4	0.15	0.03	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,210)	1:243:A:ASP:H	1:246:A:TYR:H	4	0.13	0.01	0.13
(1,3529)	1:449:A:LEU:HD21	1:494:A:ALA:H	3	0.57	0.06	0.59
(1,3529)	1:449:A:LEU:HD22	1:494:A:ALA:H	3	0.57	0.06	0.59
(1,3529)	1:449:A:LEU:HD23	1:494:A:ALA:H	3	0.57	0.06	0.59
(1,2048)	1:357:A:LEU:HD11	1:392:A:ASN:H	3	0.55	0.11	0.62
(1,2048)	1:357:A:LEU:HD12	1:392:A:ASN:H	3	0.55	0.11	0.62
(1,2048)	1:357:A:LEU:HD13	1:392:A:ASN:H	3	0.55	0.11	0.62
(1,2590)	1:390:A:PHE:HD1	1:471:A:TYR:HB2	3	0.53	0.26	0.68
(1,2590)	1:390:A:PHE:HD1	1:471:A:TYR:HB3	3	0.53	0.26	0.68
(1,2590)	1:390:A:PHE:HD2	1:471:A:TYR:HB2	3	0.53	0.26	0.68
(1,2590)	1:390:A:PHE:HD2	1:471:A:TYR:HB3	3	0.53	0.26	0.68
(1,705)	1:273:A:GLU:HG2	1:328:A:SER:H	3	0.5	0.05	0.49
(1,705)	1:273:A:GLU:HG3	1:328:A:SER:H	3	0.5	0.05	0.49
(1,2695)	1:398:A:LYS:HD2	1:475:A:PHE:HZ	3	0.49	0.11	0.56
(1,2695)	1:398:A:LYS:HD3	1:475:A:PHE:HZ	3	0.49	0.11	0.56
(1,757)	1:276:A:SER:HB2	1:355:A:ARG:HG2	3	0.48	0.12	0.4
(1,757)	1:276:A:SER:HB3	1:355:A:ARG:HG2	3	0.48	0.12	0.4
(1,1959)	1:352:A:LEU:HD21	1:356:A:VAL:H	3	0.48	0.1	0.51
(1,1959)	1:352:A:LEU:HD22	1:356:A:VAL:H	3	0.48	0.1	0.51
(1,1959)	1:352:A:LEU:HD23	1:356:A:VAL:H	3	0.48	0.1	0.51
(1,110)	1:235:A:THR:HG1	1:267:A:ARG:HD2	3	0.47	0.19	0.55
(1,110)	1:235:A:THR:HG1	1:267:A:ARG:HD3	3	0.47	0.19	0.55
(1,1317)	1:302:A:GLN:HE21	1:332:A:LEU:HD21	3	0.47	0.16	0.5
(1,1317)	1:302:A:GLN:HE21	1:332:A:LEU:HD22	3	0.47	0.16	0.5
(1,1317)	1:302:A:GLN:HE21	1:332:A:LEU:HD23	3	0.47	0.16	0.5
(1,1317)	1:302:A:GLN:HE22	1:332:A:LEU:HD21	3	0.47	0.16	0.5
(1,1317)	1:302:A:GLN:HE22	1:332:A:LEU:HD22	3	0.47	0.16	0.5
(1,1317)	1:302:A:GLN:HE22	1:332:A:LEU:HD23	3	0.47	0.16	0.5
(1,3633)	1:458:A:LEU:HD11	1:480:A:PHE:HD1	3	0.47	0.09	0.41
(1,3633)	1:458:A:LEU:HD11	1:480:A:PHE:HD2	3	0.47	0.09	0.41
(1,3633)	1:458:A:LEU:HD12	1:480:A:PHE:HD1	3	0.47	0.09	0.41
(1,3633)	1:458:A:LEU:HD12	1:480:A:PHE:HD2	3	0.47	0.09	0.41
(1,3633)	1:458:A:LEU:HD13	1:480:A:PHE:HD1	3	0.47	0.09	0.41
(1,3633)	1:458:A:LEU:HD13	1:480:A:PHE:HD2	3	0.47	0.09	0.41
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD2	3	0.47	0.03	0.47
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD3	3	0.47	0.03	0.47
(1,2381)	1:376:A:GLN:HA	1:412:A:GLN:HE21	3	0.45	0.15	0.49
(1,2381)	1:376:A:GLN:HA	1:412:A:GLN:HE22	3	0.45	0.15	0.49
(1,3482)	1:446:A:HIS:HA	1:483:A:VAL:HB	3	0.45	0.15	0.54
(1,2357)	1:375:A:TRP:HH2	1:383:A:LYS:HE2	3	0.44	0.15	0.53
(1,2357)	1:375:A:TRP:HH2	1:383:A:LYS:HE3	3	0.44	0.15	0.53
(1,2704)	1:398:A:LYS:HA	1:416:A:LEU:HD11	3	0.43	0.15	0.51

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2704)	1:398:A:LYS:HA	1:416:A:LEU:HD12	3	0.43	0.15	0.51
(1,2704)	1:398:A:LYS:HA	1:416:A:LEU:HD13	3	0.43	0.15	0.51
(1,3070)	1:423:A:MET:HA	1:456:A:GLU:H	3	0.43	0.08	0.42
(1,2432)	1:380:A:LEU:HA	1:384:A:GLU:H	3	0.4	0.12	0.35
(1,3294)	1:433:A:ILE:HB	1:441:A:ALA:HA	3	0.4	0.18	0.52
(1,3362)	1:437:A:SER:HA	1:461:A:SER:HA	3	0.4	0.19	0.49
(1,21)	1:232:A:ALA:H	1:235:A:THR:H	3	0.39	0.16	0.47
(1,2888)	1:408:A:ASP:HA	1:459:A:LEU:HD11	3	0.39	0.19	0.33
(1,2888)	1:408:A:ASP:HA	1:459:A:LEU:HD12	3	0.39	0.19	0.33
(1,2888)	1:408:A:ASP:HA	1:459:A:LEU:HD13	3	0.39	0.19	0.33
(1,1964)	1:352:A:LEU:HA	1:355:A:ARG:HD2	3	0.39	0.15	0.31
(1,1964)	1:352:A:LEU:HA	1:355:A:ARG:HD3	3	0.39	0.15	0.31
(1,3188)	1:430:A:ILE:HB	1:469:A:MET:HE1	3	0.38	0.04	0.4
(1,3188)	1:430:A:ILE:HB	1:469:A:MET:HE2	3	0.38	0.04	0.4
(1,3188)	1:430:A:ILE:HB	1:469:A:MET:HE3	3	0.38	0.04	0.4
(1,2077)	1:359:A:MET:HG2	1:363:A:LEU:H	3	0.38	0.12	0.4
(1,2077)	1:359:A:MET:HG3	1:363:A:LEU:H	3	0.38	0.12	0.4
(1,3649)	1:460:A:LEU:HD21	1:472:A:LEU:HD11	3	0.37	0.2	0.36
(1,3649)	1:460:A:LEU:HD21	1:472:A:LEU:HD12	3	0.37	0.2	0.36
(1,3649)	1:460:A:LEU:HD21	1:472:A:LEU:HD13	3	0.37	0.2	0.36
(1,3649)	1:460:A:LEU:HD22	1:472:A:LEU:HD11	3	0.37	0.2	0.36
(1,3649)	1:460:A:LEU:HD22	1:472:A:LEU:HD12	3	0.37	0.2	0.36
(1,3649)	1:460:A:LEU:HD22	1:472:A:LEU:HD13	3	0.37	0.2	0.36
(1,3649)	1:460:A:LEU:HD23	1:472:A:LEU:HD11	3	0.37	0.2	0.36
(1,3649)	1:460:A:LEU:HD23	1:472:A:LEU:HD12	3	0.37	0.2	0.36
(1,3649)	1:460:A:LEU:HD23	1:472:A:LEU:HD13	3	0.37	0.2	0.36
(1,1996)	1:354:A:LYS:HA	1:358:A:GLN:HE21	3	0.37	0.14	0.31
(1,1996)	1:354:A:LYS:HA	1:358:A:GLN:HE22	3	0.37	0.14	0.31
(1,439)	1:255:A:HIS:HE1	1:308:A:ASP:HB2	3	0.36	0.18	0.34
(1,439)	1:255:A:HIS:HE1	1:308:A:ASP:HB3	3	0.36	0.18	0.34
(1,1570)	1:317:A:TYR:HA	1:320:A:PHE:HE1	3	0.36	0.19	0.46
(1,1570)	1:317:A:TYR:HA	1:320:A:PHE:HE2	3	0.36	0.19	0.46
(1,346)	1:250:A:TYR:HB2	1:263:A:TRP:HE3	3	0.36	0.17	0.25
(1,2484)	1:383:A:LYS:HB2	1:464:A:ILE:HD11	3	0.35	0.16	0.37
(1,2484)	1:383:A:LYS:HB2	1:464:A:ILE:HD12	3	0.35	0.16	0.37
(1,2484)	1:383:A:LYS:HB2	1:464:A:ILE:HD13	3	0.35	0.16	0.37
(1,2484)	1:383:A:LYS:HB3	1:464:A:ILE:HD11	3	0.35	0.16	0.37
(1,2484)	1:383:A:LYS:HB3	1:464:A:ILE:HD12	3	0.35	0.16	0.37
(1,2484)	1:383:A:LYS:HB3	1:464:A:ILE:HD13	3	0.35	0.16	0.37
(1,3301)	1:434:A:THR:H	1:484:A:SER:H	3	0.35	0.09	0.36
(1,291)	1:248:A:GLU:HA	1:252:A:HIS:H	3	0.35	0.14	0.43
(1,1909)	1:348:A:LEU:HA	1:352:A:LEU:H	3	0.34	0.04	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3841)	1:481:A:GLN:HG2	1:489:A:SER:HA	3	0.34	0.16	0.31
(1,3841)	1:481:A:GLN:HG3	1:489:A:SER:HA	3	0.34	0.16	0.31
(1,371)	1:251:A:LYS:HE2	1:259:A:ASP:HA	3	0.33	0.04	0.36
(1,371)	1:251:A:LYS:HE3	1:259:A:ASP:HA	3	0.33	0.04	0.36
(1,549)	1:263:A:TRP:H	1:359:A:MET:HG2	3	0.33	0.14	0.35
(1,549)	1:263:A:TRP:H	1:359:A:MET:HG3	3	0.33	0.14	0.35
(1,1074)	1:295:A:HIS:HA	1:309:A:ASP:HA	3	0.33	0.21	0.19
(1,1471)	1:314:A:MET:HA	1:353:A:THR:H	3	0.32	0.04	0.32
(1,1432)	1:312:A:GLN:HE21	1:336:A:ARG:HG2	3	0.32	0.21	0.23
(1,1432)	1:312:A:GLN:HE21	1:336:A:ARG:HG3	3	0.32	0.21	0.23
(1,1432)	1:312:A:GLN:HE22	1:336:A:ARG:HG2	3	0.32	0.21	0.23
(1,1432)	1:312:A:GLN:HE22	1:336:A:ARG:HG3	3	0.32	0.21	0.23
(1,2348)	1:375:A:TRP:HZ3	1:401:A:ARG:H	3	0.32	0.09	0.34
(1,252)	1:246:A:TYR:HE1	1:263:A:TRP:HE1	3	0.31	0.06	0.32
(1,252)	1:246:A:TYR:HD1	1:263:A:TRP:HE1	3	0.31	0.06	0.32
(1,1997)	1:354:A:LYS:HB2	1:358:A:GLN:HE21	3	0.31	0.15	0.35
(1,1997)	1:354:A:LYS:HB2	1:358:A:GLN:HE22	3	0.31	0.15	0.35
(1,1997)	1:354:A:LYS:HB3	1:358:A:GLN:HE21	3	0.31	0.15	0.35
(1,1997)	1:354:A:LYS:HB3	1:358:A:GLN:HE22	3	0.31	0.15	0.35
(1,144)	1:237:A:ASN:HD21	1:238:A:LYS:H	3	0.31	0.18	0.3
(1,144)	1:237:A:ASN:HD22	1:238:A:LYS:H	3	0.31	0.18	0.3
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE21	3	0.31	0.06	0.35
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE22	3	0.31	0.06	0.35
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE21	3	0.31	0.06	0.35
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE22	3	0.31	0.06	0.35
(1,570)	1:264:A:SER:HB2	1:359:A:MET:HA	3	0.3	0.14	0.25
(1,570)	1:264:A:SER:HB3	1:359:A:MET:HA	3	0.3	0.14	0.25
(1,3918)	1:488:A:GLU:HA	1:491:A:GLU:HA	3	0.3	0.14	0.36
(1,1415)	1:312:A:GLN:HA	1:349:A:ARG:HD2	3	0.3	0.03	0.29
(1,1415)	1:312:A:GLN:HA	1:349:A:ARG:HD3	3	0.3	0.03	0.29
(1,3150)	1:429:A:LYS:HD2	1:481:A:GLN:HB2	3	0.3	0.08	0.25
(1,3150)	1:429:A:LYS:HD2	1:481:A:GLN:HB3	3	0.3	0.08	0.25
(1,3150)	1:429:A:LYS:HD3	1:481:A:GLN:HB2	3	0.3	0.08	0.25
(1,3150)	1:429:A:LYS:HD3	1:481:A:GLN:HB3	3	0.3	0.08	0.25
(1,3028)	1:419:A:TYR:HA	1:422:A:ARG:HD2	3	0.29	0.16	0.21
(1,3028)	1:419:A:TYR:HA	1:422:A:ARG:HD3	3	0.29	0.16	0.21
(1,3522)	1:448:A:GLU:HA	1:451:A:ARG:H	3	0.28	0.11	0.29
(1,525)	1:262:A:THR:HB	1:370:A:LYS:HD2	3	0.28	0.21	0.15
(1,525)	1:262:A:THR:HB	1:370:A:LYS:HD3	3	0.28	0.21	0.15
(1,2794)	1:403:A:ALA:HA	1:413:A:THR:H	3	0.28	0.08	0.23
(1,673)	1:270:A:GLY:H	1:273:A:GLU:HA	3	0.28	0.14	0.19
(1,1420)	1:312:A:GLN:HE21	1:340:A:GLN:H	3	0.28	0.12	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1420)	1:312:A:GLN:HE22	1:340:A:GLN:H	3	0.28	0.12	0.22
(1,2631)	1:393:A:GLN:HA	1:396:A:ILE:H	3	0.28	0.07	0.25
(1,3112)	1:426:A:GLY:HA2	1:428:A:GLU:HA	3	0.27	0.13	0.24
(1,3112)	1:426:A:GLY:HA3	1:428:A:GLU:HA	3	0.27	0.13	0.24
(1,3113)	1:426:A:GLY:HA2	1:428:A:GLU:HB2	3	0.27	0.11	0.2
(1,3113)	1:426:A:GLY:HA2	1:428:A:GLU:HB3	3	0.27	0.11	0.2
(1,3113)	1:426:A:GLY:HA3	1:428:A:GLU:HB2	3	0.27	0.11	0.2
(1,3113)	1:426:A:GLY:HA3	1:428:A:GLU:HB3	3	0.27	0.11	0.2
(1,3185)	1:430:A:ILE:HD11	1:475:A:PHE:H	3	0.27	0.1	0.34
(1,3185)	1:430:A:ILE:HD12	1:475:A:PHE:H	3	0.27	0.1	0.34
(1,3185)	1:430:A:ILE:HD13	1:475:A:PHE:H	3	0.27	0.1	0.34
(1,2813)	1:404:A:SER:HB2	1:458:A:LEU:HA	3	0.27	0.1	0.24
(1,2813)	1:404:A:SER:HB3	1:458:A:LEU:HA	3	0.27	0.1	0.24
(1,1578)	1:318:A:LEU:HA	1:382:A:LEU:HA	3	0.26	0.11	0.21
(1,2227)	1:368:A:ALA:HA	1:371:A:TYR:H	3	0.26	0.09	0.27
(1,2508)	1:384:A:GLU:HA	1:464:A:ILE:HD11	3	0.26	0.09	0.27
(1,2508)	1:384:A:GLU:HA	1:464:A:ILE:HD12	3	0.26	0.09	0.27
(1,2508)	1:384:A:GLU:HA	1:464:A:ILE:HD13	3	0.26	0.09	0.27
(1,2892)	1:408:A:ASP:HA	1:442:A:LYS:HE2	3	0.26	0.09	0.21
(1,2892)	1:408:A:ASP:HA	1:442:A:LYS:HE3	3	0.26	0.09	0.21
(1,353)	1:250:A:TYR:HE1	1:256:A:ASP:HB2	3	0.25	0.06	0.28
(1,353)	1:250:A:TYR:HE1	1:256:A:ASP:HB3	3	0.25	0.06	0.28
(1,353)	1:250:A:TYR:HE2	1:256:A:ASP:HB2	3	0.25	0.06	0.28
(1,353)	1:250:A:TYR:HE2	1:256:A:ASP:HB3	3	0.25	0.06	0.28
(1,648)	1:268:A:VAL:HB	1:274:A:TYR:H	3	0.25	0.04	0.24
(1,3817)	1:475:A:PHE:HE2	1:476:A:ASP:HB2	3	0.25	0.05	0.23
(1,3817)	1:475:A:PHE:HD2	1:476:A:ASP:HB2	3	0.25	0.05	0.23
(1,3817)	1:475:A:PHE:HD2	1:476:A:ASP:HB3	3	0.25	0.05	0.23
(1,8)	1:231:A:GLN:HG2	1:236:A:ARG:HG2	3	0.25	0.1	0.27
(1,8)	1:231:A:GLN:HG2	1:236:A:ARG:HG3	3	0.25	0.1	0.27
(1,8)	1:231:A:GLN:HG3	1:236:A:ARG:HG2	3	0.25	0.1	0.27
(1,8)	1:231:A:GLN:HG3	1:236:A:ARG:HG3	3	0.25	0.1	0.27
(1,2880)	1:407:A:THR:H	1:409:A:SER:H	3	0.25	0.06	0.21
(1,1353)	1:305:A:PHE:HE1	1:307:A:MET:HA	3	0.24	0.12	0.16
(1,1353)	1:305:A:PHE:HE2	1:307:A:MET:HA	3	0.24	0.12	0.16
(1,1621)	1:320:A:PHE:HE1	1:378:A:PHE:HB2	3	0.24	0.08	0.23
(1,1621)	1:320:A:PHE:HE1	1:378:A:PHE:HB3	3	0.24	0.08	0.23
(1,1621)	1:320:A:PHE:HE2	1:378:A:PHE:HB2	3	0.24	0.08	0.23
(1,1621)	1:320:A:PHE:HE2	1:378:A:PHE:HB3	3	0.24	0.08	0.23
(1,2351)	1:375:A:TRP:HE3	1:400:A:LEU:HA	3	0.24	0.04	0.22
(1,180)	1:241:A:ILE:HB	1:246:A:TYR:HD1	3	0.23	0.1	0.19
(1,180)	1:241:A:ILE:HB	1:246:A:TYR:HD2	3	0.23	0.1	0.19

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,620)	1:266:A:ASN:HB2	1:274:A:TYR:HE1	3	0.23	0.09	0.22
(1,620)	1:266:A:ASN:HB2	1:274:A:TYR:HE2	3	0.23	0.09	0.22
(1,620)	1:266:A:ASN:HB3	1:274:A:TYR:HE1	3	0.23	0.09	0.22
(1,620)	1:266:A:ASN:HB3	1:274:A:TYR:HE2	3	0.23	0.09	0.22
(1,966)	1:285:A:PRO:HD2	1:288:A:MET:HE1	3	0.23	0.11	0.19
(1,966)	1:285:A:PRO:HD2	1:288:A:MET:HE2	3	0.23	0.11	0.19
(1,966)	1:285:A:PRO:HD2	1:288:A:MET:HE3	3	0.23	0.11	0.19
(1,966)	1:285:A:PRO:HD3	1:288:A:MET:HE1	3	0.23	0.11	0.19
(1,966)	1:285:A:PRO:HD3	1:288:A:MET:HE2	3	0.23	0.11	0.19
(1,966)	1:285:A:PRO:HD3	1:288:A:MET:HE3	3	0.23	0.11	0.19
(1,3540)	1:449:A:LEU:HA	1:452:A:LYS:H	3	0.23	0.11	0.16
(1,158)	1:238:A:LYS:HA	1:241:A:ILE:HB	3	0.23	0.04	0.21
(1,347)	1:250:A:TYR:HE1	1:260:A:PRO:HA	3	0.22	0.13	0.16
(1,347)	1:250:A:TYR:HE2	1:260:A:PRO:HA	3	0.22	0.13	0.16
(1,2988)	1:417:A:GLU:HA	1:420:A:VAL:H	3	0.22	0.09	0.17
(1,1676)	1:325:A:ILE:HD11	1:327:A:SER:HB2	3	0.22	0.09	0.21
(1,1676)	1:325:A:ILE:HD11	1:327:A:SER:HB3	3	0.22	0.09	0.21
(1,1676)	1:325:A:ILE:HD12	1:327:A:SER:HB2	3	0.22	0.09	0.21
(1,1676)	1:325:A:ILE:HD12	1:327:A:SER:HB3	3	0.22	0.09	0.21
(1,1676)	1:325:A:ILE:HD13	1:327:A:SER:HB2	3	0.22	0.09	0.21
(1,1676)	1:325:A:ILE:HD13	1:327:A:SER:HB3	3	0.22	0.09	0.21
(1,1910)	1:348:A:LEU:HD11	1:352:A:LEU:H	3	0.21	0.04	0.21
(1,1910)	1:348:A:LEU:HD12	1:352:A:LEU:H	3	0.21	0.04	0.21
(1,1910)	1:348:A:LEU:HD13	1:352:A:LEU:H	3	0.21	0.04	0.21
(1,1945)	1:351:A:ALA:HA	1:355:A:ARG:H	3	0.21	0.03	0.22
(1,2913)	1:410:A:SER:HA	1:438:A:TYR:HE1	3	0.2	0.03	0.22
(1,2913)	1:410:A:SER:HA	1:438:A:TYR:HE2	3	0.2	0.03	0.22
(1,1035)	1:290:A:ASN:H	1:292:A:ASP:H	3	0.2	0.05	0.23
(1,1897)	1:347:A:ASN:HA	1:351:A:ALA:H	3	0.2	0.08	0.21
(1,3785)	1:474:A:GLU:HA	1:480:A:PHE:H	3	0.2	0.1	0.14
(1,2911)	1:410:A:SER:HA	1:438:A:TYR:HD1	3	0.17	0.04	0.17
(1,2911)	1:410:A:SER:HA	1:438:A:TYR:HD2	3	0.17	0.04	0.17
(1,127)	1:236:A:ARG:HB2	1:237:A:ASN:H	3	0.17	0.04	0.17
(1,127)	1:236:A:ARG:HB3	1:237:A:ASN:H	3	0.17	0.04	0.17
(1,1320)	1:302:A:GLN:H	1:328:A:SER:HA	3	0.16	0.04	0.16
(1,3519)	1:448:A:GLU:HB2	1:452:A:LYS:H	3	0.16	0.02	0.17
(1,3519)	1:448:A:GLU:HB3	1:452:A:LYS:H	3	0.16	0.02	0.17
(1,509)	1:261:A:LEU:H	1:282:A:SER:H	3	0.15	0.02	0.16
(1,3598)	1:453:A:LYS:HG2	1:493:A:LEU:HB2	3	0.15	0.04	0.13
(1,3598)	1:453:A:LYS:HG2	1:493:A:LEU:HB3	3	0.15	0.04	0.13
(1,1954)	1:351:A:ALA:HA	1:353:A:THR:HB	3	0.14	0.02	0.14
(1,3744)	1:469:A:MET:HA	1:472:A:LEU:H	3	0.14	0.02	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,86)	1:234:A:TRP:HD1	1:275:A:THR:HG21	3	0.13	0.0	0.13
(1,86)	1:234:A:TRP:HD1	1:275:A:THR:HG22	3	0.13	0.0	0.13
(1,86)	1:234:A:TRP:HD1	1:275:A:THR:HG23	3	0.13	0.0	0.13
(1,3103)	1:424:A:LYS:HB2	1:425:A:GLU:HG2	2	0.76	0.08	0.76
(1,3103)	1:424:A:LYS:HB2	1:425:A:GLU:HG3	2	0.76	0.08	0.76
(1,3103)	1:424:A:LYS:HB3	1:425:A:GLU:HG2	2	0.76	0.08	0.76
(1,3103)	1:424:A:LYS:HB3	1:425:A:GLU:HG3	2	0.76	0.08	0.76
(1,1425)	1:312:A:GLN:HG2	1:339:A:LEU:HA	2	0.65	0.05	0.65
(1,1425)	1:312:A:GLN:HG3	1:339:A:LEU:HA	2	0.65	0.05	0.65
(1,1638)	1:320:A:PHE:HA	1:322:A:ARG:HG2	2	0.64	0.06	0.64
(1,1638)	1:320:A:PHE:HA	1:322:A:ARG:HG3	2	0.64	0.06	0.64
(1,2505)	1:384:A:GLU:HA	1:468:A:MET:HA	2	0.61	0.03	0.61
(1,1081)	1:296:A:GLY:H	1:319:A:ARG:HA	2	0.56	0.04	0.56
(1,3480)	1:446:A:HIS:HE1	1:484:A:SER:HA	2	0.54	0.03	0.54
(1,3074)	1:423:A:MET:HE1	1:430:A:ILE:HA	2	0.54	0.12	0.54
(1,3074)	1:423:A:MET:HE2	1:430:A:ILE:HA	2	0.54	0.12	0.54
(1,3074)	1:423:A:MET:HE3	1:430:A:ILE:HA	2	0.54	0.12	0.54
(1,864)	1:280:A:ILE:HD11	1:371:A:TYR:HE1	2	0.52	0.08	0.52
(1,864)	1:280:A:ILE:HD11	1:371:A:TYR:HE2	2	0.52	0.08	0.52
(1,864)	1:280:A:ILE:HD12	1:371:A:TYR:HE1	2	0.52	0.08	0.52
(1,864)	1:280:A:ILE:HD12	1:371:A:TYR:HE2	2	0.52	0.08	0.52
(1,864)	1:280:A:ILE:HD13	1:371:A:TYR:HE1	2	0.52	0.08	0.52
(1,864)	1:280:A:ILE:HD13	1:371:A:TYR:HE2	2	0.52	0.08	0.52
(1,3126)	1:427:A:GLN:HG2	1:430:A:ILE:HA	2	0.52	0.15	0.52
(1,3126)	1:427:A:GLN:HG3	1:430:A:ILE:HA	2	0.52	0.15	0.52
(1,1430)	1:312:A:GLN:HE21	1:336:A:ARG:HA	2	0.52	0.05	0.52
(1,1430)	1:312:A:GLN:HE22	1:336:A:ARG:HA	2	0.52	0.05	0.52
(1,927)	1:283:A:GLN:HA	1:377:A:GLN:HA	2	0.5	0.03	0.5
(1,2483)	1:383:A:LYS:HD2	1:465:A:ASP:HA	2	0.5	0.18	0.5
(1,2483)	1:383:A:LYS:HD3	1:465:A:ASP:HA	2	0.5	0.18	0.5
(1,2849)	1:405:A:THR:HG21	1:457:A:VAL:HB	2	0.48	0.05	0.48
(1,2849)	1:405:A:THR:HG22	1:457:A:VAL:HB	2	0.48	0.05	0.48
(1,2849)	1:405:A:THR:HG23	1:457:A:VAL:HB	2	0.48	0.05	0.48
(1,440)	1:255:A:HIS:HB2	1:294:A:LYS:HE2	2	0.48	0.1	0.48
(1,440)	1:255:A:HIS:HB2	1:294:A:LYS:HE3	2	0.48	0.1	0.48
(1,440)	1:255:A:HIS:HB3	1:294:A:LYS:HE2	2	0.48	0.1	0.48
(1,440)	1:255:A:HIS:HB3	1:294:A:LYS:HE3	2	0.48	0.1	0.48
(1,1391)	1:309:A:ASP:HB2	1:311:A:GLU:HB2	2	0.48	0.15	0.48
(1,1391)	1:309:A:ASP:HB2	1:311:A:GLU:HB3	2	0.48	0.15	0.48
(1,1391)	1:309:A:ASP:HB3	1:311:A:GLU:HB2	2	0.48	0.15	0.48
(1,1391)	1:309:A:ASP:HB3	1:311:A:GLU:HB3	2	0.48	0.15	0.48
(1,2444)	1:381:A:VAL:HA	1:464:A:ILE:HD11	2	0.48	0.12	0.48

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2444)	1:381:A:VAL:HA	1:464:A:ILE:HD12	2	0.48	0.12	0.48
(1,2444)	1:381:A:VAL:HA	1:464:A:ILE:HD13	2	0.48	0.12	0.48
(1,3072)	1:423:A:MET:HE1	1:431:A:TYR:HD1	2	0.48	0.13	0.48
(1,3072)	1:423:A:MET:HE1	1:431:A:TYR:HD2	2	0.48	0.13	0.48
(1,3072)	1:423:A:MET:HE2	1:431:A:TYR:HD1	2	0.48	0.13	0.48
(1,3072)	1:423:A:MET:HE2	1:431:A:TYR:HD2	2	0.48	0.13	0.48
(1,3072)	1:423:A:MET:HE3	1:431:A:TYR:HD1	2	0.48	0.13	0.48
(1,3072)	1:423:A:MET:HE3	1:431:A:TYR:HD2	2	0.48	0.13	0.48
(1,3422)	1:441:A:ALA:H	1:461:A:SER:HB2	2	0.47	0.02	0.47
(1,3422)	1:441:A:ALA:H	1:461:A:SER:HB3	2	0.47	0.02	0.47
(1,1166)	1:298:A:LYS:HG2	1:309:A:ASP:H	2	0.46	0.0	0.46
(1,1166)	1:298:A:LYS:HG3	1:309:A:ASP:H	2	0.46	0.0	0.46
(1,869)	1:280:A:ILE:HD11	1:360:A:LEU:HA	2	0.45	0.01	0.45
(1,869)	1:280:A:ILE:HD12	1:360:A:LEU:HA	2	0.45	0.01	0.45
(1,869)	1:280:A:ILE:HD13	1:360:A:LEU:HA	2	0.45	0.01	0.45
(1,3079)	1:423:A:MET:HE1	1:428:A:GLU:HA	2	0.45	0.01	0.45
(1,3079)	1:423:A:MET:HE2	1:428:A:GLU:HA	2	0.45	0.01	0.45
(1,3079)	1:423:A:MET:HE3	1:428:A:GLU:HA	2	0.45	0.01	0.45
(1,3840)	1:481:A:GLN:HG2	1:489:A:SER:H	2	0.45	0.05	0.45
(1,3840)	1:481:A:GLN:HG3	1:489:A:SER:H	2	0.45	0.05	0.45
(1,1066)	1:295:A:HIS:HB2	1:320:A:PHE:HA	2	0.45	0.15	0.45
(1,1066)	1:295:A:HIS:HB3	1:320:A:PHE:HA	2	0.45	0.15	0.45
(1,1527)	1:316:A:ASN:H	1:349:A:ARG:HD2	2	0.44	0.24	0.44
(1,1527)	1:316:A:ASN:H	1:349:A:ARG:HD3	2	0.44	0.24	0.44
(1,103)	1:235:A:THR:H	1:303:A:ARG:HD2	2	0.44	0.11	0.44
(1,103)	1:235:A:THR:H	1:303:A:ARG:HD3	2	0.44	0.11	0.44
(1,3071)	1:423:A:MET:HE1	1:431:A:TYR:H	2	0.44	0.01	0.44
(1,3071)	1:423:A:MET:HE2	1:431:A:TYR:H	2	0.44	0.01	0.44
(1,3071)	1:423:A:MET:HE3	1:431:A:TYR:H	2	0.44	0.01	0.44
(1,2898)	1:409:A:SER:H	1:442:A:LYS:HE2	2	0.42	0.18	0.42
(1,2898)	1:409:A:SER:H	1:442:A:LYS:HE3	2	0.42	0.18	0.42
(1,3636)	1:458:A:LEU:HD11	1:469:A:MET:HE1	2	0.42	0.3	0.42
(1,3636)	1:458:A:LEU:HD11	1:469:A:MET:HE2	2	0.42	0.3	0.42
(1,3636)	1:458:A:LEU:HD11	1:469:A:MET:HE3	2	0.42	0.3	0.42
(1,3636)	1:458:A:LEU:HD12	1:469:A:MET:HE1	2	0.42	0.3	0.42
(1,3636)	1:458:A:LEU:HD12	1:469:A:MET:HE2	2	0.42	0.3	0.42
(1,3636)	1:458:A:LEU:HD12	1:469:A:MET:HE3	2	0.42	0.3	0.42
(1,3636)	1:458:A:LEU:HD13	1:469:A:MET:HE1	2	0.42	0.3	0.42
(1,3636)	1:458:A:LEU:HD13	1:469:A:MET:HE2	2	0.42	0.3	0.42
(1,3636)	1:458:A:LEU:HD13	1:469:A:MET:HE3	2	0.42	0.3	0.42
(1,3927)	1:489:A:SER:HB2	1:493:A:LEU:HD11	2	0.42	0.14	0.42
(1,3927)	1:489:A:SER:HB2	1:493:A:LEU:HD12	2	0.42	0.14	0.42

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Key	Atom-1	Atom-2	Models^1	Mean (Å)	SD^1 (Å)	Median (Å)
(1,3927)	1:489:A:SER:HB2	1:493:A:LEU:HD13	2	0.42	0.14	0.42
(1,3927)	1:489:A:SER:HB3	1:493:A:LEU:HD11	2	0.42	0.14	0.42
(1,3927)	1:489:A:SER:HB3	1:493:A:LEU:HD12	2	0.42	0.14	0.42
(1,3927)	1:489:A:SER:HB3	1:493:A:LEU:HD13	2	0.42	0.14	0.42
(1,3940)	1:490:A:LEU:HD21	1:493:A:LEU:HB2	2	0.41	0.02	0.41
(1,3940)	1:490:A:LEU:HD21	1:493:A:LEU:HB3	2	0.41	0.02	0.41
(1,3940)	1:490:A:LEU:HD22	1:493:A:LEU:HB2	2	0.41	0.02	0.41
(1,3940)	1:490:A:LEU:HD22	1:493:A:LEU:HB3	2	0.41	0.02	0.41
(1,3940)	1:490:A:LEU:HD23	1:493:A:LEU:HB2	2	0.41	0.02	0.41
(1,3940)	1:490:A:LEU:HD23	1:493:A:LEU:HB3	2	0.41	0.02	0.41
(1,5)	1:231:A:GLN:HG2	1:236:A:ARG:H	2	0.4	0.14	0.4
(1,5)	1:231:A:GLN:HG3	1:236:A:ARG:H	2	0.4	0.14	0.4
(1,3063)	1:422:A:ARG:HB2	1:427:A:GLN:HE21	2	0.4	0.1	0.4
(1,3063)	1:422:A:ARG:HB2	1:427:A:GLN:HE22	2	0.4	0.1	0.4
(1,3063)	1:422:A:ARG:HB3	1:427:A:GLN:HE21	2	0.4	0.1	0.4
(1,3063)	1:422:A:ARG:HB3	1:427:A:GLN:HE22	2	0.4	0.1	0.4
(1,1077)	1:295:A:HIS:HB2	1:296:A:GLY:H	2	0.4	0.02	0.4
(1,1077)	1:295:A:HIS:HB3	1:296:A:GLY:H	2	0.4	0.02	0.4
(1,3332)	1:435:A:ALA:H	1:460:A:LEU:H	2	0.4	0.19	0.4
(1,975)	1:286:A:TRP:HZ3	1:290:A:ASN:HA	2	0.4	0.01	0.4
(1,1010)	1:288:A:MET:HA	1:319:A:ARG:HD2	2	0.4	0.14	0.4
(1,1010)	1:288:A:MET:HA	1:319:A:ARG:HD3	2	0.4	0.14	0.4
(1,2882)	1:407:A:THR:HG21	1:409:A:SER:H	2	0.4	0.04	0.4
(1,2882)	1:407:A:THR:HG22	1:409:A:SER:H	2	0.4	0.04	0.4
(1,2882)	1:407:A:THR:HG23	1:409:A:SER:H	2	0.4	0.04	0.4
(1,3090)	1:424:A:LYS:HE2	1:455:A:ILE:HA	2	0.4	0.11	0.4
(1,3090)	1:424:A:LYS:HE3	1:455:A:ILE:HA	2	0.4	0.11	0.4
(1,3471)	1:445:A:PRO:HA	1:448:A:GLU:HG2	2	0.4	0.14	0.4
(1,3471)	1:445:A:PRO:HA	1:448:A:GLU:HG3	2	0.4	0.14	0.4
(1,2594)	1:390:A:PHE:HA	1:393:A:GLN:HA	2	0.39	0.18	0.39
(1,2823)	1:404:A:SER:H	1:414:A:VAL:H	2	0.39	0.03	0.39
(1,2839)	1:405:A:THR:HA	1:459:A:LEU:HD11	2	0.39	0.01	0.39
(1,2839)	1:405:A:THR:HA	1:459:A:LEU:HD12	2	0.39	0.01	0.39
(1,2839)	1:405:A:THR:HA	1:459:A:LEU:HD13	2	0.39	0.01	0.39
(1,145)	1:238:A:LYS:HD2	1:267:A:ARG:H	2	0.38	0.05	0.38
(1,145)	1:238:A:LYS:HD3	1:267:A:ARG:H	2	0.38	0.05	0.38
(1,2083)	1:359:A:MET:HA	1:362:A:LYS:HD2	2	0.38	0.16	0.38
(1,2083)	1:359:A:MET:HA	1:362:A:LYS:HD3	2	0.38	0.16	0.38
(1,2210)	1:367:A:ASP:H	1:371:A:TYR:H	2	0.38	0.19	0.38
(1,2697)	1:398:A:LYS:HA	1:475:A:PHE:HE1	2	0.38	0.26	0.38
(1,3199)	1:431:A:TYR:HE1	1:489:A:SER:HA	2	0.38	0.12	0.38
(1,3199)	1:431:A:TYR:HE2	1:489:A:SER:HA	2	0.38	0.12	0.38

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3601)	1:453:A:LYS:HG2	1:493:A:LEU:HD21	2	0.38	0.13	0.38
(1,3601)	1:453:A:LYS:HG2	1:493:A:LEU:HD22	2	0.38	0.13	0.38
(1,3601)	1:453:A:LYS:HG2	1:493:A:LEU:HD23	2	0.38	0.13	0.38
(1,3601)	1:453:A:LYS:HG3	1:493:A:LEU:HD21	2	0.38	0.13	0.38
(1,3601)	1:453:A:LYS:HG3	1:493:A:LEU:HD22	2	0.38	0.13	0.38
(1,3601)	1:453:A:LYS:HG3	1:493:A:LEU:HD23	2	0.38	0.13	0.38
(1,1298)	1:301:A:VAL:H	1:306:A:ILE:HB	2	0.38	0.09	0.38
(1,2429)	1:380:A:LEU:HA	1:462:A:ASP:HB2	2	0.38	0.03	0.38
(1,2429)	1:380:A:LEU:HA	1:462:A:ASP:HB3	2	0.38	0.03	0.38
(1,2830)	1:404:A:SER:H	1:407:A:THR:HB	2	0.38	0.2	0.38
(1,3083)	1:423:A:MET:HB2	1:427:A:GLN:HE21	2	0.38	0.12	0.38
(1,3083)	1:423:A:MET:HB2	1:427:A:GLN:HE22	2	0.38	0.12	0.38
(1,3083)	1:423:A:MET:HB3	1:427:A:GLN:HE21	2	0.38	0.12	0.38
(1,3083)	1:423:A:MET:HB3	1:427:A:GLN:HE22	2	0.38	0.12	0.38
(1,1118)	1:297:A:LEU:HA	1:322:A:ARG:HD2	2	0.37	0.12	0.37
(1,1118)	1:297:A:LEU:HA	1:322:A:ARG:HD3	2	0.37	0.12	0.37
(1,1543)	1:317:A:TYR:HD1	1:389:A:ASP:HB2	2	0.37	0.15	0.37
(1,1543)	1:317:A:TYR:HD1	1:389:A:ASP:HB3	2	0.37	0.15	0.37
(1,1543)	1:317:A:TYR:HD2	1:389:A:ASP:HB2	2	0.37	0.15	0.37
(1,1543)	1:317:A:TYR:HD2	1:389:A:ASP:HB3	2	0.37	0.15	0.37
(1,3039)	1:420:A:VAL:HB	1:475:A:PHE:HZ	2	0.36	0.04	0.36
(1,456)	1:258:A:ASN:HB2	1:283:A:GLN:HB2	2	0.36	0.21	0.36
(1,456)	1:258:A:ASN:HB2	1:283:A:GLN:HB3	2	0.36	0.21	0.36
(1,456)	1:258:A:ASN:HB3	1:283:A:GLN:HB2	2	0.36	0.21	0.36
(1,456)	1:258:A:ASN:HB3	1:283:A:GLN:HB3	2	0.36	0.21	0.36
(1,1847)	1:343:A:THR:HG21	1:347:A:ASN:HD21	2	0.36	0.18	0.36
(1,1847)	1:343:A:THR:HG21	1:347:A:ASN:HD22	2	0.36	0.18	0.36
(1,1847)	1:343:A:THR:HG22	1:347:A:ASN:HD21	2	0.36	0.18	0.36
(1,1847)	1:343:A:THR:HG22	1:347:A:ASN:HD22	2	0.36	0.18	0.36
(1,1847)	1:343:A:THR:HG23	1:347:A:ASN:HD21	2	0.36	0.18	0.36
(1,1847)	1:343:A:THR:HG23	1:347:A:ASN:HD22	2	0.36	0.18	0.36
(1,1884)	1:346:A:ARG:HA	1:350:A:ASN:H	2	0.35	0.12	0.35
(1,3096)	1:424:A:LYS:H	1:427:A:GLN:HB2	2	0.35	0.1	0.35
(1,3096)	1:424:A:LYS:H	1:427:A:GLN:HB3	2	0.35	0.1	0.35
(1,1973)	1:353:A:THR:HG21	1:392:A:ASN:HB2	2	0.34	0.05	0.34
(1,1973)	1:353:A:THR:HG21	1:392:A:ASN:HB3	2	0.34	0.05	0.34
(1,1973)	1:353:A:THR:HG22	1:392:A:ASN:HB2	2	0.34	0.05	0.34
(1,1973)	1:353:A:THR:HG22	1:392:A:ASN:HB3	2	0.34	0.05	0.34
(1,1973)	1:353:A:THR:HG23	1:392:A:ASN:HB2	2	0.34	0.05	0.34
(1,1973)	1:353:A:THR:HG23	1:392:A:ASN:HB3	2	0.34	0.05	0.34
(1,2859)	1:405:A:THR:HG21	1:442:A:LYS:HA	2	0.34	0.05	0.34
(1,2859)	1:405:A:THR:HG22	1:442:A:LYS:HA	2	0.34	0.05	0.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2859)	1:405:A:THR:HG23	1:442:A:LYS:HA	2	0.34	0.05	0.34
(1,3091)	1:424:A:LYS:HG2	1:455:A:ILE:HA	2	0.34	0.05	0.34
(1,3091)	1:424:A:LYS:HG3	1:455:A:ILE:HA	2	0.34	0.05	0.34
(1,3254)	1:433:A:ILE:HA	1:484:A:SER:H	2	0.34	0.05	0.34
(1,1003)	1:288:A:MET:HG2	1:381:A:VAL:HG21	2	0.34	0.06	0.34
(1,1003)	1:288:A:MET:HG2	1:381:A:VAL:HG22	2	0.34	0.06	0.34
(1,1003)	1:288:A:MET:HG2	1:381:A:VAL:HG23	2	0.34	0.06	0.34
(1,1003)	1:288:A:MET:HG3	1:381:A:VAL:HG21	2	0.34	0.06	0.34
(1,1003)	1:288:A:MET:HG3	1:381:A:VAL:HG22	2	0.34	0.06	0.34
(1,1003)	1:288:A:MET:HG3	1:381:A:VAL:HG23	2	0.34	0.06	0.34
(1,1008)	1:288:A:MET:HE1	1:320:A:PHE:HB2	2	0.34	0.05	0.34
(1,1008)	1:288:A:MET:HE1	1:320:A:PHE:HB3	2	0.34	0.05	0.34
(1,1008)	1:288:A:MET:HE2	1:320:A:PHE:HB2	2	0.34	0.05	0.34
(1,1008)	1:288:A:MET:HE2	1:320:A:PHE:HB3	2	0.34	0.05	0.34
(1,1008)	1:288:A:MET:HE3	1:320:A:PHE:HB2	2	0.34	0.05	0.34
(1,1008)	1:288:A:MET:HE3	1:320:A:PHE:HB3	2	0.34	0.05	0.34
(1,2737)	1:401:A:ARG:HD2	1:414:A:VAL:HA	2	0.34	0.14	0.34
(1,2737)	1:401:A:ARG:HD3	1:414:A:VAL:HA	2	0.34	0.14	0.34
(1,3000)	1:418:A:ASP:HA	1:421:A:SER:HB2	2	0.34	0.02	0.34
(1,3000)	1:418:A:ASP:HA	1:421:A:SER:HB3	2	0.34	0.02	0.34
(1,961)	1:285:A:PRO:HG2	1:294:A:LYS:HB2	2	0.33	0.2	0.33
(1,961)	1:285:A:PRO:HG2	1:294:A:LYS:HB3	2	0.33	0.2	0.33
(1,961)	1:285:A:PRO:HG3	1:294:A:LYS:HB2	2	0.33	0.2	0.33
(1,961)	1:285:A:PRO:HG3	1:294:A:LYS:HB3	2	0.33	0.2	0.33
(1,3477)	1:446:A:HIS:HD2	1:490:A:LEU:HD11	2	0.33	0.17	0.33
(1,3477)	1:446:A:HIS:HD2	1:490:A:LEU:HD12	2	0.33	0.17	0.33
(1,3477)	1:446:A:HIS:HD2	1:490:A:LEU:HD13	2	0.33	0.17	0.33
(1,3530)	1:449:A:LEU:HD11	1:494:A:ALA:HA	2	0.33	0.18	0.33
(1,3530)	1:449:A:LEU:HD12	1:494:A:ALA:HA	2	0.33	0.18	0.33
(1,3530)	1:449:A:LEU:HD13	1:494:A:ALA:HA	2	0.33	0.18	0.33
(1,3530)	1:449:A:LEU:HD21	1:494:A:ALA:HA	2	0.33	0.18	0.33
(1,3530)	1:449:A:LEU:HD22	1:494:A:ALA:HA	2	0.33	0.18	0.33
(1,3530)	1:449:A:LEU:HD23	1:494:A:ALA:HA	2	0.33	0.18	0.33
(1,2336)	1:375:A:TRP:HZ2	1:468:A:MET:HE1	2	0.33	0.03	0.33
(1,2336)	1:375:A:TRP:HZ2	1:468:A:MET:HE2	2	0.33	0.03	0.33
(1,2336)	1:375:A:TRP:HZ2	1:468:A:MET:HE3	2	0.33	0.03	0.33
(1,3389)	1:438:A:TYR:HE1	1:442:A:LYS:HD2	2	0.32	0.01	0.32
(1,3389)	1:438:A:TYR:HE1	1:442:A:LYS:HD3	2	0.32	0.01	0.32
(1,3389)	1:438:A:TYR:HE2	1:442:A:LYS:HD2	2	0.32	0.01	0.32
(1,3389)	1:438:A:TYR:HE2	1:442:A:LYS:HD3	2	0.32	0.01	0.32
(1,1493)	1:314:A:MET:HB2	1:316:A:ASN:HA	2	0.32	0.04	0.32
(1,1493)	1:314:A:MET:HB3	1:316:A:ASN:HA	2	0.32	0.04	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,693)	1:272:A:GLN:HB2	1:274:A:TYR:H	2	0.32	0.0	0.32
(1,693)	1:272:A:GLN:HB3	1:274:A:TYR:H	2	0.32	0.0	0.32
(1,2620)	1:393:A:GLN:HE21	1:474:A:GLU:HB2	2	0.32	0.03	0.32
(1,2620)	1:393:A:GLN:HE21	1:474:A:GLU:HB3	2	0.32	0.03	0.32
(1,2620)	1:393:A:GLN:HE22	1:474:A:GLU:HB2	2	0.32	0.03	0.32
(1,2620)	1:393:A:GLN:HE22	1:474:A:GLU:HB3	2	0.32	0.03	0.32
(1,473)	1:260:A:PRO:HA	1:281:A:PRO:HA	2	0.32	0.12	0.32
(1,963)	1:285:A:PRO:HG2	1:288:A:MET:H	2	0.32	0.12	0.32
(1,963)	1:285:A:PRO:HG3	1:288:A:MET:H	2	0.32	0.12	0.32
(1,1871)	1:345:A:THR:HA	1:349:A:ARG:H	2	0.32	0.12	0.32
(1,2642)	1:394:A:GLU:HA	1:398:A:LYS:H	2	0.32	0.08	0.32
(1,2696)	1:398:A:LYS:HA	1:475:A:PHE:HE1	2	0.32	0.16	0.32
(1,2696)	1:398:A:LYS:HA	1:475:A:PHE:HE2	2	0.32	0.16	0.32
(1,3095)	1:424:A:LYS:H	1:427:A:GLN:H	2	0.32	0.08	0.32
(1,1373)	1:307:A:MET:HE1	1:335:A:SER:H	2	0.31	0.12	0.31
(1,1373)	1:307:A:MET:HE2	1:335:A:SER:H	2	0.31	0.12	0.31
(1,1373)	1:307:A:MET:HE3	1:335:A:SER:H	2	0.31	0.12	0.31
(1,1701)	1:329:A:ASP:HB2	1:344:A:VAL:HG21	2	0.3	0.08	0.3
(1,1701)	1:329:A:ASP:HB2	1:344:A:VAL:HG22	2	0.3	0.08	0.3
(1,1701)	1:329:A:ASP:HB2	1:344:A:VAL:HG23	2	0.3	0.08	0.3
(1,1701)	1:329:A:ASP:HB3	1:344:A:VAL:HG21	2	0.3	0.08	0.3
(1,1701)	1:329:A:ASP:HB3	1:344:A:VAL:HG22	2	0.3	0.08	0.3
(1,1701)	1:329:A:ASP:HB3	1:344:A:VAL:HG23	2	0.3	0.08	0.3
(1,3523)	1:448:A:GLU:HA	1:451:A:ARG:HB2	2	0.3	0.02	0.3
(1,3523)	1:448:A:GLU:HA	1:451:A:ARG:HB3	2	0.3	0.02	0.3
(1,970)	1:285:A:PRO:HG2	1:287:A:ASP:H	2	0.3	0.03	0.3
(1,970)	1:285:A:PRO:HG3	1:287:A:ASP:H	2	0.3	0.03	0.3
(1,1445)	1:313:A:PHE:HA	1:349:A:ARG:H	2	0.3	0.07	0.3
(1,1506)	1:315:A:PRO:HA	1:349:A:ARG:HD2	2	0.3	0.16	0.3
(1,1506)	1:315:A:PRO:HA	1:349:A:ARG:HD3	2	0.3	0.16	0.3
(1,1816)	1:339:A:LEU:HA	1:342:A:SER:H	2	0.3	0.12	0.3
(1,2797)	1:403:A:ALA:HA	1:412:A:GLN:HA	2	0.29	0.02	0.29
(1,2910)	1:410:A:SER:HA	1:459:A:LEU:HD11	2	0.29	0.15	0.29
(1,2910)	1:410:A:SER:HA	1:459:A:LEU:HD12	2	0.29	0.15	0.29
(1,2910)	1:410:A:SER:HA	1:459:A:LEU:HD13	2	0.29	0.15	0.29
(1,3605)	1:453:A:LYS:HG2	1:455:A:ILE:HD11	2	0.29	0.07	0.29
(1,3605)	1:453:A:LYS:HG2	1:455:A:ILE:HD12	2	0.29	0.07	0.29
(1,3605)	1:453:A:LYS:HG2	1:455:A:ILE:HD13	2	0.29	0.07	0.29
(1,3605)	1:453:A:LYS:HG3	1:455:A:ILE:HD11	2	0.29	0.07	0.29
(1,3605)	1:453:A:LYS:HG3	1:455:A:ILE:HD12	2	0.29	0.07	0.29
(1,3605)	1:453:A:LYS:HG3	1:455:A:ILE:HD13	2	0.29	0.07	0.29
(1,408)	1:253:A:ILE:HB	1:298:A:LYS:H	2	0.29	0.06	0.29

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2838)	1:405:A:THR:H	1:459:A:LEU:H	2	0.29	0.0	0.29
(1,3700)	1:465:A:ASP:HA	1:468:A:MET:H	2	0.29	0.08	0.29
(1,3942)	1:490:A:LEU:H	1:492:A:LYS:H	2	0.29	0.18	0.29
(1,222)	1:244:A:GLU:H	1:247:A:LYS:H	2	0.28	0.18	0.28
(1,2810)	1:404:A:SER:HA	1:459:A:LEU:HD11	2	0.28	0.08	0.28
(1,2810)	1:404:A:SER:HA	1:459:A:LEU:HD12	2	0.28	0.08	0.28
(1,2810)	1:404:A:SER:HA	1:459:A:LEU:HD13	2	0.28	0.08	0.28
(1,3099)	1:424:A:LYS:HG2	1:427:A:GLN:HE21	2	0.28	0.08	0.28
(1,3099)	1:424:A:LYS:HG2	1:427:A:GLN:HE22	2	0.28	0.08	0.28
(1,3099)	1:424:A:LYS:HG3	1:427:A:GLN:HE21	2	0.28	0.08	0.28
(1,3099)	1:424:A:LYS:HG3	1:427:A:GLN:HE22	2	0.28	0.08	0.28
(1,3788)	1:474:A:GLU:HA	1:479:A:PRO:HA	2	0.28	0.03	0.28
(1,2314)	1:374:A:PHE:HZ	1:399:A:LEU:HD11	2	0.28	0.13	0.28
(1,2314)	1:374:A:PHE:HZ	1:399:A:LEU:HD12	2	0.28	0.13	0.28
(1,2314)	1:374:A:PHE:HZ	1:399:A:LEU:HD13	2	0.28	0.13	0.28
(1,1958)	1:352:A:LEU:HA	1:356:A:VAL:H	2	0.28	0.12	0.28
(1,2825)	1:404:A:SER:H	1:414:A:VAL:HG11	2	0.28	0.08	0.28
(1,2825)	1:404:A:SER:H	1:414:A:VAL:HG12	2	0.28	0.08	0.28
(1,2825)	1:404:A:SER:H	1:414:A:VAL:HG13	2	0.28	0.08	0.28
(1,1419)	1:312:A:GLN:HB2	1:345:A:THR:HG21	2	0.27	0.11	0.27
(1,1419)	1:312:A:GLN:HB2	1:345:A:THR:HG22	2	0.27	0.11	0.27
(1,1419)	1:312:A:GLN:HB2	1:345:A:THR:HG23	2	0.27	0.11	0.27
(1,1419)	1:312:A:GLN:HB3	1:345:A:THR:HG21	2	0.27	0.11	0.27
(1,1419)	1:312:A:GLN:HB3	1:345:A:THR:HG22	2	0.27	0.11	0.27
(1,1419)	1:312:A:GLN:HB3	1:345:A:THR:HG23	2	0.27	0.11	0.27
(1,423)	1:254:A:ALA:HA	1:323:A:GLY:H	2	0.26	0.01	0.26
(1,685)	1:272:A:GLN:HE21	1:351:A:ALA:HB1	2	0.26	0.12	0.26
(1,685)	1:272:A:GLN:HE21	1:351:A:ALA:HB2	2	0.26	0.12	0.26
(1,685)	1:272:A:GLN:HE21	1:351:A:ALA:HB3	2	0.26	0.12	0.26
(1,685)	1:272:A:GLN:HE22	1:351:A:ALA:HB1	2	0.26	0.12	0.26
(1,685)	1:272:A:GLN:HE22	1:351:A:ALA:HB2	2	0.26	0.12	0.26
(1,685)	1:272:A:GLN:HE22	1:351:A:ALA:HB3	2	0.26	0.12	0.26
(1,2132)	1:361:A:GLU:HA	1:371:A:TYR:HE1	2	0.26	0.06	0.26
(1,2862)	1:405:A:THR:HG21	1:408:A:ASP:HA	2	0.26	0.08	0.26
(1,2862)	1:405:A:THR:HG22	1:408:A:ASP:HA	2	0.26	0.08	0.26
(1,2862)	1:405:A:THR:HG23	1:408:A:ASP:HA	2	0.26	0.08	0.26
(1,3351)	1:436:A:ASP:HA	1:463:A:ARG:HA	2	0.26	0.04	0.26
(1,3917)	1:488:A:GLU:HA	1:491:A:GLU:H	2	0.26	0.16	0.26
(1,690)	1:272:A:GLN:HG2	1:344:A:VAL:HG11	2	0.26	0.13	0.26
(1,690)	1:272:A:GLN:HG2	1:344:A:VAL:HG12	2	0.26	0.13	0.26
(1,690)	1:272:A:GLN:HG2	1:344:A:VAL:HG13	2	0.26	0.13	0.26
(1,690)	1:272:A:GLN:HG3	1:344:A:VAL:HG11	2	0.26	0.13	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,690)	1:272:A:GLN:HG3	1:344:A:VAL:HG12	2	0.26	0.13	0.26
(1,690)	1:272:A:GLN:HG3	1:344:A:VAL:HG13	2	0.26	0.13	0.26
(1,1154)	1:298:A:LYS:HB2	1:324:A:LEU:HB2	2	0.26	0.02	0.26
(1,1154)	1:298:A:LYS:HB2	1:324:A:LEU:HB3	2	0.26	0.02	0.26
(1,1154)	1:298:A:LYS:HB3	1:324:A:LEU:HB2	2	0.26	0.02	0.26
(1,1154)	1:298:A:LYS:HB3	1:324:A:LEU:HB3	2	0.26	0.02	0.26
(1,3478)	1:446:A:HIS:HD2	1:486:A:VAL:HG21	2	0.26	0.1	0.26
(1,3478)	1:446:A:HIS:HD2	1:486:A:VAL:HG22	2	0.26	0.1	0.26
(1,3478)	1:446:A:HIS:HD2	1:486:A:VAL:HG23	2	0.26	0.1	0.26
(1,130)	1:237:A:ASN:HA	1:265:A:HIS:HE1	2	0.25	0.01	0.25
(1,2365)	1:375:A:TRP:HA	1:379:A:GLY:H	2	0.25	0.06	0.25
(1,707)	1:273:A:GLU:H	1:327:A:SER:HA	2	0.24	0.08	0.24
(1,1215)	1:299:A:LEU:H	1:307:A:MET:H	2	0.24	0.12	0.24
(1,2360)	1:375:A:TRP:HZ2	1:383:A:LYS:HG2	2	0.24	0.15	0.24
(1,2360)	1:375:A:TRP:HZ2	1:383:A:LYS:HG3	2	0.24	0.15	0.24
(1,3915)	1:488:A:GLU:HA	1:492:A:LYS:H	2	0.24	0.05	0.24
(1,958)	1:285:A:PRO:HG2	1:320:A:PHE:HA	2	0.24	0.04	0.24
(1,958)	1:285:A:PRO:HG3	1:320:A:PHE:HA	2	0.24	0.04	0.24
(1,2323)	1:374:A:PHE:HZ	1:378:A:PHE:HB2	2	0.24	0.04	0.24
(1,2323)	1:374:A:PHE:HZ	1:378:A:PHE:HB3	2	0.24	0.04	0.24
(1,1132)	1:297:A:LEU:H	1:310:A:ALA:H	2	0.24	0.07	0.24
(1,2811)	1:404:A:SER:HB2	1:458:A:LEU:H	2	0.24	0.11	0.24
(1,2811)	1:404:A:SER:HB3	1:458:A:LEU:H	2	0.24	0.11	0.24
(1,3078)	1:423:A:MET:HE1	1:428:A:GLU:H	2	0.24	0.11	0.24
(1,3078)	1:423:A:MET:HE2	1:428:A:GLU:H	2	0.24	0.11	0.24
(1,3078)	1:423:A:MET:HE3	1:428:A:GLU:H	2	0.24	0.11	0.24
(1,914)	1:282:A:SER:H	1:378:A:PHE:HZ	2	0.24	0.0	0.24
(1,2893)	1:408:A:ASP:HB2	1:442:A:LYS:HE2	2	0.24	0.13	0.24
(1,2893)	1:408:A:ASP:HB2	1:442:A:LYS:HE3	2	0.24	0.13	0.24
(1,2893)	1:408:A:ASP:HB3	1:442:A:LYS:HE2	2	0.24	0.13	0.24
(1,2893)	1:408:A:ASP:HB3	1:442:A:LYS:HE3	2	0.24	0.13	0.24
(1,112)	1:235:A:THR:HA	1:265:A:HIS:HE1	2	0.23	0.11	0.23
(1,2793)	1:403:A:ALA:H	1:413:A:THR:H	2	0.23	0.05	0.23
(1,23)	1:232:A:ALA:HB1	1:235:A:THR:HB	2	0.23	0.08	0.23
(1,23)	1:232:A:ALA:HB2	1:235:A:THR:HB	2	0.23	0.08	0.23
(1,23)	1:232:A:ALA:HB3	1:235:A:THR:HB	2	0.23	0.08	0.23
(1,3365)	1:437:A:SER:H	1:441:A:ALA:H	2	0.23	0.07	0.23
(1,2593)	1:390:A:PHE:HA	1:393:A:GLN:H	2	0.22	0.08	0.22
(1,675)	1:270:A:GLY:H	1:272:A:GLN:H	2	0.22	0.08	0.22
(1,2781)	1:403:A:ALA:H	1:459:A:LEU:H	2	0.22	0.02	0.22
(1,2640)	1:394:A:GLU:HA	1:475:A:PHE:HA	2	0.22	0.06	0.22
(1,723)	1:274:A:TYR:H	1:328:A:SER:H	2	0.22	0.08	0.22

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Key	Atom-1	Atom-2	Models^1	Mean (Å)	SD^1 (Å)	Median (Å)
(1,3255)	1:433:A:ILE:HB	1:484:A:SER:H	2	0.22	0.01	0.22
(1,701)	1:273:A:GLU:H	1:329:A:ASP:HA	2	0.21	0.05	0.21
(1,3570)	1:450:A:LEU:HA	1:453:A:LYS:H	2	0.21	0.01	0.21
(1,84)	1:234:A:TRP:HD1	1:275:A:THR:HB	2	0.21	0.03	0.21
(1,1130)	1:297:A:LEU:H	1:311:A:GLU:HA	2	0.21	0.09	0.21
(1,2358)	1:375:A:TRP:HZ2	1:383:A:LYS:HE2	2	0.2	0.1	0.2
(1,2358)	1:375:A:TRP:HZ2	1:383:A:LYS:HE3	2	0.2	0.1	0.2
(1,2808)	1:404:A:SER:HB2	1:459:A:LEU:H	2	0.2	0.05	0.2
(1,2808)	1:404:A:SER:HB3	1:459:A:LEU:H	2	0.2	0.05	0.2
(1,2945)	1:415:A:SER:H	1:419:A:TYR:H	2	0.2	0.1	0.2
(1,653)	1:268:A:VAL:HB	1:273:A:GLU:HA	2	0.2	0.09	0.2
(1,877)	1:280:A:ILE:HA	1:322:A:ARG:H	2	0.2	0.02	0.2
(1,1883)	1:345:A:THR:HB	1:346:A:ARG:HB2	2	0.2	0.01	0.2
(1,1883)	1:345:A:THR:HB	1:346:A:ARG:HB3	2	0.2	0.01	0.2
(1,2199)	1:365:A:LYS:HA	1:368:A:ALA:H	2	0.2	0.02	0.2
(1,2448)	1:381:A:VAL:HA	1:384:A:GLU:H	2	0.19	0.04	0.19
(1,3364)	1:437:A:SER:HA	1:461:A:SER:HB2	2	0.19	0.04	0.19
(1,3364)	1:437:A:SER:HA	1:461:A:SER:HB3	2	0.19	0.04	0.19
(1,2831)	1:404:A:SER:H	1:406:A:HIS:H	2	0.18	0.02	0.18
(1,876)	1:280:A:ILE:H	1:322:A:ARG:H	2	0.18	0.01	0.18
(1,1197)	1:299:A:LEU:HA	1:325:A:ILE:H	2	0.18	0.01	0.18
(1,1278)	1:301:A:VAL:HG11	1:332:A:LEU:HD11	2	0.18	0.01	0.18
(1,1278)	1:301:A:VAL:HG11	1:332:A:LEU:HD12	2	0.18	0.01	0.18
(1,1278)	1:301:A:VAL:HG11	1:332:A:LEU:HD13	2	0.18	0.01	0.18
(1,1278)	1:301:A:VAL:HG12	1:332:A:LEU:HD11	2	0.18	0.01	0.18
(1,1278)	1:301:A:VAL:HG12	1:332:A:LEU:HD12	2	0.18	0.01	0.18
(1,1278)	1:301:A:VAL:HG12	1:332:A:LEU:HD13	2	0.18	0.01	0.18
(1,1278)	1:301:A:VAL:HG13	1:332:A:LEU:HD11	2	0.18	0.01	0.18
(1,1278)	1:301:A:VAL:HG13	1:332:A:LEU:HD12	2	0.18	0.01	0.18
(1,1278)	1:301:A:VAL:HG13	1:332:A:LEU:HD13	2	0.18	0.01	0.18
(1,752)	1:275:A:THR:HG21	1:324:A:LEU:HD21	2	0.18	0.06	0.18
(1,752)	1:275:A:THR:HG21	1:324:A:LEU:HD22	2	0.18	0.06	0.18
(1,752)	1:275:A:THR:HG21	1:324:A:LEU:HD23	2	0.18	0.06	0.18
(1,752)	1:275:A:THR:HG22	1:324:A:LEU:HD21	2	0.18	0.06	0.18
(1,752)	1:275:A:THR:HG22	1:324:A:LEU:HD22	2	0.18	0.06	0.18
(1,752)	1:275:A:THR:HG22	1:324:A:LEU:HD23	2	0.18	0.06	0.18
(1,752)	1:275:A:THR:HG23	1:324:A:LEU:HD21	2	0.18	0.06	0.18
(1,752)	1:275:A:THR:HG23	1:324:A:LEU:HD22	2	0.18	0.06	0.18
(1,752)	1:275:A:THR:HG23	1:324:A:LEU:HD23	2	0.18	0.06	0.18
(1,1791)	1:337:A:GLU:H	1:340:A:GLN:H	2	0.18	0.03	0.18
(1,2260)	1:371:A:TYR:HE1	1:399:A:LEU:HA	2	0.18	0.06	0.18
(1,2260)	1:371:A:TYR:HE2	1:399:A:LEU:HA	2	0.18	0.06	0.18

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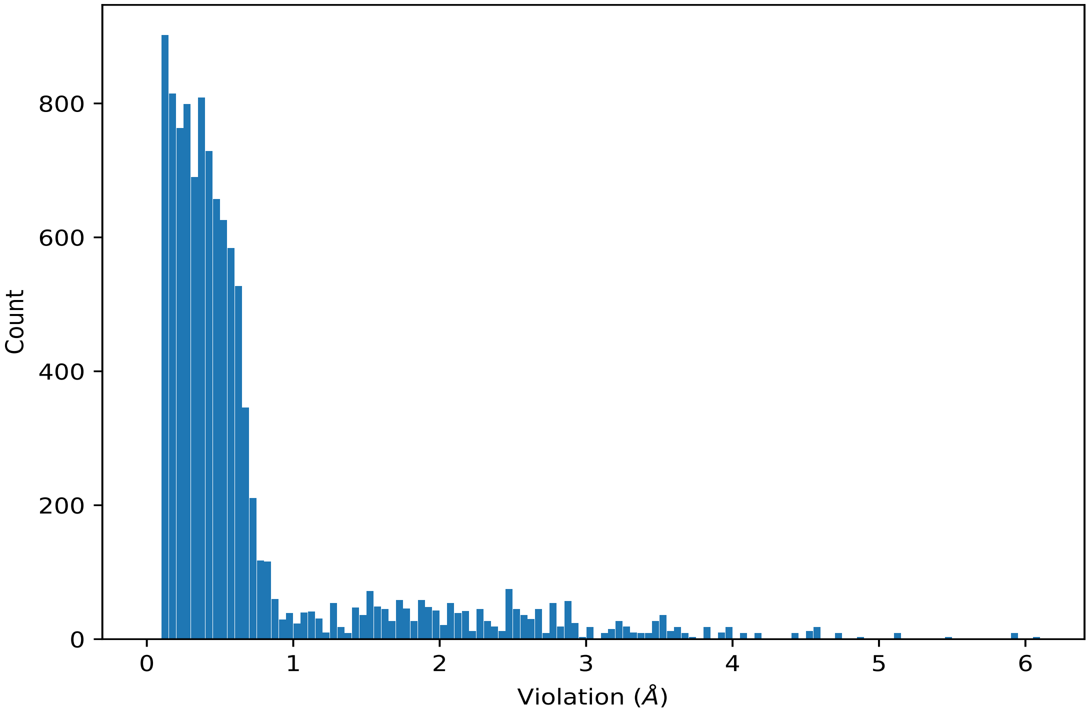
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2433)	1:380:A:LEU:H	1:383:A:LYS:H	2	0.18	0.03	0.18
(1,3777)	1:473:A:THR:HB	1:480:A:PHE:H	2	0.18	0.08	0.18
(1,282)	1:247:A:LYS:HA	1:250:A:TYR:H	2	0.17	0.06	0.17
(1,2807)	1:404:A:SER:HA	1:459:A:LEU:H	2	0.17	0.06	0.17
(1,3238)	1:432:A:TYR:HB2	1:460:A:LEU:H	2	0.17	0.06	0.17
(1,3238)	1:432:A:TYR:HB3	1:460:A:LEU:H	2	0.17	0.06	0.17
(1,3688)	1:464:A:ILE:HD11	1:467:A:TRP:HE3	2	0.17	0.06	0.17
(1,3688)	1:464:A:ILE:HD12	1:467:A:TRP:HE3	2	0.17	0.06	0.17
(1,3688)	1:464:A:ILE:HD13	1:467:A:TRP:HE3	2	0.17	0.06	0.17
(1,1479)	1:314:A:MET:H	1:349:A:ARG:HD2	2	0.17	0.07	0.17
(1,1479)	1:314:A:MET:H	1:349:A:ARG:HD3	2	0.17	0.07	0.17
(1,3858)	1:482:A:SER:H	1:485:A:LYS:H	2	0.17	0.04	0.17
(1,1827)	1:340:A:GLN:HA	1:342:A:SER:H	2	0.16	0.04	0.16
(1,52)	1:233:A:LEU:HA	1:235:A:THR:H	2	0.15	0.04	0.15
(1,740)	1:275:A:THR:H	1:328:A:SER:H	2	0.15	0.04	0.15
(1,2340)	1:375:A:TRP:HD1	1:412:A:GLN:HE21	2	0.15	0.0	0.15
(1,2340)	1:375:A:TRP:HD1	1:412:A:GLN:HE22	2	0.15	0.0	0.15
(1,1610)	1:319:A:ARG:HA	1:321:A:VAL:HB	2	0.15	0.04	0.15
(1,2544)	1:386:A:PRO:HG2	1:397:A:ALA:H	2	0.14	0.02	0.14
(1,2544)	1:386:A:PRO:HG3	1:397:A:ALA:H	2	0.14	0.02	0.14
(1,2739)	1:401:A:ARG:HD2	1:413:A:THR:HA	2	0.14	0.03	0.14
(1,2739)	1:401:A:ARG:HD3	1:413:A:THR:HA	2	0.14	0.03	0.14
(1,2816)	1:404:A:SER:HA	1:457:A:VAL:HB	2	0.14	0.02	0.14
(1,2961)	1:416:A:LEU:HB2	1:475:A:PHE:HZ	2	0.13	0.02	0.13
(1,2961)	1:416:A:LEU:HB3	1:475:A:PHE:HZ	2	0.13	0.02	0.13
(1,3171)	1:430:A:ILE:HA	1:481:A:GLN:H	2	0.13	0.01	0.13
(1,3742)	1:469:A:MET:HE1	1:473:A:THR:HA	2	0.13	0.02	0.13
(1,3742)	1:469:A:MET:HE2	1:473:A:THR:HA	2	0.13	0.02	0.13
(1,3742)	1:469:A:MET:HE3	1:473:A:THR:HA	2	0.13	0.02	0.13
(1,24)	1:232:A:ALA:H	1:235:A:THR:HG21	2	0.12	0.02	0.12
(1,24)	1:232:A:ALA:H	1:235:A:THR:HG22	2	0.12	0.02	0.12
(1,24)	1:232:A:ALA:H	1:235:A:THR:HG23	2	0.12	0.02	0.12
(1,3563)	1:450:A:LEU:HA	1:455:A:ILE:H	2	0.12	0.02	0.12
(1,3622)	1:456:A:GLU:HG2	1:457:A:VAL:H	2	0.12	0.01	0.12
(1,3622)	1:456:A:GLU:HG3	1:457:A:VAL:H	2	0.12	0.01	0.12
(1,1277)	1:301:A:VAL:HB	1:332:A:LEU:HD11	2	0.12	0.01	0.12
(1,1277)	1:301:A:VAL:HB	1:332:A:LEU:HD12	2	0.12	0.01	0.12
(1,1277)	1:301:A:VAL:HB	1:332:A:LEU:HD13	2	0.12	0.01	0.12
(1,1788)	1:337:A:GLU:HA	1:341:A:ASP:H	2	0.12	0.01	0.12
(1,3405)	1:439:A:ALA:HA	1:442:A:LYS:HB2	2	0.12	0.01	0.12
(1,3405)	1:439:A:ALA:HA	1:442:A:LYS:HB3	2	0.12	0.01	0.12
(1,452)	1:257:A:PHE:H	1:258:A:ASN:H	2	0.12	0.0	0.12

^{1}Number of violated models, ^{2}Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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 ⓘ

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)
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	2	6.06
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	2	6.06
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	2	6.06
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	5	5.92
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	5	5.92
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	5	5.92
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	5	5.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	5	5.92
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	5	5.92
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	5	5.92
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	5	5.92
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	5	5.92
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG11	5	5.46
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG12	5	5.46
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG13	5	5.46
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	9	5.13
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	9	5.13
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	9	5.13
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	9	5.13
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	9	5.13
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	9	5.13
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	9	5.13
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	9	5.13
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	9	5.13
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG11	9	4.88
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG12	9	4.88
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG13	9	4.88
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	9	4.7
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	9	4.7
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	9	4.7
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	9	4.7
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	9	4.7
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	9	4.7
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	9	4.7
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	9	4.7
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	9	4.7
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	7	4.59
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	7	4.59
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	7	4.59
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	7	4.59
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	7	4.59
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	7	4.59
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	7	4.59
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	7	4.59
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	7	4.59
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	5	4.57
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	5	4.57
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	5	4.57
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	5	4.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	5	4.57
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	5	4.57
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	5	4.57
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	5	4.57
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	5	4.57
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	15	4.54
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	15	4.54
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	15	4.54
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	10	4.51
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	10	4.51
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	10	4.51
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	10	4.51
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	10	4.51
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	10	4.51
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	10	4.51
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	10	4.51
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	10	4.51
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	14	4.41
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	14	4.41
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	14	4.41
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	14	4.41
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	14	4.41
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	14	4.41
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	14	4.41
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	14	4.41
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	14	4.41
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	20	4.18
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	20	4.18
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	20	4.18
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	20	4.18
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	20	4.18
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	20	4.18
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	20	4.18
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	20	4.18
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	20	4.18
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	8	4.07
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	8	4.07
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	8	4.07
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	8	4.07
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	8	4.07
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	8	4.07
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	8	4.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	8	4.07
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	8	4.07
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	9	3.99
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	9	3.99
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	9	3.99
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	9	3.99
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	9	3.99
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	9	3.99
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	9	3.99
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	9	3.99
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	9	3.99
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	16	3.98
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	16	3.98
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	16	3.98
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	16	3.98
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	16	3.98
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	16	3.98
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	16	3.98
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	16	3.98
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	16	3.98
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	8	3.93
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	8	3.92
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	8	3.92
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	8	3.92
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	8	3.92
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	8	3.92
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	8	3.92
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	8	3.92
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	8	3.92
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	8	3.92
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	4	3.84
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	4	3.84
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	4	3.84
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	4	3.84
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	4	3.84
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	4	3.84
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	4	3.84
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	4	3.84
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	4	3.84
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	15	3.83
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	15	3.83
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	15	3.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	15	3.83
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	15	3.83
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	15	3.83
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	15	3.83
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	15	3.83
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	15	3.83
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	18	3.71
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	18	3.71
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	18	3.71
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	8	3.65
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	8	3.65
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	8	3.65
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	8	3.65
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	8	3.65
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	8	3.65
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	8	3.65
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	8	3.65
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	8	3.65
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	12	3.64
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	12	3.64
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	12	3.64
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	12	3.64
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	12	3.64
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	12	3.64
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	12	3.64
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	12	3.64
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	12	3.64
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	18	3.6
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	18	3.6
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	18	3.6
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	18	3.6
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	18	3.6
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	18	3.6
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	18	3.6
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	18	3.6
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	18	3.6
(1,3972)	1:318:A:LEU:HD11	2:622:B:TYR:HE1	2	3.57
(1,3972)	1:318:A:LEU:HD12	2:622:B:TYR:HE1	2	3.57
(1,3972)	1:318:A:LEU:HD13	2:622:B:TYR:HE1	2	3.57
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	3	3.55
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	3	3.55
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	3	3.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	3	3.55
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	3	3.55
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	3	3.55
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	3	3.55
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	3	3.55
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	3	3.55
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	11	3.54
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	11	3.54
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	11	3.54
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	11	3.54
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	11	3.54
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	11	3.54
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	11	3.54
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	11	3.54
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	11	3.54
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	7	3.52
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	7	3.52
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	7	3.52
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	7	3.52
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	7	3.52
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	7	3.52
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	7	3.52
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	7	3.52
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	7	3.52
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	9	3.51
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	9	3.51
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	9	3.51
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	9	3.51
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	9	3.51
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	9	3.51
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	9	3.51
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	9	3.51
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	9	3.51
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	10	3.51
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	10	3.51
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	10	3.51
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	10	3.51
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	10	3.51
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	10	3.51
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	10	3.51
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	10	3.51
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	10	3.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	4	3.49
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	4	3.49
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	4	3.49
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	4	3.49
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	4	3.49
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	4	3.49
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	4	3.49
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	4	3.49
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	4	3.49
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	20	3.46
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	20	3.46
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	20	3.46
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	20	3.46
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	20	3.46
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	20	3.46
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	20	3.46
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	20	3.46
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	20	3.46
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG11	12	3.45
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG12	12	3.45
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG13	12	3.45
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG11	12	3.45
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG12	12	3.45
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG13	12	3.45
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG11	12	3.45
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG12	12	3.45
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG13	12	3.45
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	11	3.44
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	11	3.44
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	11	3.44
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	11	3.44
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	11	3.44
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	11	3.44
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	11	3.44
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	11	3.44
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	11	3.44
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	17	3.36
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	17	3.36
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	17	3.36
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	17	3.36
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	17	3.36
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	17	3.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	17	3.36
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	17	3.36
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	17	3.36
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	18	3.32
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG11	6	3.3
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG12	6	3.3
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG13	6	3.3
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG11	6	3.3
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG12	6	3.3
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG13	6	3.3
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG11	6	3.3
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG12	6	3.3
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG13	6	3.3
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	10	3.29
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	5	3.26
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	5	3.26
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	5	3.26
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	5	3.26
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	5	3.26
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	5	3.26
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	5	3.26
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	5	3.26
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	5	3.26
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	11	3.25
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	11	3.25
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	11	3.25
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	11	3.25
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	11	3.25
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	11	3.25
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	11	3.25
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	11	3.25
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	11	3.25
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB1	11	3.23
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB2	11	3.23
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB3	11	3.23
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB1	11	3.23
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB2	11	3.23
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB3	11	3.23
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB1	11	3.23
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB2	11	3.23
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB3	11	3.23
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	17	3.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	17	3.21
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	17	3.21
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	17	3.21
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	17	3.21
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	17	3.21
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	17	3.21
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	17	3.21
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	17	3.21
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	13	3.2
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	13	3.2
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	13	3.2
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	13	3.2
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	13	3.2
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	13	3.2
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	13	3.2
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	13	3.2
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	13	3.2
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	6	3.19
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	6	3.19
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	6	3.19
(1,3972)	1:318:A:LEU:HD11	2:622:B:TYR:HE1	17	3.17
(1,3972)	1:318:A:LEU:HD12	2:622:B:TYR:HE1	17	3.17
(1,3972)	1:318:A:LEU:HD13	2:622:B:TYR:HE1	17	3.17
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	5	3.16
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	5	3.16
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	5	3.16
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	5	3.16
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	5	3.16
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	5	3.16
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	5	3.16
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	5	3.16
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	5	3.16
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	5	3.14
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	5	3.14
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	5	3.14
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	5	3.14
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	5	3.14
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	5	3.14
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	5	3.14
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	5	3.14
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	5	3.14
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	12	3.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	12	3.03
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	12	3.03
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	12	3.03
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	12	3.03
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	12	3.03
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	12	3.03
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	12	3.03
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	12	3.03
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	9	3.0
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	9	3.0
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	9	3.0
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	9	3.0
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	9	3.0
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	9	3.0
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	9	3.0
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	9	3.0
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	9	3.0
(1,3972)	1:318:A:LEU:HD11	2:622:B:TYR:HE1	15	2.96
(1,3972)	1:318:A:LEU:HD12	2:622:B:TYR:HE1	15	2.96
(1,3972)	1:318:A:LEU:HD13	2:622:B:TYR:HE1	15	2.96
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	12	2.93
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	12	2.93
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	12	2.93
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	11	2.92
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	11	2.92
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	11	2.92
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	11	2.92
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	11	2.92
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	11	2.92
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	11	2.92
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	11	2.92
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	11	2.92
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG11	15	2.9
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG12	15	2.9
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG13	15	2.9
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	6	2.9
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	6	2.9
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	6	2.9
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	6	2.9
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	6	2.9
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	6	2.9
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	6	2.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	6	2.9
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	6	2.9
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	20	2.89
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	20	2.89
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	20	2.89
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	20	2.89
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	20	2.89
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	20	2.89
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	20	2.89
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	20	2.89
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	20	2.89
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	6	2.88
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	6	2.88
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	6	2.88
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	6	2.88
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	6	2.88
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	6	2.88
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	6	2.88
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	6	2.88
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	6	2.88
(1,3972)	1:318:A:LEU:HD11	2:622:B:TYR:HE1	10	2.88
(1,3972)	1:318:A:LEU:HD12	2:622:B:TYR:HE1	10	2.88
(1,3972)	1:318:A:LEU:HD13	2:622:B:TYR:HE1	10	2.88
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	17	2.88
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	17	2.88
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	17	2.88
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	17	2.88
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	17	2.88
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	17	2.88
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	17	2.88
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	17	2.88
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	17	2.88
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	3	2.88
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	3	2.88
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	3	2.88
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	3	2.88
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	3	2.88
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	3	2.88
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	3	2.88
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	3	2.88
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	3	2.88
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	7	2.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	7	2.86
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	7	2.86
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	7	2.86
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	7	2.86
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	7	2.86
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	7	2.86
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	7	2.86
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	7	2.86
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	15	2.86
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	15	2.86
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	15	2.86
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	15	2.86
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	15	2.86
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	15	2.86
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	15	2.86
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	15	2.86
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	15	2.86
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	4	2.84
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	17	2.83
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	17	2.83
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	17	2.83
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	17	2.83
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	17	2.83
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	17	2.83
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	17	2.83
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	17	2.83
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	17	2.83
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	7	2.82
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	7	2.82
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	7	2.82
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	7	2.82
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	7	2.82
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	7	2.82
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	7	2.82
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	7	2.82
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	7	2.82
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG11	5	2.79
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG12	5	2.79
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG13	5	2.79
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG11	5	2.79
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG12	5	2.79
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG13	5	2.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG11	5	2.79
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG12	5	2.79
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG13	5	2.79
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	6	2.79
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	6	2.79
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	6	2.79
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	6	2.79
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	6	2.79
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	6	2.79
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	6	2.79
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	6	2.79
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	6	2.79
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	1	2.78
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	1	2.78
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	1	2.78
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	1	2.78
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	1	2.78
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	1	2.78
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	1	2.78
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	1	2.78
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	1	2.78
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	20	2.77
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	20	2.77
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	20	2.77
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	20	2.77
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	20	2.77
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	20	2.77
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	20	2.77
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	20	2.77
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	20	2.77
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	15	2.75
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	15	2.75
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	15	2.75
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	15	2.75
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	15	2.75
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	15	2.75
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	15	2.75
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	15	2.75
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	15	2.75
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	11	2.75
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	11	2.75
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	11	2.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	11	2.75
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	11	2.75
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	11	2.75
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	11	2.75
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	11	2.75
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	11	2.75
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	16	2.72
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	16	2.72
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	16	2.72
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	16	2.72
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	16	2.72
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	16	2.72
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	16	2.72
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	16	2.72
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	16	2.72
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	8	2.68
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	8	2.68
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	8	2.68
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	8	2.68
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	8	2.68
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	8	2.68
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	8	2.68
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	8	2.68
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	8	2.68
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	12	2.67
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	12	2.67
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	12	2.67
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	12	2.67
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	12	2.67
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	12	2.67
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	12	2.67
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	12	2.67
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	12	2.67
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	20	2.67
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	20	2.67
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	20	2.67
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	20	2.67
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	20	2.67
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	20	2.67
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	20	2.67
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	20	2.67
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	20	2.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	3	2.66
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	3	2.66
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	3	2.66
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	3	2.66
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	3	2.66
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	3	2.66
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	3	2.66
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	3	2.66
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	3	2.66
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	5	2.65
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	5	2.65
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	5	2.65
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	5	2.65
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	5	2.65
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	5	2.65
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	5	2.65
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	5	2.65
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	5	2.65
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	14	2.64
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	14	2.64
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	14	2.64
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	14	2.64
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	14	2.64
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	14	2.64
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	14	2.64
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	14	2.64
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	14	2.64
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	4	2.64
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	4	2.64
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	4	2.64
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	4	2.64
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	4	2.64
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	4	2.64
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	4	2.64
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	4	2.64
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	4	2.64
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	10	2.64
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	10	2.64
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	10	2.64
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	10	2.61
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	10	2.61
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	10	2.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	10	2.61
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	10	2.61
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	10	2.61
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	10	2.61
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	10	2.61
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	10	2.61
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	14	2.59
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	14	2.59
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	14	2.59
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	14	2.59
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	14	2.59
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	14	2.59
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	14	2.59
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	14	2.59
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	14	2.59
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	19	2.58
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	19	2.58
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	19	2.58
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	19	2.58
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	19	2.58
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	19	2.58
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	19	2.58
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	19	2.58
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	19	2.58
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	17	2.56
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	17	2.56
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	17	2.56
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	17	2.56
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	17	2.56
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	17	2.56
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	17	2.56
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	17	2.56
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	17	2.56
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	7	2.55
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	7	2.55
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	7	2.55
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	7	2.55
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	7	2.55
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	7	2.55
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	7	2.55
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	7	2.55
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	7	2.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG11	18	2.54
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG12	18	2.54
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG13	18	2.54
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG11	18	2.54
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG12	18	2.54
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG13	18	2.54
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG11	18	2.54
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG12	18	2.54
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG13	18	2.54
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG21	18	2.54
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG22	18	2.54
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG23	18	2.54
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG21	18	2.54
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG22	18	2.54
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG23	18	2.54
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG21	18	2.54
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG22	18	2.54
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG23	18	2.54
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	18	2.52
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	18	2.52
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	18	2.52
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	18	2.52
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	18	2.52
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	18	2.52
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	18	2.52
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	18	2.52
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	18	2.52
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	5	2.52
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	5	2.52
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	5	2.52
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	5	2.52
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	5	2.52
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	5	2.52
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	5	2.52
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	5	2.52
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	5	2.52
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	3	2.5
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	3	2.5
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	3	2.5
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	3	2.5
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	3	2.5
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	3	2.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	3	2.5
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	3	2.5
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	3	2.5
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	10	2.49
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	10	2.49
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	10	2.49
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	10	2.49
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	10	2.49
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	10	2.49
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	10	2.49
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	10	2.49
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	10	2.49
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	20	2.49
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	20	2.49
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	20	2.49
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	20	2.49
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	20	2.49
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	20	2.49
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	20	2.49
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	20	2.49
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	20	2.49
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	15	2.48
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	15	2.48
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	15	2.48
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	15	2.48
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	15	2.48
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	15	2.48
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	15	2.48
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	15	2.48
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	15	2.48
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	13	2.47
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	13	2.47
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	13	2.47
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	13	2.47
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	13	2.47
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	13	2.47
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	13	2.47
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	13	2.47
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	13	2.47
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	18	2.47
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	18	2.47
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	18	2.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	18	2.47
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	18	2.47
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	18	2.47
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	18	2.47
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	18	2.47
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	18	2.47
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	6	2.46
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	6	2.46
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	6	2.46
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	6	2.46
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	6	2.46
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	6	2.46
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	6	2.46
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	6	2.46
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	6	2.46
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	5	2.46
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	5	2.46
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	5	2.46
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	5	2.46
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	5	2.46
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	5	2.46
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	5	2.46
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	5	2.46
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	5	2.46
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	10	2.45
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	10	2.45
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	10	2.45
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	10	2.45
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	10	2.45
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	10	2.45
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	10	2.45
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	10	2.45
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	10	2.45
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	16	2.45
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	16	2.45
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	16	2.45
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG11	7	2.43
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG12	7	2.43
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG13	7	2.43
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	15	2.42
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	15	2.42
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	15	2.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	15	2.42
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	15	2.42
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	15	2.42
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	15	2.42
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	15	2.42
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	15	2.42
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	2	2.37
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	17	2.36
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	17	2.36
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	17	2.36
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	17	2.36
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	17	2.36
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	17	2.36
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	17	2.36
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	17	2.36
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	17	2.36
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	11	2.35
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	11	2.35
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	11	2.35
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	11	2.35
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	11	2.35
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	11	2.35
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	11	2.35
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	11	2.35
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	11	2.35
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	19	2.31
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	19	2.31
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	19	2.31
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	19	2.31
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	19	2.31
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	19	2.31
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	19	2.31
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	19	2.31
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	19	2.31
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	8	2.31
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	8	2.31
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	8	2.31
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	8	2.31
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	8	2.31
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	8	2.31
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	8	2.31
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	8	2.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	8	2.31
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	6	2.3
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	6	2.3
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	6	2.3
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	6	2.3
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	6	2.3
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	6	2.3
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	6	2.3
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	6	2.3
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	6	2.3
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	14	2.29
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	14	2.29
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	14	2.29
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	14	2.29
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	14	2.29
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	14	2.29
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	14	2.29
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	14	2.29
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	14	2.29
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	7	2.28
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	7	2.28
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	7	2.28
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	7	2.28
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	7	2.28
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	7	2.28
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	7	2.28
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	7	2.28
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	7	2.28
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	5	2.28
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	5	2.28
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	5	2.28
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	5	2.28
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	5	2.28
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	5	2.28
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	5	2.28
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	5	2.28
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	5	2.28
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	1	2.27
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	1	2.27
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	1	2.27
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	1	2.27
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	1	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	1	2.27
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	1	2.27
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	1	2.27
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	1	2.27
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	6	2.25
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	6	2.25
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	6	2.25
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	6	2.25
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	6	2.25
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	6	2.25
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	6	2.25
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	6	2.25
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	6	2.25
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	7	2.24
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	7	2.24
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	7	2.24
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	7	2.24
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	7	2.24
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	7	2.24
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	7	2.24
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	7	2.24
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	7	2.24
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	8	2.21
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	8	2.21
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	8	2.21
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	1	2.18
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	1	2.18
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	1	2.18
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	1	2.18
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	1	2.18
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	1	2.18
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	1	2.18
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	1	2.18
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	1	2.18
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	17	2.18
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	17	2.18
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	17	2.18
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	17	2.18
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	17	2.18
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	17	2.18
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	17	2.18
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	17	2.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	17	2.18
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	7	2.18
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	7	2.18
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	7	2.18
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	12	2.17
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	12	2.17
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	12	2.17
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	12	2.17
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	12	2.17
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	12	2.17
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	12	2.17
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	12	2.17
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	12	2.17
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	1	2.16
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	1	2.16
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	1	2.16
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	20	2.16
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	20	2.16
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	20	2.16
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	20	2.16
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	20	2.16
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	20	2.16
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	20	2.16
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	20	2.16
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	20	2.16
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	14	2.11
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	14	2.11
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	14	2.11
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	14	2.11
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	14	2.11
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	14	2.11
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	14	2.11
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	14	2.11
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	14	2.11
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	4	2.1
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	4	2.1
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	4	2.1
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	17	2.1
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	17	2.1
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	17	2.1
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	17	2.1
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	17	2.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	17	2.1
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	17	2.1
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	17	2.1
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	17	2.1
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	19	2.1
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	19	2.1
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	19	2.1
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	19	2.1
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	19	2.1
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	19	2.1
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	19	2.1
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	19	2.1
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	19	2.1
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	15	2.1
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	15	2.1
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	15	2.1
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	15	2.1
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	15	2.1
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	15	2.1
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	15	2.1
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	15	2.1
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	15	2.1
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB1	19	2.09
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB2	19	2.09
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB3	19	2.09
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB1	19	2.09
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB2	19	2.09
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB3	19	2.09
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB1	19	2.09
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB2	19	2.09
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB3	19	2.09
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	18	2.08
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	18	2.08
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	18	2.08
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	18	2.08
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	18	2.08
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	18	2.08
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	18	2.08
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	18	2.08
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	18	2.08
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	3	2.07
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	3	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	3	2.07
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	3	2.07
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	3	2.07
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	3	2.07
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	3	2.07
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	3	2.07
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	3	2.07
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	8	2.07
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	8	2.07
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	8	2.07
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	8	2.07
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	8	2.07
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	8	2.07
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	8	2.07
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	8	2.07
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	8	2.07
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	12	2.06
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	12	2.06
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	12	2.06
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	12	2.06
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	12	2.06
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	12	2.06
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	12	2.06
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	12	2.06
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	12	2.06
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	6	2.06
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	6	2.06
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	6	2.06
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	6	2.06
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	6	2.06
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	6	2.06
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	6	2.06
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	6	2.06
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	6	2.06
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	17	2.04
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	17	2.04
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	17	2.04
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	17	2.04
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	17	2.04
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	17	2.04
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	17	2.04
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	17	2.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	17	2.04
(1,3970)	1:357:A:LEU:HD11	2:620:B:LEU:HD21	5	2.04
(1,3970)	1:357:A:LEU:HD11	2:620:B:LEU:HD22	5	2.04
(1,3970)	1:357:A:LEU:HD11	2:620:B:LEU:HD23	5	2.04
(1,3970)	1:357:A:LEU:HD12	2:620:B:LEU:HD21	5	2.04
(1,3970)	1:357:A:LEU:HD12	2:620:B:LEU:HD22	5	2.04
(1,3970)	1:357:A:LEU:HD12	2:620:B:LEU:HD23	5	2.04
(1,3970)	1:357:A:LEU:HD13	2:620:B:LEU:HD21	5	2.04
(1,3970)	1:357:A:LEU:HD13	2:620:B:LEU:HD22	5	2.04
(1,3970)	1:357:A:LEU:HD13	2:620:B:LEU:HD23	5	2.04
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG11	17	2.03
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG12	17	2.03
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG13	17	2.03
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	3	1.99
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	3	1.99
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	3	1.99
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	6	1.99
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	11	1.98
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	11	1.98
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	11	1.98
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	14	1.97
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	14	1.97
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	14	1.97
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	14	1.97
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	14	1.97
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	14	1.97
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	14	1.97
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	14	1.97
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	14	1.97
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	13	1.97
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	13	1.97
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	13	1.97
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	13	1.97
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	13	1.97
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	13	1.97
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	13	1.97
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	13	1.97
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	13	1.97
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	2	1.96
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	2	1.96
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	2	1.96
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	2	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	2	1.96
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	2	1.96
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	2	1.96
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	2	1.96
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	2	1.96
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	20	1.96
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	20	1.96
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	20	1.96
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	20	1.96
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	20	1.96
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	20	1.96
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	20	1.96
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	20	1.96
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	20	1.96
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	2	1.93
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	2	1.93
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	2	1.93
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	2	1.93
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	2	1.93
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	2	1.93
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	2	1.93
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	2	1.93
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	2	1.93
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	16	1.92
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	16	1.92
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	16	1.92
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	16	1.92
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	16	1.92
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	16	1.92
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	16	1.92
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	16	1.92
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	16	1.92
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	4	1.91
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	4	1.91
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	4	1.91
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	4	1.91
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	4	1.91
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	4	1.91
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	4	1.91
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	4	1.91
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	4	1.91
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	2	1.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	2	1.9
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	2	1.9
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	2	1.9
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	2	1.9
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	2	1.9
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	2	1.9
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	2	1.9
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	2	1.9
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	13	1.9
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	13	1.9
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	13	1.9
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	7	1.9
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	7	1.9
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	7	1.9
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	7	1.9
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	7	1.9
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	7	1.9
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	7	1.9
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	7	1.9
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	7	1.9
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	10	1.89
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	10	1.89
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	10	1.89
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	10	1.89
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	10	1.89
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	10	1.89
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	10	1.89
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	10	1.89
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	10	1.89
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	19	1.89
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	19	1.88
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	19	1.88
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	19	1.88
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	19	1.88
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	19	1.88
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	19	1.88
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	19	1.88
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	19	1.88
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	19	1.88
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	17	1.88
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	17	1.88
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	17	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	17	1.88
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	17	1.88
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	17	1.88
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	17	1.88
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	17	1.88
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	17	1.88
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB1	14	1.86
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB2	14	1.86
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB3	14	1.86
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB1	14	1.86
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB2	14	1.86
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB3	14	1.86
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB1	14	1.86
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB2	14	1.86
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB3	14	1.86
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG11	15	1.86
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG12	15	1.86
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG13	15	1.86
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG11	15	1.86
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG12	15	1.86
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG13	15	1.86
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG11	15	1.86
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG12	15	1.86
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG13	15	1.86
(1,3972)	1:318:A:LEU:HD11	2:622:B:TYR:HE1	20	1.86
(1,3972)	1:318:A:LEU:HD12	2:622:B:TYR:HE1	20	1.86
(1,3972)	1:318:A:LEU:HD13	2:622:B:TYR:HE1	20	1.86
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	18	1.85
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	18	1.85
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	18	1.85
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	18	1.85
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	18	1.85
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	18	1.85
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	18	1.85
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	18	1.85
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	18	1.85
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	4	1.84
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	4	1.84
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	4	1.84
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	4	1.84
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	4	1.84
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	4	1.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	4	1.84
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	4	1.84
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	4	1.84
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	15	1.83
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	15	1.83
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	15	1.83
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	15	1.83
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	15	1.83
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	15	1.83
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	15	1.83
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	15	1.83
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	15	1.83
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	3	1.82
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	3	1.82
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	3	1.82
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	3	1.82
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	3	1.82
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	3	1.82
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	3	1.82
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	3	1.82
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	3	1.82
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	2	1.79
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	2	1.79
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	2	1.79
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	2	1.79
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	2	1.79
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	2	1.79
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	2	1.79
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	2	1.79
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	2	1.79
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	1	1.78
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	1	1.78
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	1	1.78
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	1	1.78
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	1	1.78
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	1	1.78
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	1	1.78
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	1	1.78
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	1	1.78
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	15	1.78
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	15	1.78
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	15	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	15	1.78
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	15	1.78
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	15	1.78
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	15	1.78
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	15	1.78
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	15	1.78
(1,3635)	1:458:A:LEU:HD12	1:480:A:PHE:HE1	16	1.78
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG11	11	1.77
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG12	11	1.77
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG13	11	1.77
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG11	11	1.77
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG12	11	1.77
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG13	11	1.77
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG11	11	1.77
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG12	11	1.77
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG13	11	1.77
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG21	11	1.77
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG22	11	1.77
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG23	11	1.77
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG21	11	1.77
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG22	11	1.77
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG23	11	1.77
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG21	11	1.77
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG22	11	1.77
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG23	11	1.77
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	14	1.74
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	14	1.74
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	14	1.74
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	14	1.74
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	14	1.74
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	14	1.74
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	14	1.74
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	14	1.74
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	14	1.74
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	16	1.73
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	16	1.73
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	16	1.73
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	16	1.73
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	16	1.73
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	16	1.73
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	16	1.73
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	16	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	16	1.73
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	19	1.73
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	19	1.73
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	19	1.73
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	19	1.73
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	19	1.73
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	19	1.73
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	19	1.73
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	19	1.73
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	19	1.73
(1,3635)	1:458:A:LEU:HD11	1:480:A:PHE:HD1	3	1.72
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	4	1.71
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	4	1.71
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	4	1.71
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	4	1.71
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	4	1.71
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	4	1.71
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	4	1.71
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	4	1.71
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	4	1.71
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	10	1.71
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	10	1.71
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	10	1.71
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	10	1.71
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	10	1.71
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	10	1.71
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	10	1.71
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	10	1.71
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	10	1.71
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	19	1.7
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	19	1.7
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	19	1.7
(1,3970)	1:357:A:LEU:HD11	2:620:B:LEU:HD21	4	1.7
(1,3970)	1:357:A:LEU:HD11	2:620:B:LEU:HD22	4	1.7
(1,3970)	1:357:A:LEU:HD11	2:620:B:LEU:HD23	4	1.7
(1,3970)	1:357:A:LEU:HD12	2:620:B:LEU:HD21	4	1.7
(1,3970)	1:357:A:LEU:HD12	2:620:B:LEU:HD22	4	1.7
(1,3970)	1:357:A:LEU:HD12	2:620:B:LEU:HD23	4	1.7
(1,3970)	1:357:A:LEU:HD13	2:620:B:LEU:HD21	4	1.7
(1,3970)	1:357:A:LEU:HD13	2:620:B:LEU:HD22	4	1.7
(1,3970)	1:357:A:LEU:HD13	2:620:B:LEU:HD23	4	1.7
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB1	6	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB2	6	1.66
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB3	6	1.66
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB1	6	1.66
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB2	6	1.66
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB3	6	1.66
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB1	6	1.66
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB2	6	1.66
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB3	6	1.66
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB1	8	1.66
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB2	8	1.66
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB3	8	1.66
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB1	8	1.66
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB2	8	1.66
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB3	8	1.66
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB1	8	1.66
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB2	8	1.66
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB3	8	1.66
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	14	1.65
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	14	1.65
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	14	1.65
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	14	1.65
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	14	1.65
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	14	1.65
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	14	1.65
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	14	1.65
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	14	1.65
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	3	1.62
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	3	1.62
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	3	1.62
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	3	1.62
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	3	1.62
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	3	1.62
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	3	1.62
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	3	1.62
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	3	1.62
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	6	1.62
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	6	1.62
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	6	1.62
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	6	1.62
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	6	1.62
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	6	1.62
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	6	1.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	6	1.62
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	6	1.62
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	20	1.62
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	20	1.62
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	20	1.62
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	20	1.62
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	20	1.62
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	20	1.62
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	20	1.62
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	20	1.62
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	20	1.62
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	9	1.62
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	9	1.62
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	9	1.62
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	9	1.62
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	9	1.62
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	9	1.62
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	9	1.62
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	9	1.62
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	9	1.62
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	11	1.61
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	11	1.61
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	11	1.61
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	11	1.61
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	11	1.61
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	11	1.61
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	11	1.61
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	11	1.61
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	11	1.61
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB1	10	1.59
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB2	10	1.59
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB3	10	1.59
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB1	10	1.59
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB2	10	1.59
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB3	10	1.59
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB1	10	1.59
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB2	10	1.59
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB3	10	1.59
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	11	1.59
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	11	1.59
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	11	1.59
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	11	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	11	1.59
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	11	1.59
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	11	1.59
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	11	1.59
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	11	1.59
(1,2565)	1:387:A:ALA:HB1	1:471:A:TYR:HD1	10	1.59
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	9	1.58
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	9	1.58
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	9	1.58
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	9	1.58
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	9	1.58
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	9	1.58
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	9	1.58
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	9	1.58
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	9	1.58
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	1	1.58
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	1	1.58
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	1	1.58
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	1	1.58
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	1	1.58
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	1	1.58
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	1	1.58
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	1	1.58
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	1	1.58
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	16	1.57
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	16	1.57
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	16	1.57
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	16	1.57
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	16	1.57
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	16	1.57
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	16	1.57
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	16	1.57
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	16	1.57
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	14	1.56
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	14	1.56
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	14	1.56
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	2	1.54
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	2	1.54
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	2	1.54
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	2	1.54
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	2	1.54
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	2	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	2	1.54
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	2	1.54
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	2	1.54
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	13	1.54
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	13	1.54
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	13	1.54
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	13	1.54
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	13	1.54
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	13	1.54
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	13	1.54
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	13	1.54
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	13	1.54
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	12	1.54
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	12	1.54
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	12	1.54
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	12	1.54
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	12	1.54
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	12	1.54
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	12	1.54
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	12	1.54
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	12	1.54
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	1	1.54
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	1	1.54
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	1	1.54
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	1	1.54
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	1	1.54
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	1	1.54
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	1	1.54
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	1	1.54
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	1	1.54
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	20	1.53
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	20	1.53
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	20	1.53
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	20	1.53
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	20	1.53
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	20	1.53
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	20	1.53
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	20	1.53
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	20	1.53
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB1	16	1.51
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB2	16	1.51
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB3	16	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB1	16	1.51
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB2	16	1.51
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB3	16	1.51
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB1	16	1.51
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB2	16	1.51
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB3	16	1.51
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG11	2	1.51
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG12	2	1.51
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG13	2	1.51
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG11	2	1.51
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG12	2	1.51
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG13	2	1.51
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG11	2	1.51
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG12	2	1.51
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG13	2	1.51
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	16	1.51
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	16	1.51
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	16	1.51
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	16	1.51
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	16	1.51
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	16	1.51
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	16	1.51
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	16	1.51
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	16	1.51
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	7	1.48
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	7	1.48
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	7	1.48
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	7	1.48
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	7	1.48
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	7	1.48
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	7	1.48
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	7	1.48
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	7	1.48
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	13	1.48
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	13	1.48
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	13	1.48
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	13	1.48
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	13	1.48
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	13	1.48
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	13	1.48
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	13	1.48
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	13	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	2	1.48
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	2	1.48
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	2	1.48
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	2	1.48
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	2	1.48
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	2	1.48
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	2	1.48
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	2	1.48
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	2	1.48
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG11	9	1.47
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG12	9	1.47
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG13	9	1.47
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG11	9	1.47
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG12	9	1.47
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG13	9	1.47
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG11	9	1.47
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG12	9	1.47
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG13	9	1.47
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	11	1.43
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	11	1.43
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	11	1.43
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	11	1.43
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	11	1.43
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	11	1.43
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	11	1.43
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	11	1.43
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	11	1.43
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	13	1.43
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	13	1.43
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	13	1.43
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	13	1.43
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	13	1.43
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	13	1.43
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	13	1.43
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	13	1.43
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	13	1.43
(1,3635)	1:458:A:LEU:HD13	1:480:A:PHE:HE2	19	1.43
(1,3635)	1:458:A:LEU:HD12	1:480:A:PHE:HE1	4	1.42
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	11	1.41
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	11	1.41
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	11	1.41
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	11	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	11	1.41
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	11	1.41
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	11	1.41
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	11	1.41
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	11	1.41
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG11	14	1.4
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG12	14	1.4
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG13	14	1.4
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG11	14	1.4
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG12	14	1.4
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG13	14	1.4
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG11	14	1.4
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG12	14	1.4
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG13	14	1.4
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG21	14	1.4
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG22	14	1.4
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG23	14	1.4
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG21	14	1.4
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG22	14	1.4
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG23	14	1.4
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG21	14	1.4
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG22	14	1.4
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG23	14	1.4
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	19	1.38
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	19	1.38
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	19	1.38
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	19	1.38
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	19	1.38
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	19	1.38
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	19	1.38
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	19	1.38
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	19	1.38
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB1	13	1.33
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB2	13	1.33
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB3	13	1.33
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB1	13	1.33
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB2	13	1.33
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB3	13	1.33
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB1	13	1.33
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB2	13	1.33
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB3	13	1.33
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	14	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	14	1.33
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	14	1.33
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	14	1.33
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	14	1.33
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	14	1.33
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	14	1.33
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	14	1.33
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	14	1.33
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG11	10	1.29
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG12	10	1.29
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG13	10	1.29
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG11	10	1.29
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG12	10	1.29
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG13	10	1.29
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG11	10	1.29
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG12	10	1.29
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG13	10	1.29
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG11	16	1.28
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG12	16	1.28
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG13	16	1.28
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG11	16	1.28
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG12	16	1.28
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG13	16	1.28
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG11	16	1.28
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG12	16	1.28
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG13	16	1.28
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	1	1.28
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	1	1.28
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	1	1.28
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	1	1.28
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	1	1.28
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	1	1.28
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	1	1.28
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	1	1.28
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	1	1.28
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	12	1.27
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	12	1.27
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	12	1.27
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	12	1.27
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	12	1.27
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	12	1.27
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	12	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	12	1.27
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	12	1.27
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	2	1.26
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	2	1.26
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	2	1.26
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	2	1.26
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	2	1.26
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	2	1.26
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	2	1.26
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	2	1.26
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	2	1.26
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	1	1.25
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	1	1.25
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	1	1.25
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	1	1.25
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	1	1.25
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	1	1.25
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	1	1.25
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	1	1.25
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	1	1.25
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	18	1.24
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	18	1.24
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	18	1.24
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	18	1.24
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	18	1.24
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	18	1.24
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	18	1.24
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	18	1.24
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	18	1.24
(1,2565)	1:387:A:ALA:HB3	1:471:A:TYR:HD1	12	1.21
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	9	1.18
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	9	1.18
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	9	1.18
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	9	1.18
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	9	1.18
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	9	1.18
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	9	1.18
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	9	1.18
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	9	1.18
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	17	1.17
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	17	1.17
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	17	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	15	1.17
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	15	1.17
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	15	1.17
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	15	1.17
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	15	1.17
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	15	1.17
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	15	1.17
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	15	1.17
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	15	1.17
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	5	1.15
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	5	1.15
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	5	1.15
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	5	1.15
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	5	1.15
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	5	1.15
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	5	1.15
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	5	1.15
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	5	1.15
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	1	1.15
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	10	1.14
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	10	1.14
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	10	1.14
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	10	1.14
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	10	1.14
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	10	1.14
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	10	1.14
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	10	1.14
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	10	1.14
(1,2565)	1:387:A:ALA:HB1	1:471:A:TYR:HD2	14	1.14
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	8	1.12
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	8	1.12
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	8	1.12
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	8	1.12
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	8	1.12
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	8	1.12
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	8	1.12
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	8	1.12
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	8	1.12
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	10	1.12
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	10	1.12
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	10	1.12
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	10	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	10	1.12
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	10	1.12
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	10	1.12
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	10	1.12
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	10	1.12
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG11	10	1.11
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG12	10	1.11
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG13	10	1.11
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	8	1.11
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	8	1.11
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	8	1.11
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	8	1.11
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	8	1.11
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	8	1.11
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	8	1.11
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	8	1.11
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	8	1.11
(1,2755)	1:402:A:PHE:HD2	1:460:A:LEU:HD11	14	1.1
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD21	13	1.09
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD22	13	1.09
(1,3969)	1:399:A:LEU:HD11	2:620:B:LEU:HD23	13	1.09
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD21	13	1.09
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD22	13	1.09
(1,3969)	1:399:A:LEU:HD12	2:620:B:LEU:HD23	13	1.09
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD21	13	1.09
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD22	13	1.09
(1,3969)	1:399:A:LEU:HD13	2:620:B:LEU:HD23	13	1.09
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	12	1.09
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	12	1.09
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	12	1.09
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	12	1.09
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	12	1.09
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	12	1.09
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	12	1.09
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	12	1.09
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	12	1.09
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	5	1.08
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	5	1.08
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	5	1.08
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG11	14	1.07
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG12	14	1.07
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG13	14	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG11	14	1.07
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG12	14	1.07
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG13	14	1.07
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG11	14	1.07
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG12	14	1.07
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG13	14	1.07
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	14	1.07
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	14	1.07
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	14	1.07
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	14	1.07
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	14	1.07
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	14	1.07
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	14	1.07
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	14	1.07
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	14	1.07
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	5	1.05
(1,2565)	1:387:A:ALA:HB3	1:471:A:TYR:HD1	4	1.04
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	16	1.02
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	16	1.02
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	16	1.02
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	16	1.02
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	16	1.02
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	16	1.02
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	16	1.02
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	16	1.02
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	16	1.02
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	20	1.01
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	20	1.01
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	20	1.01
(1,3970)	1:357:A:LEU:HD11	2:620:B:LEU:HD21	17	1.0
(1,3970)	1:357:A:LEU:HD11	2:620:B:LEU:HD22	17	1.0
(1,3970)	1:357:A:LEU:HD11	2:620:B:LEU:HD23	17	1.0
(1,3970)	1:357:A:LEU:HD12	2:620:B:LEU:HD21	17	1.0
(1,3970)	1:357:A:LEU:HD12	2:620:B:LEU:HD22	17	1.0
(1,3970)	1:357:A:LEU:HD12	2:620:B:LEU:HD23	17	1.0
(1,3970)	1:357:A:LEU:HD13	2:620:B:LEU:HD21	17	1.0
(1,3970)	1:357:A:LEU:HD13	2:620:B:LEU:HD22	17	1.0
(1,3970)	1:357:A:LEU:HD13	2:620:B:LEU:HD23	17	1.0
(1,2565)	1:387:A:ALA:HB1	1:471:A:TYR:HD1	18	1.0
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	19	0.99
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	19	0.99
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	19	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	19	0.99
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	19	0.99
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	19	0.99
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	19	0.99
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	19	0.99
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	19	0.99
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	12	0.97
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	12	0.97
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	12	0.97
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	12	0.97
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	12	0.97
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	12	0.97
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	12	0.97
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	12	0.97
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	12	0.97
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	8	0.97
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	8	0.97
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	8	0.97
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	8	0.97
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	8	0.97
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	8	0.97
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	8	0.97
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	8	0.97
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	8	0.97
(1,3971)	1:314:A:MET:HE1	2:622:B:TYR:HE2	9	0.96
(1,3971)	1:314:A:MET:HE2	2:622:B:TYR:HE2	9	0.96
(1,3971)	1:314:A:MET:HE3	2:622:B:TYR:HE2	9	0.96
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG21	16	0.95
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG22	16	0.95
(1,3976)	1:464:A:ILE:HD11	2:630:B:VAL:HG23	16	0.95
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG21	16	0.95
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG22	16	0.95
(1,3976)	1:464:A:ILE:HD12	2:630:B:VAL:HG23	16	0.95
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG21	16	0.95
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG22	16	0.95
(1,3976)	1:464:A:ILE:HD13	2:630:B:VAL:HG23	16	0.95
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB1	4	0.94
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB2	4	0.94
(1,3967)	1:396:A:ILE:HD11	2:621:B:ALA:HB3	4	0.94
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB1	4	0.94
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB2	4	0.94
(1,3967)	1:396:A:ILE:HD12	2:621:B:ALA:HB3	4	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB1	4	0.94
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB2	4	0.94
(1,3967)	1:396:A:ILE:HD13	2:621:B:ALA:HB3	4	0.94
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG11	1	0.92
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG12	1	0.92
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG13	1	0.92
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG11	1	0.92
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG12	1	0.92
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG13	1	0.92
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG11	1	0.92
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG12	1	0.92
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG13	1	0.92
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	14	0.92
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	2	0.9
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	2	0.9
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	2	0.9
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	2	0.9
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	2	0.9
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	2	0.9
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	2	0.9
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	2	0.9
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	2	0.9
(1,2565)	1:387:A:ALA:HB2	1:471:A:TYR:HD2	17	0.9
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG11	20	0.89
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG12	20	0.89
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG13	20	0.89
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG11	20	0.89
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG12	20	0.89
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG13	20	0.89
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG11	20	0.89
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG12	20	0.89
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG13	20	0.89
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	3	0.89
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	3	0.89
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	3	0.89
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	3	0.89
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	3	0.89
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	3	0.89
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	3	0.89
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	3	0.89
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	3	0.89
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD2	7	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD3	7	0.88
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG11	10	0.87
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG12	10	0.87
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG13	10	0.87
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG11	10	0.87
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG12	10	0.87
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG13	10	0.87
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG11	10	0.87
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG12	10	0.87
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG13	10	0.87
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG21	10	0.87
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG22	10	0.87
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG23	10	0.87
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG21	10	0.87
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG22	10	0.87
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG23	10	0.87
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG21	10	0.87
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG22	10	0.87
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG23	10	0.87
(1,3972)	1:318:A:LEU:HD11	2:622:B:TYR:HE1	9	0.87
(1,3972)	1:318:A:LEU:HD12	2:622:B:TYR:HE1	9	0.87
(1,3972)	1:318:A:LEU:HD13	2:622:B:TYR:HE1	9	0.87
(1,3118)	1:427:A:GLN:HG2	1:493:A:LEU:HD11	15	0.87
(1,3118)	1:427:A:GLN:HG2	1:493:A:LEU:HD12	15	0.87
(1,3118)	1:427:A:GLN:HG2	1:493:A:LEU:HD13	15	0.87
(1,3118)	1:427:A:GLN:HG3	1:493:A:LEU:HD11	15	0.87
(1,3118)	1:427:A:GLN:HG3	1:493:A:LEU:HD12	15	0.87
(1,3118)	1:427:A:GLN:HG3	1:493:A:LEU:HD13	15	0.87
(1,2997)	1:418:A:ASP:HA	1:422:A:ARG:HG2	3	0.87
(1,2997)	1:418:A:ASP:HA	1:422:A:ARG:HG3	3	0.87
(1,447)	1:256:A:ASP:HA	1:258:A:ASN:HD21	3	0.86
(1,447)	1:256:A:ASP:HA	1:258:A:ASN:HD22	3	0.86
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	17	0.85
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	17	0.85
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	17	0.85
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	17	0.85
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	17	0.85
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	17	0.85
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	17	0.85
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	17	0.85
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	17	0.85
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG11	4	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG12	4	0.84
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG13	4	0.84
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG11	4	0.84
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG12	4	0.84
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG13	4	0.84
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG11	4	0.84
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG12	4	0.84
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG13	4	0.84
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG21	4	0.84
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG22	4	0.84
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG23	4	0.84
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG21	4	0.84
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG22	4	0.84
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG23	4	0.84
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG21	4	0.84
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG22	4	0.84
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG23	4	0.84
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	12	0.84
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	12	0.84
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	12	0.84
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	12	0.84
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	12	0.84
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	12	0.84
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	12	0.84
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	12	0.84
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	12	0.84
(1,3103)	1:424:A:LYS:HB2	1:425:A:GLU:HG2	8	0.84
(1,3103)	1:424:A:LYS:HB2	1:425:A:GLU:HG3	8	0.84
(1,3103)	1:424:A:LYS:HB3	1:425:A:GLU:HG2	8	0.84
(1,3103)	1:424:A:LYS:HB3	1:425:A:GLU:HG3	8	0.84
(1,2915)	1:410:A:SER:HB3	1:438:A:TYR:HD1	7	0.84
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	3	0.84
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	3	0.83
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	3	0.83
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	3	0.83
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	3	0.83
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	3	0.83
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	3	0.83
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	3	0.83
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	3	0.83
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	3	0.83
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	11	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	11	0.83
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	11	0.83
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	11	0.83
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	2	0.82
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	2	0.82
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	2	0.82
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	2	0.82
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	2	0.82
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	2	0.82
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	2	0.82
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	2	0.82
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	2	0.82
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	3	0.82
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	3	0.82
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	3	0.82
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	3	0.82
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	3	0.82
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	3	0.82
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	3	0.82
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	3	0.82
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	3	0.82
(1,3147)	1:429:A:LYS:HD2	1:488:A:GLU:HG2	15	0.82
(1,3147)	1:429:A:LYS:HD2	1:488:A:GLU:HG3	15	0.82
(1,3147)	1:429:A:LYS:HD3	1:488:A:GLU:HG2	15	0.82
(1,3147)	1:429:A:LYS:HD3	1:488:A:GLU:HG3	15	0.82
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	3	0.81
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	3	0.81
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	3	0.81
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	3	0.81
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	3	0.81
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	3	0.81
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	3	0.81
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	3	0.81
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	3	0.81
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	7	0.81
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	7	0.81
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	7	0.81
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	7	0.81
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	7	0.81
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	7	0.81
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	7	0.81
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	7	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	7	0.81
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	18	0.81
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	18	0.81
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	18	0.81
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	18	0.81
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	18	0.81
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	18	0.81
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	18	0.81
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	18	0.81
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	18	0.81
(1,3635)	1:458:A:LEU:HD11	1:480:A:PHE:HE2	18	0.81
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	14	0.8
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	14	0.8
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	14	0.8
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	14	0.8
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	14	0.8
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	14	0.8
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	14	0.8
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	14	0.8
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	14	0.8
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	9	0.8
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	9	0.8
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	9	0.8
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	9	0.8
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	9	0.8
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	9	0.8
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	9	0.8
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	9	0.8
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	9	0.8
(1,3165)	1:429:A:LYS:HB3	1:431:A:TYR:HE2	7	0.8
(1,349)	1:250:A:TYR:HD2	1:260:A:PRO:HB3	4	0.8
(1,2938)	1:414:A:VAL:HG21	1:418:A:ASP:H	8	0.79
(1,2938)	1:414:A:VAL:HG22	1:418:A:ASP:H	8	0.79
(1,2938)	1:414:A:VAL:HG23	1:418:A:ASP:H	8	0.79
(1,3315)	1:434:A:THR:HA	1:461:A:SER:HA	13	0.78
(1,2938)	1:414:A:VAL:HG21	1:418:A:ASP:H	3	0.78
(1,2938)	1:414:A:VAL:HG22	1:418:A:ASP:H	3	0.78
(1,2938)	1:414:A:VAL:HG23	1:418:A:ASP:H	3	0.78
(1,2927)	1:412:A:GLN:HA	1:414:A:VAL:HB	11	0.78
(1,2699)	1:398:A:LYS:HE2	1:417:A:GLU:HG2	12	0.78
(1,2699)	1:398:A:LYS:HE2	1:417:A:GLU:HG3	12	0.78
(1,2699)	1:398:A:LYS:HE3	1:417:A:GLU:HG2	12	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2699)	1:398:A:LYS:HE3	1:417:A:GLU:HG3	12	0.78
(1,1946)	1:351:A:ALA:HA	1:355:A:ARG:HD2	16	0.78
(1,1946)	1:351:A:ALA:HA	1:355:A:ARG:HD3	16	0.78
(1,447)	1:256:A:ASP:HA	1:258:A:ASN:HD21	1	0.78
(1,447)	1:256:A:ASP:HA	1:258:A:ASN:HD22	1	0.78
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB1	12	0.77
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB2	12	0.77
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB3	12	0.77
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB1	12	0.77
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB2	12	0.77
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB3	12	0.77
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB1	12	0.77
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB2	12	0.77
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB3	12	0.77
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB2	4	0.77
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB3	4	0.77
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB1	14	0.77
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB2	14	0.77
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB3	14	0.77
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB1	14	0.77
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB2	14	0.77
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB3	14	0.77
(1,1811)	1:339:A:LEU:HD21	1:345:A:THR:H	14	0.77
(1,1811)	1:339:A:LEU:HD22	1:345:A:THR:H	14	0.77
(1,1811)	1:339:A:LEU:HD23	1:345:A:THR:H	14	0.77
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	7	0.77
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG21	8	0.76
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG22	8	0.76
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG23	8	0.76
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG21	8	0.76
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG22	8	0.76
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG23	8	0.76
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG21	8	0.76
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG22	8	0.76
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG23	8	0.76
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	6	0.76
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	6	0.76
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	6	0.76
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	6	0.76
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	6	0.76
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	6	0.76
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	6	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	6	0.76
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	6	0.76
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD21	19	0.76
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD22	19	0.76
(1,3977)	1:458:A:LEU:HD11	2:634:B:LEU:HD23	19	0.76
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD21	19	0.76
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD22	19	0.76
(1,3977)	1:458:A:LEU:HD12	2:634:B:LEU:HD23	19	0.76
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD21	19	0.76
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD22	19	0.76
(1,3977)	1:458:A:LEU:HD13	2:634:B:LEU:HD23	19	0.76
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	16	0.76
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	16	0.76
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	16	0.76
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	16	0.76
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	16	0.76
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	16	0.76
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	16	0.76
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	16	0.76
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	16	0.76
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	10	0.76
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	10	0.76
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	10	0.76
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	10	0.76
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB2	12	0.76
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB3	12	0.76
(1,1013)	1:288:A:MET:HA	1:294:A:LYS:H	11	0.76
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	9	0.75
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	9	0.75
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	9	0.75
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	9	0.75
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	9	0.75
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	9	0.75
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	9	0.75
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	9	0.75
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	9	0.75
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	14	0.75
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	14	0.75
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	14	0.75
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	14	0.75
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	14	0.75
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	14	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	14	0.75
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	14	0.75
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	14	0.75
(1,3110)	1:426:A:GLY:HA2	1:492:A:LYS:HD3	19	0.75
(1,3110)	1:426:A:GLY:HA3	1:492:A:LYS:HD3	19	0.75
(1,2628)	1:393:A:GLN:HG2	1:397:A:ALA:H	9	0.75
(1,2628)	1:393:A:GLN:HG3	1:397:A:ALA:H	9	0.75
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	3	0.75
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	3	0.75
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	3	0.75
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	3	0.75
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	3	0.75
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	3	0.75
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	3	0.75
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	3	0.75
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	3	0.75
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD2	19	0.75
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD3	19	0.75
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	1	0.75
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	14	0.75
(1,684)	1:272:A:GLN:HE21	1:351:A:ALA:H	7	0.75
(1,684)	1:272:A:GLN:HE22	1:351:A:ALA:H	7	0.75
(2,5)	1:290:A:ASN:HB2	1:293:A:HIS:HA	12	0.74
(2,5)	1:290:A:ASN:HB3	1:293:A:HIS:HA	12	0.74
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	13	0.74
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	13	0.74
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	13	0.74
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	13	0.74
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	13	0.74
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	13	0.74
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	13	0.74
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	13	0.74
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	13	0.74
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG11	4	0.74
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG12	4	0.74
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG13	4	0.74
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG11	4	0.74
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG12	4	0.74
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG13	4	0.74
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG11	4	0.74
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG12	4	0.74
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG13	4	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3110)	1:426:A:GLY:HA2	1:492:A:LYS:HD3	5	0.74
(1,3110)	1:426:A:GLY:HA3	1:492:A:LYS:HD3	5	0.74
(1,2997)	1:418:A:ASP:HA	1:422:A:ARG:HG2	20	0.74
(1,2997)	1:418:A:ASP:HA	1:422:A:ARG:HG3	20	0.74
(1,2938)	1:414:A:VAL:HG21	1:418:A:ASP:H	17	0.74
(1,2938)	1:414:A:VAL:HG22	1:418:A:ASP:H	17	0.74
(1,2938)	1:414:A:VAL:HG23	1:418:A:ASP:H	17	0.74
(1,2938)	1:414:A:VAL:HG21	1:418:A:ASP:H	18	0.74
(1,2938)	1:414:A:VAL:HG22	1:418:A:ASP:H	18	0.74
(1,2938)	1:414:A:VAL:HG23	1:418:A:ASP:H	18	0.74
(1,2595)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	14	0.74
(1,2595)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	14	0.74
(1,2595)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	14	0.74
(1,2595)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	14	0.74
(1,2590)	1:390:A:PHE:HD1	1:471:A:TYR:HB2	18	0.74
(1,2590)	1:390:A:PHE:HD1	1:471:A:TYR:HB3	18	0.74
(1,2590)	1:390:A:PHE:HD2	1:471:A:TYR:HB2	18	0.74
(1,2590)	1:390:A:PHE:HD2	1:471:A:TYR:HB3	18	0.74
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	12	0.74
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	20	0.74
(2,5)	1:290:A:ASN:HB2	1:293:A:HIS:HA	9	0.73
(2,5)	1:290:A:ASN:HB3	1:293:A:HIS:HA	9	0.73
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	4	0.73
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	4	0.73
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	4	0.73
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	4	0.73
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	4	0.73
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	4	0.73
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	4	0.73
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	4	0.73
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	4	0.73
(1,3636)	1:458:A:LEU:HD11	1:469:A:MET:HE1	18	0.73
(1,3636)	1:458:A:LEU:HD11	1:469:A:MET:HE2	18	0.73
(1,3636)	1:458:A:LEU:HD11	1:469:A:MET:HE3	18	0.73
(1,3636)	1:458:A:LEU:HD12	1:469:A:MET:HE1	18	0.73
(1,3636)	1:458:A:LEU:HD12	1:469:A:MET:HE2	18	0.73
(1,3636)	1:458:A:LEU:HD12	1:469:A:MET:HE3	18	0.73
(1,3636)	1:458:A:LEU:HD13	1:469:A:MET:HE1	18	0.73
(1,3636)	1:458:A:LEU:HD13	1:469:A:MET:HE2	18	0.73
(1,3636)	1:458:A:LEU:HD13	1:469:A:MET:HE3	18	0.73
(1,3360)	1:437:A:SER:HA	1:462:A:ASP:HA	15	0.73
(1,3110)	1:426:A:GLY:HA2	1:492:A:LYS:HD3	6	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3110)	1:426:A:GLY:HA3	1:492:A:LYS:HD3	6	0.73
(1,3110)	1:426:A:GLY:HA2	1:492:A:LYS:HD3	9	0.73
(1,3110)	1:426:A:GLY:HA3	1:492:A:LYS:HD3	9	0.73
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB2	19	0.73
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB3	19	0.73
(1,2595)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	4	0.73
(1,2595)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	4	0.73
(1,2595)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	4	0.73
(1,2595)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	4	0.73
(1,2565)	1:387:A:ALA:HB3	1:471:A:TYR:HD1	2	0.73
(1,684)	1:272:A:GLN:HE21	1:351:A:ALA:H	4	0.73
(1,684)	1:272:A:GLN:HE22	1:351:A:ALA:H	4	0.73
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	19	0.72
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	19	0.72
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	19	0.72
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	19	0.72
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	19	0.72
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	19	0.72
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	19	0.72
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	19	0.72
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	19	0.72
(1,3635)	1:458:A:LEU:HD13	1:480:A:PHE:HE2	14	0.72
(1,3479)	1:446:A:HIS:HD2	1:484:A:SER:H	13	0.72
(1,3178)	1:430:A:ILE:HD11	1:479:A:PRO:HA	19	0.72
(1,3178)	1:430:A:ILE:HD12	1:479:A:PRO:HA	19	0.72
(1,3178)	1:430:A:ILE:HD13	1:479:A:PRO:HA	19	0.72
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG2	13	0.72
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG3	13	0.72
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG2	13	0.72
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG3	13	0.72
(1,3110)	1:426:A:GLY:HA2	1:492:A:LYS:HD3	13	0.72
(1,3110)	1:426:A:GLY:HA3	1:492:A:LYS:HD3	13	0.72
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB2	10	0.72
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB3	10	0.72
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA2	7	0.72
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA3	7	0.72
(1,1044)	1:291:A:ARG:HA	1:293:A:HIS:HA	7	0.72
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	2	0.72
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	13	0.72
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	20	0.72
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	20	0.72
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	20	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG21	7	0.71
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG22	7	0.71
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG23	7	0.71
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG21	7	0.71
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG22	7	0.71
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG23	7	0.71
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG21	7	0.71
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG22	7	0.71
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG23	7	0.71
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	5	0.71
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	5	0.71
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	5	0.71
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	5	0.71
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	5	0.71
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	5	0.71
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	5	0.71
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	5	0.71
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	5	0.71
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG11	7	0.71
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG12	7	0.71
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG13	7	0.71
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG11	7	0.71
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG12	7	0.71
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG13	7	0.71
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG11	7	0.71
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG12	7	0.71
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG13	7	0.71
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG21	7	0.71
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG22	7	0.71
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG23	7	0.71
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG21	7	0.71
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG22	7	0.71
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG23	7	0.71
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG21	7	0.71
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG22	7	0.71
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG23	7	0.71
(1,3898)	1:486:A:VAL:HG11	1:488:A:GLU:HA	6	0.71
(1,3898)	1:486:A:VAL:HG12	1:488:A:GLU:HA	6	0.71
(1,3898)	1:486:A:VAL:HG13	1:488:A:GLU:HA	6	0.71
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	16	0.71
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	16	0.71
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	16	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	16	0.71
(1,3110)	1:426:A:GLY:HA2	1:492:A:LYS:HD3	8	0.71
(1,3110)	1:426:A:GLY:HA3	1:492:A:LYS:HD3	8	0.71
(1,3110)	1:426:A:GLY:HA2	1:492:A:LYS:HD3	15	0.71
(1,3110)	1:426:A:GLY:HA3	1:492:A:LYS:HD3	15	0.71
(1,2997)	1:418:A:ASP:HA	1:422:A:ARG:HG2	6	0.71
(1,2997)	1:418:A:ASP:HA	1:422:A:ARG:HG3	6	0.71
(1,2889)	1:408:A:ASP:HB3	1:451:A:ARG:HH22	4	0.71
(1,2436)	1:380:A:LEU:HA	1:383:A:LYS:HD2	13	0.71
(1,2436)	1:380:A:LEU:HA	1:383:A:LYS:HD3	13	0.71
(1,2122)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	6	0.71
(1,2122)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	13	0.71
(1,1452)	1:313:A:PHE:HZ	1:345:A:THR:HA	20	0.71
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	18	0.71
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	16	0.71
(2,9)	1:338:A:ILE:HD11	1:342:A:SER:H	17	0.7
(2,9)	1:338:A:ILE:HD12	1:342:A:SER:H	17	0.7
(2,9)	1:338:A:ILE:HD13	1:342:A:SER:H	17	0.7
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB1	5	0.7
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB2	5	0.7
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB3	5	0.7
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB1	5	0.7
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB2	5	0.7
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB3	5	0.7
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB1	5	0.7
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB2	5	0.7
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB3	5	0.7
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB2	7	0.7
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB3	7	0.7
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB2	7	0.7
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB3	7	0.7
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB2	7	0.7
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB3	7	0.7
(1,3634)	1:458:A:LEU:HD11	1:480:A:PHE:HE1	16	0.7
(1,3634)	1:458:A:LEU:HD11	1:480:A:PHE:HE2	16	0.7
(1,3634)	1:458:A:LEU:HD12	1:480:A:PHE:HE1	16	0.7
(1,3634)	1:458:A:LEU:HD12	1:480:A:PHE:HE2	16	0.7
(1,3634)	1:458:A:LEU:HD13	1:480:A:PHE:HE1	16	0.7
(1,3634)	1:458:A:LEU:HD13	1:480:A:PHE:HE2	16	0.7
(1,3315)	1:434:A:THR:HA	1:461:A:SER:HA	12	0.7
(1,3007)	1:419:A:TYR:HE2	1:478:A:LYS:HG2	19	0.7
(1,3007)	1:419:A:TYR:HE2	1:478:A:LYS:HG3	19	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	4	0.7
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	4	0.7
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	4	0.7
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	4	0.7
(1,1638)	1:320:A:PHE:HA	1:322:A:ARG:HG2	4	0.7
(1,1638)	1:320:A:PHE:HA	1:322:A:ARG:HG3	4	0.7
(1,1511)	1:315:A:PRO:HG2	1:319:A:ARG:H	7	0.7
(1,1511)	1:315:A:PRO:HG3	1:319:A:ARG:H	7	0.7
(1,1425)	1:312:A:GLN:HG2	1:339:A:LEU:HA	18	0.7
(1,1425)	1:312:A:GLN:HG3	1:339:A:LEU:HA	18	0.7
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD2	9	0.7
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD3	9	0.7
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD2	10	0.7
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD3	10	0.7
(1,988)	1:287:A:ASP:HB2	1:293:A:HIS:HA	9	0.7
(1,988)	1:287:A:ASP:HB3	1:293:A:HIS:HA	9	0.7
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	15	0.7
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	18	0.7
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	3	0.7
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	3	0.7
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	3	0.7
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	12	0.7
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	12	0.7
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	4	0.69
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	4	0.69
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	4	0.69
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	4	0.69
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	4	0.69
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	4	0.69
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	4	0.69
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	4	0.69
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	4	0.69
(1,3882)	1:485:A:LYS:HB2	1:487:A:ASP:HB3	14	0.69
(1,3627)	1:457:A:VAL:HB	1:459:A:LEU:HD21	16	0.69
(1,3627)	1:457:A:VAL:HB	1:459:A:LEU:HD22	16	0.69
(1,3627)	1:457:A:VAL:HB	1:459:A:LEU:HD23	16	0.69
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG2	7	0.69
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG3	7	0.69
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG2	7	0.69
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG3	7	0.69
(1,3007)	1:419:A:TYR:HE2	1:478:A:LYS:HG2	13	0.69
(1,3007)	1:419:A:TYR:HE2	1:478:A:LYS:HG3	13	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2938)	1:414:A:VAL:HG21	1:418:A:ASP:H	12	0.69
(1,2938)	1:414:A:VAL:HG22	1:418:A:ASP:H	12	0.69
(1,2938)	1:414:A:VAL:HG23	1:418:A:ASP:H	12	0.69
(1,2873)	1:406:A:HIS:HA	1:422:A:ARG:HD2	15	0.69
(1,2873)	1:406:A:HIS:HA	1:422:A:ARG:HD3	15	0.69
(1,2755)	1:402:A:PHE:HD1	1:460:A:LEU:HD12	17	0.69
(1,2196)	1:365:A:LYS:HE2	1:398:A:LYS:HE2	7	0.69
(1,2196)	1:365:A:LYS:HE2	1:398:A:LYS:HE3	7	0.69
(1,2196)	1:365:A:LYS:HE3	1:398:A:LYS:HE2	7	0.69
(1,2196)	1:365:A:LYS:HE3	1:398:A:LYS:HE3	7	0.69
(1,2122)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	11	0.69
(1,1072)	1:295:A:HIS:HE1	1:311:A:GLU:HA	14	0.69
(1,1072)	1:295:A:HIS:HE1	1:311:A:GLU:HA	16	0.69
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD2	2	0.69
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD3	2	0.69
(1,1013)	1:288:A:MET:HA	1:294:A:LYS:H	3	0.69
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	2	0.69
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	2	0.69
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	2	0.69
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD2	11	0.69
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD3	11	0.69
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	13	0.69
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG21	2	0.69
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG22	2	0.69
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG23	2	0.69
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	15	0.68
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	15	0.68
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	15	0.68
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	15	0.68
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	15	0.68
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	15	0.68
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	15	0.68
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	15	0.68
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	15	0.68
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	18	0.68
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	18	0.68
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	18	0.68
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	18	0.68
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	18	0.68
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	18	0.68
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	18	0.68
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	18	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	18	0.68
(1,3315)	1:434:A:THR:HA	1:461:A:SER:HA	1	0.68
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	16	0.68
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	16	0.68
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	16	0.68
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	16	0.68
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG2	1	0.68
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG3	1	0.68
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG2	1	0.68
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG3	1	0.68
(1,2997)	1:418:A:ASP:HA	1:422:A:ARG:HG2	9	0.68
(1,2997)	1:418:A:ASP:HA	1:422:A:ARG:HG3	9	0.68
(1,2889)	1:408:A:ASP:HB3	1:451:A:ARG:HH22	11	0.68
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB2	16	0.68
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB3	16	0.68
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB2	17	0.68
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB3	17	0.68
(1,2590)	1:390:A:PHE:HD1	1:471:A:TYR:HB2	12	0.68
(1,2590)	1:390:A:PHE:HD1	1:471:A:TYR:HB3	12	0.68
(1,2590)	1:390:A:PHE:HD2	1:471:A:TYR:HB2	12	0.68
(1,2590)	1:390:A:PHE:HD2	1:471:A:TYR:HB3	12	0.68
(1,2122)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	7	0.68
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD21	9	0.68
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD22	9	0.68
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD21	9	0.68
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD22	9	0.68
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD21	18	0.68
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD22	18	0.68
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD21	18	0.68
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD22	18	0.68
(1,1946)	1:351:A:ALA:HA	1:355:A:ARG:HD2	9	0.68
(1,1946)	1:351:A:ALA:HA	1:355:A:ARG:HD3	9	0.68
(1,1935)	1:350:A:ASN:HA	1:354:A:LYS:HG2	1	0.68
(1,1935)	1:350:A:ASN:HA	1:354:A:LYS:HG3	1	0.68
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	11	0.68
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	11	0.68
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	11	0.68
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	11	0.68
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	11	0.68
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	11	0.68
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	11	0.68
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	11	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	11	0.68
(1,1527)	1:316:A:ASN:H	1:349:A:ARG:HD2	15	0.68
(1,1527)	1:316:A:ASN:H	1:349:A:ARG:HD3	15	0.68
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD11	19	0.68
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD12	19	0.68
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD13	19	0.68
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	10	0.68
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	19	0.68
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	6	0.68
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	1	0.68
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	10	0.67
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	10	0.67
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	10	0.67
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	10	0.67
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	10	0.67
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	10	0.67
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	10	0.67
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	10	0.67
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	10	0.67
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	17	0.67
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	17	0.67
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	17	0.67
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	17	0.67
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	17	0.67
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	17	0.67
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	17	0.67
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	17	0.67
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	17	0.67
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	13	0.67
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	13	0.67
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	13	0.67
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	13	0.67
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	13	0.67
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	13	0.67
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	13	0.67
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	13	0.67
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	13	0.67
(1,3479)	1:446:A:HIS:HD2	1:484:A:SER:H	4	0.67
(1,3479)	1:446:A:HIS:HD2	1:484:A:SER:H	19	0.67
(1,3360)	1:437:A:SER:HA	1:462:A:ASP:HA	5	0.67
(1,3353)	1:436:A:ASP:HA	1:461:A:SER:HA	20	0.67
(1,3207)	1:431:A:TYR:HA	1:482:A:SER:HA	18	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3126)	1:427:A:GLN:HG2	1:430:A:ILE:HA	11	0.67
(1,3126)	1:427:A:GLN:HG3	1:430:A:ILE:HA	11	0.67
(1,3103)	1:424:A:LYS:HB2	1:425:A:GLU:HG2	9	0.67
(1,3103)	1:424:A:LYS:HB2	1:425:A:GLU:HG3	9	0.67
(1,3103)	1:424:A:LYS:HB3	1:425:A:GLU:HG2	9	0.67
(1,3103)	1:424:A:LYS:HB3	1:425:A:GLU:HG3	9	0.67
(1,2986)	1:417:A:GLU:HA	1:421:A:SER:HB2	10	0.67
(1,2986)	1:417:A:GLU:HA	1:421:A:SER:HB3	10	0.67
(1,2938)	1:414:A:VAL:HG21	1:418:A:ASP:H	16	0.67
(1,2938)	1:414:A:VAL:HG22	1:418:A:ASP:H	16	0.67
(1,2938)	1:414:A:VAL:HG23	1:418:A:ASP:H	16	0.67
(1,2483)	1:383:A:LYS:HD2	1:465:A:ASP:HA	17	0.67
(1,2483)	1:383:A:LYS:HD3	1:465:A:ASP:HA	17	0.67
(1,2045)	1:357:A:LEU:HD21	1:395:A:ALA:H	15	0.67
(1,2045)	1:357:A:LEU:HD22	1:395:A:ALA:H	15	0.67
(1,2045)	1:357:A:LEU:HD23	1:395:A:ALA:H	15	0.67
(1,1886)	1:346:A:ARG:HG2	1:350:A:ASN:HD21	13	0.67
(1,1886)	1:346:A:ARG:HG2	1:350:A:ASN:HD22	13	0.67
(1,1886)	1:346:A:ARG:HG3	1:350:A:ASN:HD21	13	0.67
(1,1886)	1:346:A:ARG:HG3	1:350:A:ASN:HD22	13	0.67
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD21	9	0.67
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD22	9	0.67
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	14	0.67
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	14	0.67
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	14	0.67
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	14	0.67
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	14	0.67
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	14	0.67
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	14	0.67
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	14	0.67
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	14	0.67
(1,988)	1:287:A:ASP:HB2	1:293:A:HIS:HA	1	0.67
(1,988)	1:287:A:ASP:HB3	1:293:A:HIS:HA	1	0.67
(1,986)	1:287:A:ASP:HB2	1:294:A:LYS:H	12	0.67
(1,986)	1:287:A:ASP:HB3	1:294:A:LYS:H	12	0.67
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	6	0.67
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	8	0.67
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	8	0.67
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	8	0.67
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	20	0.67
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD2	11	0.67
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD3	11	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD2	11	0.67
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD3	11	0.67
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD2	11	0.67
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD3	11	0.67
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	5	0.67
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	9	0.67
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	10	0.67
(1,37)	1:233:A:LEU:HD11	1:249:A:PHE:H	5	0.67
(1,37)	1:233:A:LEU:HD12	1:249:A:PHE:H	5	0.67
(1,37)	1:233:A:LEU:HD13	1:249:A:PHE:H	5	0.67
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	1	0.66
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	1	0.66
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	1	0.66
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	1	0.66
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	1	0.66
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	1	0.66
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	1	0.66
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	1	0.66
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	1	0.66
(1,3550)	1:450:A:LEU:HD21	1:490:A:LEU:HA	14	0.66
(1,3550)	1:450:A:LEU:HD22	1:490:A:LEU:HA	14	0.66
(1,3550)	1:450:A:LEU:HD23	1:490:A:LEU:HA	14	0.66
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	14	0.66
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	14	0.66
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	14	0.66
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	14	0.66
(1,3135)	1:428:A:GLU:HA	1:478:A:LYS:HA	8	0.66
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG2	13	0.66
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG3	13	0.66
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG2	13	0.66
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG3	13	0.66
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD11	4	0.66
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD12	4	0.66
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD13	4	0.66
(1,2938)	1:414:A:VAL:HG21	1:418:A:ASP:H	1	0.66
(1,2938)	1:414:A:VAL:HG22	1:418:A:ASP:H	1	0.66
(1,2938)	1:414:A:VAL:HG23	1:418:A:ASP:H	1	0.66
(1,2938)	1:414:A:VAL:HG21	1:418:A:ASP:H	19	0.66
(1,2938)	1:414:A:VAL:HG22	1:418:A:ASP:H	19	0.66
(1,2938)	1:414:A:VAL:HG23	1:418:A:ASP:H	19	0.66
(1,2914)	1:410:A:SER:HA	1:438:A:TYR:HE1	12	0.66
(1,2873)	1:406:A:HIS:HA	1:422:A:ARG:HD2	8	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2873)	1:406:A:HIS:HA	1:422:A:ARG:HD3	8	0.66
(1,2595)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	1	0.66
(1,2595)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	1	0.66
(1,2595)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	1	0.66
(1,2595)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	1	0.66
(1,2135)	1:361:A:GLU:HG2	1:365:A:LYS:HG2	11	0.66
(1,2135)	1:361:A:GLU:HG2	1:365:A:LYS:HG3	11	0.66
(1,2135)	1:361:A:GLU:HG3	1:365:A:LYS:HG2	11	0.66
(1,2135)	1:361:A:GLU:HG3	1:365:A:LYS:HG3	11	0.66
(1,1946)	1:351:A:ALA:HA	1:355:A:ARG:HD2	5	0.66
(1,1946)	1:351:A:ALA:HA	1:355:A:ARG:HD3	5	0.66
(1,1935)	1:350:A:ASN:HA	1:354:A:LYS:HG2	8	0.66
(1,1935)	1:350:A:ASN:HA	1:354:A:LYS:HG3	8	0.66
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD2	20	0.66
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD3	20	0.66
(1,988)	1:287:A:ASP:HB2	1:293:A:HIS:HA	3	0.66
(1,988)	1:287:A:ASP:HB3	1:293:A:HIS:HA	3	0.66
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	13	0.66
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	13	0.66
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	13	0.66
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	17	0.66
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	17	0.66
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	17	0.66
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	6	0.66
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	13	0.66
(1,110)	1:235:A:THR:HG1	1:267:A:ARG:HD2	5	0.66
(1,110)	1:235:A:THR:HG1	1:267:A:ARG:HD3	5	0.66
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	3	0.66
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	4	0.66
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	18	0.66
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	6	0.65
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	6	0.65
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	6	0.65
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	6	0.65
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	6	0.65
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	6	0.65
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	6	0.65
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	6	0.65
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	6	0.65
(1,3479)	1:446:A:HIS:HD2	1:484:A:SER:H	2	0.65
(1,3479)	1:446:A:HIS:HD2	1:484:A:SER:H	12	0.65
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD21	19	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD22	19	0.65
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD23	19	0.65
(1,3110)	1:426:A:GLY:HA2	1:492:A:LYS:HD3	1	0.65
(1,3110)	1:426:A:GLY:HA3	1:492:A:LYS:HD3	1	0.65
(1,3110)	1:426:A:GLY:HA2	1:492:A:LYS:HD3	2	0.65
(1,3110)	1:426:A:GLY:HA3	1:492:A:LYS:HD3	2	0.65
(1,3074)	1:423:A:MET:HE1	1:430:A:ILE:HA	2	0.65
(1,3074)	1:423:A:MET:HE2	1:430:A:ILE:HA	2	0.65
(1,3074)	1:423:A:MET:HE3	1:430:A:ILE:HA	2	0.65
(1,2927)	1:412:A:GLN:HA	1:414:A:VAL:HB	15	0.65
(1,2888)	1:408:A:ASP:HA	1:459:A:LEU:HD11	8	0.65
(1,2888)	1:408:A:ASP:HA	1:459:A:LEU:HD12	8	0.65
(1,2888)	1:408:A:ASP:HA	1:459:A:LEU:HD13	8	0.65
(1,2875)	1:406:A:HIS:HB2	1:414:A:VAL:HB	15	0.65
(1,2875)	1:406:A:HIS:HB3	1:414:A:VAL:HB	15	0.65
(1,2595)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	17	0.65
(1,2595)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	17	0.65
(1,2595)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	17	0.65
(1,2595)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	17	0.65
(1,2427)	1:380:A:LEU:HD11	1:463:A:ARG:H	11	0.65
(1,2427)	1:380:A:LEU:HD12	1:463:A:ARG:H	11	0.65
(1,2427)	1:380:A:LEU:HD13	1:463:A:ARG:H	11	0.65
(1,2427)	1:380:A:LEU:HD11	1:463:A:ARG:H	13	0.65
(1,2427)	1:380:A:LEU:HD12	1:463:A:ARG:H	13	0.65
(1,2427)	1:380:A:LEU:HD13	1:463:A:ARG:H	13	0.65
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	16	0.65
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	16	0.65
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	16	0.65
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	16	0.65
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB1	11	0.65
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB2	11	0.65
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB3	11	0.65
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB1	11	0.65
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB2	11	0.65
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB3	11	0.65
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB1	13	0.65
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB2	13	0.65
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB3	13	0.65
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB1	13	0.65
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB2	13	0.65
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB3	13	0.65
(1,1726)	1:331:A:PRO:HB2	1:338:A:ILE:HB	19	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1726)	1:331:A:PRO:HB3	1:338:A:ILE:HB	19	0.65
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	18	0.65
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	18	0.65
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	18	0.65
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	18	0.65
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	18	0.65
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	18	0.65
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	18	0.65
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	18	0.65
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	18	0.65
(1,1511)	1:315:A:PRO:HG2	1:319:A:ARG:H	10	0.65
(1,1511)	1:315:A:PRO:HG3	1:319:A:ARG:H	10	0.65
(1,1505)	1:315:A:PRO:HD2	1:350:A:ASN:HA	10	0.65
(1,1505)	1:315:A:PRO:HD3	1:350:A:ASN:HA	10	0.65
(1,1317)	1:302:A:GLN:HE21	1:332:A:LEU:HD21	18	0.65
(1,1317)	1:302:A:GLN:HE21	1:332:A:LEU:HD22	18	0.65
(1,1317)	1:302:A:GLN:HE21	1:332:A:LEU:HD23	18	0.65
(1,1317)	1:302:A:GLN:HE22	1:332:A:LEU:HD21	18	0.65
(1,1317)	1:302:A:GLN:HE22	1:332:A:LEU:HD22	18	0.65
(1,1317)	1:302:A:GLN:HE22	1:332:A:LEU:HD23	18	0.65
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	9	0.65
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	9	0.65
(1,988)	1:287:A:ASP:HB2	1:293:A:HIS:HA	2	0.65
(1,988)	1:287:A:ASP:HB3	1:293:A:HIS:HA	2	0.65
(1,988)	1:287:A:ASP:HB2	1:293:A:HIS:HA	17	0.65
(1,988)	1:287:A:ASP:HB3	1:293:A:HIS:HA	17	0.65
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	5	0.65
(1,757)	1:276:A:SER:HB2	1:355:A:ARG:HG2	7	0.65
(1,757)	1:276:A:SER:HB3	1:355:A:ARG:HG2	7	0.65
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	12	0.65
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	12	0.65
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	12	0.65
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	12	0.65
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	8	0.64
(1,3479)	1:446:A:HIS:HD2	1:484:A:SER:H	1	0.64
(1,3479)	1:446:A:HIS:HD2	1:484:A:SER:H	7	0.64
(1,3479)	1:446:A:HIS:HD2	1:484:A:SER:H	18	0.64
(1,3315)	1:434:A:THR:HA	1:461:A:SER:HA	19	0.64
(1,3313)	1:434:A:THR:HA	1:465:A:ASP:HB2	4	0.64
(1,3313)	1:434:A:THR:HA	1:465:A:ASP:HB3	4	0.64
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD21	18	0.64
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD22	18	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD23	18	0.64
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB2	17	0.64
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB3	17	0.64
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB2	17	0.64
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB3	17	0.64
(1,3110)	1:426:A:GLY:HA2	1:492:A:LYS:HD3	17	0.64
(1,3110)	1:426:A:GLY:HA3	1:492:A:LYS:HD3	17	0.64
(1,3110)	1:426:A:GLY:HA2	1:492:A:LYS:HD3	18	0.64
(1,3110)	1:426:A:GLY:HA3	1:492:A:LYS:HD3	18	0.64
(1,2901)	1:409:A:SER:HB2	1:413:A:THR:HG21	18	0.64
(1,2901)	1:409:A:SER:HB2	1:413:A:THR:HG22	18	0.64
(1,2901)	1:409:A:SER:HB2	1:413:A:THR:HG23	18	0.64
(1,2901)	1:409:A:SER:HB3	1:413:A:THR:HG21	18	0.64
(1,2901)	1:409:A:SER:HB3	1:413:A:THR:HG22	18	0.64
(1,2901)	1:409:A:SER:HB3	1:413:A:THR:HG23	18	0.64
(1,2889)	1:408:A:ASP:HB3	1:451:A:ARG:HH22	16	0.64
(1,2860)	1:405:A:THR:HG21	1:442:A:LYS:HG2	12	0.64
(1,2860)	1:405:A:THR:HG21	1:442:A:LYS:HG3	12	0.64
(1,2860)	1:405:A:THR:HG22	1:442:A:LYS:HG2	12	0.64
(1,2860)	1:405:A:THR:HG22	1:442:A:LYS:HG3	12	0.64
(1,2860)	1:405:A:THR:HG23	1:442:A:LYS:HG2	12	0.64
(1,2860)	1:405:A:THR:HG23	1:442:A:LYS:HG3	12	0.64
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG11	1	0.64
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG12	1	0.64
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG13	1	0.64
(1,2697)	1:398:A:LYS:HA	1:475:A:PHE:HE1	7	0.64
(1,2538)	1:386:A:PRO:HA	1:471:A:TYR:HB2	7	0.64
(1,2538)	1:386:A:PRO:HA	1:471:A:TYR:HB3	7	0.64
(1,2505)	1:384:A:GLU:HA	1:468:A:MET:HA	10	0.64
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG2	6	0.64
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG3	6	0.64
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG2	6	0.64
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG3	6	0.64
(1,1935)	1:350:A:ASN:HA	1:354:A:LYS:HG2	14	0.64
(1,1935)	1:350:A:ASN:HA	1:354:A:LYS:HG3	14	0.64
(1,1726)	1:331:A:PRO:HB2	1:338:A:ILE:HB	11	0.64
(1,1726)	1:331:A:PRO:HB3	1:338:A:ILE:HB	11	0.64
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	5	0.64
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	5	0.64
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	5	0.64
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	5	0.64
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	5	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	5	0.64
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	5	0.64
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	5	0.64
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	5	0.64
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	8	0.64
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	8	0.64
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	8	0.64
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	8	0.64
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	8	0.64
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	8	0.64
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	8	0.64
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	8	0.64
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	8	0.64
(1,1511)	1:315:A:PRO:HG2	1:319:A:ARG:H	12	0.64
(1,1511)	1:315:A:PRO:HG3	1:319:A:ARG:H	12	0.64
(1,1367)	1:307:A:MET:HE1	1:339:A:LEU:H	18	0.64
(1,1367)	1:307:A:MET:HE2	1:339:A:LEU:H	18	0.64
(1,1367)	1:307:A:MET:HE3	1:339:A:LEU:H	18	0.64
(1,1072)	1:295:A:HIS:HE1	1:311:A:GLU:HA	17	0.64
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	1	0.64
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	1	0.64
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD2	13	0.64
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD3	13	0.64
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	11	0.64
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	10	0.64
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	10	0.64
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	10	0.64
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	2	0.64
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	11	0.64
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG21	17	0.64
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG22	17	0.64
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG23	17	0.64
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG21	20	0.64
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG22	20	0.64
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG23	20	0.64
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	1	0.63
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	1	0.63
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	1	0.63
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	1	0.63
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	1	0.63
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	1	0.63
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	1	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	1	0.63
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	1	0.63
(1,3882)	1:485:A:LYS:HB2	1:487:A:ASP:HB3	20	0.63
(1,3649)	1:460:A:LEU:HD21	1:472:A:LEU:HD11	7	0.63
(1,3649)	1:460:A:LEU:HD21	1:472:A:LEU:HD12	7	0.63
(1,3649)	1:460:A:LEU:HD21	1:472:A:LEU:HD13	7	0.63
(1,3649)	1:460:A:LEU:HD22	1:472:A:LEU:HD11	7	0.63
(1,3649)	1:460:A:LEU:HD22	1:472:A:LEU:HD12	7	0.63
(1,3649)	1:460:A:LEU:HD22	1:472:A:LEU:HD13	7	0.63
(1,3649)	1:460:A:LEU:HD23	1:472:A:LEU:HD11	7	0.63
(1,3649)	1:460:A:LEU:HD23	1:472:A:LEU:HD12	7	0.63
(1,3649)	1:460:A:LEU:HD23	1:472:A:LEU:HD13	7	0.63
(1,3326)	1:435:A:ALA:H	1:465:A:ASP:HB2	4	0.63
(1,3326)	1:435:A:ALA:H	1:465:A:ASP:HB3	4	0.63
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG2	9	0.63
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG3	9	0.63
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG2	9	0.63
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG3	9	0.63
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG2	17	0.63
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG3	17	0.63
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG2	17	0.63
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG3	17	0.63
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	1	0.63
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	1	0.63
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	1	0.63
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	1	0.63
(1,3110)	1:426:A:GLY:HA2	1:492:A:LYS:HD3	3	0.63
(1,3110)	1:426:A:GLY:HA3	1:492:A:LYS:HD3	3	0.63
(1,3110)	1:426:A:GLY:HA2	1:492:A:LYS:HD3	20	0.63
(1,3110)	1:426:A:GLY:HA3	1:492:A:LYS:HD3	20	0.63
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD11	3	0.63
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD12	3	0.63
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD13	3	0.63
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD11	3	0.63
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD12	3	0.63
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD13	3	0.63
(1,3007)	1:419:A:TYR:HE2	1:478:A:LYS:HG2	20	0.63
(1,3007)	1:419:A:TYR:HE2	1:478:A:LYS:HG3	20	0.63
(1,2997)	1:418:A:ASP:HA	1:422:A:ARG:HG2	2	0.63
(1,2997)	1:418:A:ASP:HA	1:422:A:ARG:HG3	2	0.63
(1,2938)	1:414:A:VAL:HG21	1:418:A:ASP:H	5	0.63
(1,2938)	1:414:A:VAL:HG22	1:418:A:ASP:H	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2938)	1:414:A:VAL:HG23	1:418:A:ASP:H	5	0.63
(1,2889)	1:408:A:ASP:HB3	1:451:A:ARG:HH22	5	0.63
(1,2427)	1:380:A:LEU:HD11	1:463:A:ARG:H	2	0.63
(1,2427)	1:380:A:LEU:HD12	1:463:A:ARG:H	2	0.63
(1,2427)	1:380:A:LEU:HD13	1:463:A:ARG:H	2	0.63
(1,2427)	1:380:A:LEU:HD11	1:463:A:ARG:H	3	0.63
(1,2427)	1:380:A:LEU:HD12	1:463:A:ARG:H	3	0.63
(1,2427)	1:380:A:LEU:HD13	1:463:A:ARG:H	3	0.63
(1,2426)	1:380:A:LEU:HD22	1:464:A:ILE:H	11	0.63
(1,2335)	1:375:A:TRP:HH2	1:468:A:MET:HE1	17	0.63
(1,2335)	1:375:A:TRP:HH2	1:468:A:MET:HE2	17	0.63
(1,2335)	1:375:A:TRP:HH2	1:468:A:MET:HE3	17	0.63
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA2	4	0.63
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA3	4	0.63
(1,2288)	1:372:A:GLN:HE21	1:376:A:GLN:H	12	0.63
(1,2288)	1:372:A:GLN:HE22	1:376:A:GLN:H	12	0.63
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	7	0.63
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	7	0.63
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	7	0.63
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	7	0.63
(1,2048)	1:357:A:LEU:HD11	1:392:A:ASN:H	14	0.63
(1,2048)	1:357:A:LEU:HD12	1:392:A:ASN:H	14	0.63
(1,2048)	1:357:A:LEU:HD13	1:392:A:ASN:H	14	0.63
(1,1946)	1:351:A:ALA:HA	1:355:A:ARG:HD2	20	0.63
(1,1946)	1:351:A:ALA:HA	1:355:A:ARG:HD3	20	0.63
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD21	3	0.63
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD22	3	0.63
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD21	14	0.63
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD22	14	0.63
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD21	16	0.63
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD22	16	0.63
(1,1391)	1:309:A:ASP:HB2	1:311:A:GLU:HB2	18	0.63
(1,1391)	1:309:A:ASP:HB2	1:311:A:GLU:HB3	18	0.63
(1,1391)	1:309:A:ASP:HB3	1:311:A:GLU:HB2	18	0.63
(1,1391)	1:309:A:ASP:HB3	1:311:A:GLU:HB3	18	0.63
(1,1013)	1:288:A:MET:HA	1:294:A:LYS:H	15	0.63
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	6	0.63
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	19	0.63
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	9	0.63
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG21	19	0.63
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG22	19	0.63
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG23	19	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:338:A:ILE:HD11	1:342:A:SER:H	7	0.62
(2,9)	1:338:A:ILE:HD12	1:342:A:SER:H	7	0.62
(2,9)	1:338:A:ILE:HD13	1:342:A:SER:H	7	0.62
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	11	0.62
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	11	0.62
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	11	0.62
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	11	0.62
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	11	0.62
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	11	0.62
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	11	0.62
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	11	0.62
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	11	0.62
(2,5)	1:290:A:ASN:HB2	1:293:A:HIS:HA	7	0.62
(2,5)	1:290:A:ASN:HB3	1:293:A:HIS:HA	7	0.62
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	20	0.62
(1,3904)	1:487:A:ASP:HA	1:491:A:GLU:HB2	14	0.62
(1,3904)	1:487:A:ASP:HA	1:491:A:GLU:HB3	14	0.62
(1,3888)	1:486:A:VAL:HG11	1:491:A:GLU:HA	14	0.62
(1,3888)	1:486:A:VAL:HG12	1:491:A:GLU:HA	14	0.62
(1,3888)	1:486:A:VAL:HG13	1:491:A:GLU:HA	14	0.62
(1,3882)	1:485:A:LYS:HB2	1:487:A:ASP:HB3	12	0.62
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB2	3	0.62
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB3	3	0.62
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB2	3	0.62
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB3	3	0.62
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB2	3	0.62
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB3	3	0.62
(1,3529)	1:449:A:LEU:HD21	1:494:A:ALA:H	16	0.62
(1,3529)	1:449:A:LEU:HD22	1:494:A:ALA:H	16	0.62
(1,3529)	1:449:A:LEU:HD23	1:494:A:ALA:H	16	0.62
(1,3164)	1:429:A:LYS:HB2	1:431:A:TYR:HE1	7	0.62
(1,3164)	1:429:A:LYS:HB2	1:431:A:TYR:HE2	7	0.62
(1,3164)	1:429:A:LYS:HB3	1:431:A:TYR:HE1	7	0.62
(1,3164)	1:429:A:LYS:HB3	1:431:A:TYR:HE2	7	0.62
(1,3145)	1:429:A:LYS:HB2	1:489:A:SER:HB2	7	0.62
(1,3145)	1:429:A:LYS:HB2	1:489:A:SER:HB3	7	0.62
(1,3145)	1:429:A:LYS:HB3	1:489:A:SER:HB2	7	0.62
(1,3145)	1:429:A:LYS:HB3	1:489:A:SER:HB3	7	0.62
(1,3136)	1:428:A:GLU:HG2	1:478:A:LYS:HA	16	0.62
(1,3136)	1:428:A:GLU:HG3	1:478:A:LYS:HA	16	0.62
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	15	0.62
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	15	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	15	0.62
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	15	0.62
(1,3080)	1:423:A:MET:HB2	1:427:A:GLN:HB2	7	0.62
(1,3080)	1:423:A:MET:HB2	1:427:A:GLN:HB3	7	0.62
(1,3080)	1:423:A:MET:HB3	1:427:A:GLN:HB2	7	0.62
(1,3080)	1:423:A:MET:HB3	1:427:A:GLN:HB3	7	0.62
(1,2997)	1:418:A:ASP:HA	1:422:A:ARG:HG2	8	0.62
(1,2997)	1:418:A:ASP:HA	1:422:A:ARG:HG3	8	0.62
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG11	5	0.62
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG12	5	0.62
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG13	5	0.62
(1,2700)	1:398:A:LYS:HG2	1:417:A:GLU:HG2	10	0.62
(1,2700)	1:398:A:LYS:HG2	1:417:A:GLU:HG3	10	0.62
(1,2700)	1:398:A:LYS:HG3	1:417:A:GLU:HG2	10	0.62
(1,2700)	1:398:A:LYS:HG3	1:417:A:GLU:HG3	10	0.62
(1,2426)	1:380:A:LEU:HD22	1:464:A:ILE:H	5	0.62
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	20	0.62
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	20	0.62
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	20	0.62
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	20	0.62
(1,2122)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	19	0.62
(1,2048)	1:357:A:LEU:HD11	1:392:A:ASN:H	20	0.62
(1,2048)	1:357:A:LEU:HD12	1:392:A:ASN:H	20	0.62
(1,2048)	1:357:A:LEU:HD13	1:392:A:ASN:H	20	0.62
(1,2045)	1:357:A:LEU:HD21	1:395:A:ALA:H	18	0.62
(1,2045)	1:357:A:LEU:HD22	1:395:A:ALA:H	18	0.62
(1,2045)	1:357:A:LEU:HD23	1:395:A:ALA:H	18	0.62
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	14	0.62
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	16	0.62
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	16	0.62
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	16	0.62
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	16	0.62
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	16	0.62
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	16	0.62
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	16	0.62
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	16	0.62
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	16	0.62
(1,1486)	1:314:A:MET:HB2	1:319:A:ARG:H	8	0.62
(1,1486)	1:314:A:MET:HB3	1:319:A:ARG:H	8	0.62
(1,1452)	1:313:A:PHE:HZ	1:345:A:THR:HA	4	0.62
(1,1074)	1:295:A:HIS:HA	1:309:A:ASP:HA	18	0.62
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD2	6	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD3	6	0.62
(1,989)	1:287:A:ASP:HB2	1:292:A:ASP:H	3	0.62
(1,989)	1:287:A:ASP:HB3	1:292:A:ASP:H	3	0.62
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	4	0.62
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	6	0.62
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	6	0.62
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	6	0.62
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	19	0.62
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	19	0.62
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	19	0.62
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	20	0.62
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	10	0.62
(1,352)	1:250:A:TYR:HE1	1:256:A:ASP:H	3	0.62
(1,352)	1:250:A:TYR:HE2	1:256:A:ASP:H	3	0.62
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	9	0.62
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	11	0.62
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	8	0.62
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG21	4	0.62
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG22	4	0.62
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG23	4	0.62
(1,37)	1:233:A:LEU:HD11	1:249:A:PHE:H	18	0.62
(1,37)	1:233:A:LEU:HD12	1:249:A:PHE:H	18	0.62
(1,37)	1:233:A:LEU:HD13	1:249:A:PHE:H	18	0.62
(2,9)	1:338:A:ILE:HD11	1:342:A:SER:H	15	0.61
(2,9)	1:338:A:ILE:HD12	1:342:A:SER:H	15	0.61
(2,9)	1:338:A:ILE:HD13	1:342:A:SER:H	15	0.61
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	10	0.61
(1,3479)	1:446:A:HIS:HD2	1:484:A:SER:H	8	0.61
(1,3353)	1:436:A:ASP:HA	1:461:A:SER:HA	16	0.61
(1,3072)	1:423:A:MET:HE1	1:431:A:TYR:HD1	18	0.61
(1,3072)	1:423:A:MET:HE1	1:431:A:TYR:HD2	18	0.61
(1,3072)	1:423:A:MET:HE2	1:431:A:TYR:HD1	18	0.61
(1,3072)	1:423:A:MET:HE2	1:431:A:TYR:HD2	18	0.61
(1,3072)	1:423:A:MET:HE3	1:431:A:TYR:HD1	18	0.61
(1,3072)	1:423:A:MET:HE3	1:431:A:TYR:HD2	18	0.61
(1,2938)	1:414:A:VAL:HG21	1:418:A:ASP:H	2	0.61
(1,2938)	1:414:A:VAL:HG22	1:418:A:ASP:H	2	0.61
(1,2938)	1:414:A:VAL:HG23	1:418:A:ASP:H	2	0.61
(1,2938)	1:414:A:VAL:HG21	1:418:A:ASP:H	4	0.61
(1,2938)	1:414:A:VAL:HG22	1:418:A:ASP:H	4	0.61
(1,2938)	1:414:A:VAL:HG23	1:418:A:ASP:H	4	0.61
(1,2938)	1:414:A:VAL:HG21	1:418:A:ASP:H	7	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2938)	1:414:A:VAL:HG22	1:418:A:ASP:H	7	0.61
(1,2938)	1:414:A:VAL:HG23	1:418:A:ASP:H	7	0.61
(1,2938)	1:414:A:VAL:HG21	1:418:A:ASP:H	14	0.61
(1,2938)	1:414:A:VAL:HG22	1:418:A:ASP:H	14	0.61
(1,2938)	1:414:A:VAL:HG23	1:418:A:ASP:H	14	0.61
(1,2889)	1:408:A:ASP:HB3	1:451:A:ARG:HH22	1	0.61
(1,2425)	1:380:A:LEU:HB2	1:464:A:ILE:H	2	0.61
(1,2425)	1:380:A:LEU:HB3	1:464:A:ILE:H	2	0.61
(1,2381)	1:376:A:GLN:HA	1:412:A:GLN:HE21	7	0.61
(1,2381)	1:376:A:GLN:HA	1:412:A:GLN:HE22	7	0.61
(1,2379)	1:376:A:GLN:HE21	1:413:A:THR:HG21	2	0.61
(1,2379)	1:376:A:GLN:HE21	1:413:A:THR:HG22	2	0.61
(1,2379)	1:376:A:GLN:HE21	1:413:A:THR:HG23	2	0.61
(1,2379)	1:376:A:GLN:HE22	1:413:A:THR:HG21	2	0.61
(1,2379)	1:376:A:GLN:HE22	1:413:A:THR:HG22	2	0.61
(1,2379)	1:376:A:GLN:HE22	1:413:A:THR:HG23	2	0.61
(1,2317)	1:374:A:PHE:HZ	1:382:A:LEU:H	19	0.61
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	5	0.61
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	5	0.61
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	5	0.61
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	5	0.61
(1,2045)	1:357:A:LEU:HD21	1:395:A:ALA:H	19	0.61
(1,2045)	1:357:A:LEU:HD22	1:395:A:ALA:H	19	0.61
(1,2045)	1:357:A:LEU:HD23	1:395:A:ALA:H	19	0.61
(1,1989)	1:354:A:LYS:HA	1:392:A:ASN:HD21	2	0.61
(1,1989)	1:354:A:LYS:HA	1:392:A:ASN:HD22	2	0.61
(1,1951)	1:351:A:ALA:HA	1:354:A:LYS:HD2	20	0.61
(1,1951)	1:351:A:ALA:HA	1:354:A:LYS:HD3	20	0.61
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	1	0.61
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	17	0.61
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	17	0.61
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	17	0.61
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	17	0.61
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	17	0.61
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	17	0.61
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	17	0.61
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	17	0.61
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	17	0.61
(1,1432)	1:312:A:GLN:HE21	1:336:A:ARG:HG2	9	0.61
(1,1432)	1:312:A:GLN:HE21	1:336:A:ARG:HG3	9	0.61
(1,1432)	1:312:A:GLN:HE22	1:336:A:ARG:HG2	9	0.61
(1,1432)	1:312:A:GLN:HE22	1:336:A:ARG:HG3	9	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1167)	1:298:A:LYS:HA	1:309:A:ASP:HA	9	0.61
(1,1081)	1:296:A:GLY:H	1:319:A:ARG:HA	6	0.61
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD2	15	0.61
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD3	15	0.61
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	7	0.61
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	7	0.61
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	7	0.61
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD2	1	0.61
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD3	1	0.61
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD2	1	0.61
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD3	1	0.61
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD2	1	0.61
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD3	1	0.61
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	14	0.61
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	4	0.61
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	9	0.61
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	15	0.61
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	15	0.61
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG21	4	0.61
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG22	4	0.61
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG23	4	0.61
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	16	0.6
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	16	0.6
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	16	0.6
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	16	0.6
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	16	0.6
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	16	0.6
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	16	0.6
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	16	0.6
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	16	0.6
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB1	18	0.6
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB2	18	0.6
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB3	18	0.6
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB1	18	0.6
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB2	18	0.6
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB3	18	0.6
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB1	18	0.6
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB2	18	0.6
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB3	18	0.6
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	5	0.6
(1,3761)	1:471:A:TYR:HA	1:473:A:THR:HG21	10	0.6
(1,3761)	1:471:A:TYR:HA	1:473:A:THR:HG22	10	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3761)	1:471:A:TYR:HA	1:473:A:THR:HG23	10	0.6
(1,3633)	1:458:A:LEU:HD11	1:480:A:PHE:HD1	16	0.6
(1,3633)	1:458:A:LEU:HD11	1:480:A:PHE:HD2	16	0.6
(1,3633)	1:458:A:LEU:HD12	1:480:A:PHE:HD1	16	0.6
(1,3633)	1:458:A:LEU:HD12	1:480:A:PHE:HD2	16	0.6
(1,3633)	1:458:A:LEU:HD13	1:480:A:PHE:HD1	16	0.6
(1,3633)	1:458:A:LEU:HD13	1:480:A:PHE:HD2	16	0.6
(1,3479)	1:446:A:HIS:HD2	1:484:A:SER:H	15	0.6
(1,3315)	1:434:A:THR:HA	1:461:A:SER:HA	9	0.6
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	12	0.6
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	12	0.6
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	12	0.6
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	12	0.6
(1,3178)	1:430:A:ILE:HD11	1:479:A:PRO:HA	17	0.6
(1,3178)	1:430:A:ILE:HD12	1:479:A:PRO:HA	17	0.6
(1,3178)	1:430:A:ILE:HD13	1:479:A:PRO:HA	17	0.6
(1,3144)	1:429:A:LYS:HD2	1:489:A:SER:HA	1	0.6
(1,3144)	1:429:A:LYS:HD3	1:489:A:SER:HA	1	0.6
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG2	18	0.6
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG3	18	0.6
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG2	18	0.6
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG3	18	0.6
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD11	3	0.6
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD12	3	0.6
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD13	3	0.6
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD11	3	0.6
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD12	3	0.6
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD13	3	0.6
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD11	9	0.6
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD12	9	0.6
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD13	9	0.6
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD11	9	0.6
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD12	9	0.6
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD13	9	0.6
(1,3081)	1:423:A:MET:HE1	1:427:A:GLN:HB2	4	0.6
(1,3081)	1:423:A:MET:HE1	1:427:A:GLN:HB3	4	0.6
(1,3081)	1:423:A:MET:HE2	1:427:A:GLN:HB2	4	0.6
(1,3081)	1:423:A:MET:HE2	1:427:A:GLN:HB3	4	0.6
(1,3081)	1:423:A:MET:HE3	1:427:A:GLN:HB2	4	0.6
(1,3081)	1:423:A:MET:HE3	1:427:A:GLN:HB3	4	0.6
(1,2986)	1:417:A:GLU:HA	1:421:A:SER:HB2	5	0.6
(1,2986)	1:417:A:GLU:HA	1:421:A:SER:HB3	5	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2984)	1:417:A:GLU:HA	1:421:A:SER:H	4	0.6
(1,2898)	1:409:A:SER:H	1:442:A:LYS:HE2	2	0.6
(1,2898)	1:409:A:SER:H	1:442:A:LYS:HE3	2	0.6
(1,2889)	1:408:A:ASP:HB3	1:451:A:ARG:HH22	10	0.6
(1,2855)	1:405:A:THR:HB	1:451:A:ARG:HA	13	0.6
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG11	2	0.6
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG12	2	0.6
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG13	2	0.6
(1,2595)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	12	0.6
(1,2595)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	12	0.6
(1,2595)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	12	0.6
(1,2595)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	12	0.6
(1,2444)	1:381:A:VAL:HA	1:464:A:ILE:HD11	17	0.6
(1,2444)	1:381:A:VAL:HA	1:464:A:ILE:HD12	17	0.6
(1,2444)	1:381:A:VAL:HA	1:464:A:ILE:HD13	17	0.6
(1,2122)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	17	0.6
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB1	19	0.6
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB2	19	0.6
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB3	19	0.6
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB1	19	0.6
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB2	19	0.6
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB3	19	0.6
(1,1964)	1:352:A:LEU:HA	1:355:A:ARG:HD2	20	0.6
(1,1964)	1:352:A:LEU:HA	1:355:A:ARG:HD3	20	0.6
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	17	0.6
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	1	0.6
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	1	0.6
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	1	0.6
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	1	0.6
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	1	0.6
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	1	0.6
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	1	0.6
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	1	0.6
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	1	0.6
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	13	0.6
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	13	0.6
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	13	0.6
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	13	0.6
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	13	0.6
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	13	0.6
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	13	0.6
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	13	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	13	0.6
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	20	0.6
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	20	0.6
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	20	0.6
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	20	0.6
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	20	0.6
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	20	0.6
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	20	0.6
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	20	0.6
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	20	0.6
(1,1452)	1:313:A:PHE:HZ	1:345:A:THR:HA	15	0.6
(1,1425)	1:312:A:GLN:HG2	1:339:A:LEU:HA	16	0.6
(1,1425)	1:312:A:GLN:HG3	1:339:A:LEU:HA	16	0.6
(1,1367)	1:307:A:MET:HE1	1:339:A:LEU:H	16	0.6
(1,1367)	1:307:A:MET:HE2	1:339:A:LEU:H	16	0.6
(1,1367)	1:307:A:MET:HE3	1:339:A:LEU:H	16	0.6
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE1	9	0.6
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE2	9	0.6
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	12	0.6
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	12	0.6
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	13	0.6
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	13	0.6
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HA	18	0.6
(1,1066)	1:295:A:HIS:HB2	1:320:A:PHE:HA	9	0.6
(1,1066)	1:295:A:HIS:HB3	1:320:A:PHE:HA	9	0.6
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD2	14	0.6
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD3	14	0.6
(1,1044)	1:291:A:ARG:HA	1:293:A:HIS:HA	12	0.6
(1,1020)	1:289:A:TRP:HH2	1:384:A:GLU:HG2	9	0.6
(1,1020)	1:289:A:TRP:HH2	1:384:A:GLU:HG3	9	0.6
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	16	0.6
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	14	0.6
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	1	0.6
(1,864)	1:280:A:ILE:HD11	1:371:A:TYR:HE1	11	0.6
(1,864)	1:280:A:ILE:HD11	1:371:A:TYR:HE2	11	0.6
(1,864)	1:280:A:ILE:HD12	1:371:A:TYR:HE1	11	0.6
(1,864)	1:280:A:ILE:HD12	1:371:A:TYR:HE2	11	0.6
(1,864)	1:280:A:ILE:HD13	1:371:A:TYR:HE1	11	0.6
(1,864)	1:280:A:ILE:HD13	1:371:A:TYR:HE2	11	0.6
(1,700)	1:273:A:GLU:HB2	1:329:A:ASP:H	8	0.6
(1,700)	1:273:A:GLU:HB3	1:329:A:ASP:H	8	0.6
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB2	1	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB3	1	0.6
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	5	0.6
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	5	0.6
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	5	0.6
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	8	0.6
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	8	0.6
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	20	0.6
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	20	0.6
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	5	0.6
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	10	0.6
(1,147)	1:238:A:LYS:HD2	1:266:A:ASN:HD21	9	0.6
(1,147)	1:238:A:LYS:HD2	1:266:A:ASN:HD22	9	0.6
(1,147)	1:238:A:LYS:HD3	1:266:A:ASN:HD21	9	0.6
(1,147)	1:238:A:LYS:HD3	1:266:A:ASN:HD22	9	0.6
(2,14)	1:442:A:LYS:H	1:461:A:SER:HB2	8	0.59
(2,14)	1:442:A:LYS:H	1:461:A:SER:HB3	8	0.59
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	13	0.59
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	20	0.59
(1,3538)	1:449:A:LEU:HD11	1:453:A:LYS:HB2	20	0.59
(1,3538)	1:449:A:LEU:HD11	1:453:A:LYS:HB3	20	0.59
(1,3538)	1:449:A:LEU:HD12	1:453:A:LYS:HB2	20	0.59
(1,3538)	1:449:A:LEU:HD12	1:453:A:LYS:HB3	20	0.59
(1,3538)	1:449:A:LEU:HD13	1:453:A:LYS:HB2	20	0.59
(1,3538)	1:449:A:LEU:HD13	1:453:A:LYS:HB3	20	0.59
(1,3529)	1:449:A:LEU:HD21	1:494:A:ALA:H	10	0.59
(1,3529)	1:449:A:LEU:HD22	1:494:A:ALA:H	10	0.59
(1,3529)	1:449:A:LEU:HD23	1:494:A:ALA:H	10	0.59
(1,3479)	1:446:A:HIS:HD2	1:484:A:SER:H	3	0.59
(1,3332)	1:435:A:ALA:H	1:460:A:LEU:H	20	0.59
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG2	3	0.59
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG3	3	0.59
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG2	3	0.59
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG3	3	0.59
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	3	0.59
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	3	0.59
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	3	0.59
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	3	0.59
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	19	0.59
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	19	0.59
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	19	0.59
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	19	0.59
(1,3089)	1:424:A:LYS:H	1:455:A:ILE:HA	1	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2871)	1:406:A:HIS:HA	1:456:A:GLU:HG2	7	0.59
(1,2871)	1:406:A:HIS:HA	1:456:A:GLU:HG3	7	0.59
(1,2595)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	5	0.59
(1,2595)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	5	0.59
(1,2595)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	5	0.59
(1,2595)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	5	0.59
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB2	4	0.59
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB3	4	0.59
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA2	20	0.59
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA3	20	0.59
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	4	0.59
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	19	0.59
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	19	0.59
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	19	0.59
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	19	0.59
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	19	0.59
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	19	0.59
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	19	0.59
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	19	0.59
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	19	0.59
(1,1452)	1:313:A:PHE:HZ	1:345:A:THR:HA	16	0.59
(1,1367)	1:307:A:MET:HE1	1:339:A:LEU:H	9	0.59
(1,1367)	1:307:A:MET:HE2	1:339:A:LEU:H	9	0.59
(1,1367)	1:307:A:MET:HE3	1:339:A:LEU:H	9	0.59
(1,1315)	1:302:A:GLN:HE21	1:332:A:LEU:HD11	18	0.59
(1,1315)	1:302:A:GLN:HE21	1:332:A:LEU:HD12	18	0.59
(1,1315)	1:302:A:GLN:HE21	1:332:A:LEU:HD13	18	0.59
(1,1315)	1:302:A:GLN:HE22	1:332:A:LEU:HD11	18	0.59
(1,1315)	1:302:A:GLN:HE22	1:332:A:LEU:HD12	18	0.59
(1,1315)	1:302:A:GLN:HE22	1:332:A:LEU:HD13	18	0.59
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD11	4	0.59
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD12	4	0.59
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD13	4	0.59
(1,1013)	1:288:A:MET:HA	1:294:A:LYS:H	19	0.59
(1,990)	1:287:A:ASP:HB2	1:292:A:ASP:HB2	3	0.59
(1,990)	1:287:A:ASP:HB2	1:292:A:ASP:HB3	3	0.59
(1,990)	1:287:A:ASP:HB3	1:292:A:ASP:HB2	3	0.59
(1,990)	1:287:A:ASP:HB3	1:292:A:ASP:HB3	3	0.59
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	1	0.59
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	1	0.59
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	1	0.59
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD21	20	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD22	20	0.59
(1,439)	1:255:A:HIS:HE1	1:308:A:ASP:HB2	9	0.59
(1,439)	1:255:A:HIS:HE1	1:308:A:ASP:HB3	9	0.59
(1,346)	1:250:A:TYR:HB2	1:263:A:TRP:HE3	18	0.59
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	3	0.59
(1,139)	1:237:A:ASN:HD21	1:239:A:SER:H	1	0.59
(1,139)	1:237:A:ASN:HD22	1:239:A:SER:H	1	0.59
(1,102)	1:234:A:TRP:HE1	1:235:A:THR:HB	4	0.59
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	18	0.58
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	18	0.58
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	18	0.58
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	18	0.58
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	18	0.58
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	18	0.58
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	18	0.58
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	18	0.58
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	18	0.58
(1,3882)	1:485:A:LYS:HB2	1:487:A:ASP:HB3	4	0.58
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB2	6	0.58
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB3	6	0.58
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB2	6	0.58
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB3	6	0.58
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB2	6	0.58
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB3	6	0.58
(1,3536)	1:449:A:LEU:HA	1:453:A:LYS:H	20	0.58
(1,3480)	1:446:A:HIS:HE1	1:484:A:SER:HA	13	0.58
(1,3362)	1:437:A:SER:HA	1:461:A:SER:HA	20	0.58
(1,3154)	1:429:A:LYS:HA	1:480:A:PHE:HA	14	0.58
(1,2938)	1:414:A:VAL:HG21	1:418:A:ASP:H	9	0.58
(1,2938)	1:414:A:VAL:HG22	1:418:A:ASP:H	9	0.58
(1,2938)	1:414:A:VAL:HG23	1:418:A:ASP:H	9	0.58
(1,2875)	1:406:A:HIS:HB2	1:414:A:VAL:HB	2	0.58
(1,2875)	1:406:A:HIS:HB3	1:414:A:VAL:HB	2	0.58
(1,2830)	1:404:A:SER:H	1:407:A:THR:HB	13	0.58
(1,2764)	1:402:A:PHE:H	1:414:A:VAL:HB	11	0.58
(1,2695)	1:398:A:LYS:HD2	1:475:A:PHE:HZ	9	0.58
(1,2695)	1:398:A:LYS:HD3	1:475:A:PHE:HZ	9	0.58
(1,2694)	1:398:A:LYS:HA	1:475:A:PHE:HZ	18	0.58
(1,2594)	1:390:A:PHE:HA	1:393:A:GLN:HA	5	0.58
(1,2563)	1:387:A:ALA:HA	1:471:A:TYR:HE1	4	0.58
(1,2563)	1:387:A:ALA:HA	1:471:A:TYR:HE2	4	0.58
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB2	1	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB3	1	0.58
(1,2505)	1:384:A:GLU:HA	1:468:A:MET:HA	13	0.58
(1,2426)	1:380:A:LEU:HD22	1:464:A:ILE:H	3	0.58
(1,2426)	1:380:A:LEU:HD22	1:464:A:ILE:H	17	0.58
(1,2425)	1:380:A:LEU:HB2	1:464:A:ILE:H	7	0.58
(1,2425)	1:380:A:LEU:HB3	1:464:A:ILE:H	7	0.58
(1,2382)	1:376:A:GLN:HG2	1:412:A:GLN:HE21	9	0.58
(1,2382)	1:376:A:GLN:HG2	1:412:A:GLN:HE22	9	0.58
(1,2382)	1:376:A:GLN:HG3	1:412:A:GLN:HE21	9	0.58
(1,2382)	1:376:A:GLN:HG3	1:412:A:GLN:HE22	9	0.58
(1,2379)	1:376:A:GLN:HE21	1:413:A:THR:HG21	6	0.58
(1,2379)	1:376:A:GLN:HE21	1:413:A:THR:HG22	6	0.58
(1,2379)	1:376:A:GLN:HE21	1:413:A:THR:HG23	6	0.58
(1,2379)	1:376:A:GLN:HE22	1:413:A:THR:HG21	6	0.58
(1,2379)	1:376:A:GLN:HE22	1:413:A:THR:HG22	6	0.58
(1,2379)	1:376:A:GLN:HE22	1:413:A:THR:HG23	6	0.58
(1,2337)	1:375:A:TRP:HD1	1:413:A:THR:HA	14	0.58
(1,2210)	1:367:A:ASP:H	1:371:A:TYR:H	12	0.58
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD21	3	0.58
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD22	3	0.58
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD21	3	0.58
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD22	3	0.58
(1,1959)	1:352:A:LEU:HD21	1:356:A:VAL:H	2	0.58
(1,1959)	1:352:A:LEU:HD22	1:356:A:VAL:H	2	0.58
(1,1959)	1:352:A:LEU:HD23	1:356:A:VAL:H	2	0.58
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	18	0.58
(1,1745)	1:333:A:ASN:HD21	1:338:A:ILE:HD11	13	0.58
(1,1745)	1:333:A:ASN:HD21	1:338:A:ILE:HD12	13	0.58
(1,1745)	1:333:A:ASN:HD21	1:338:A:ILE:HD13	13	0.58
(1,1745)	1:333:A:ASN:HD22	1:338:A:ILE:HD11	13	0.58
(1,1745)	1:333:A:ASN:HD22	1:338:A:ILE:HD12	13	0.58
(1,1745)	1:333:A:ASN:HD22	1:338:A:ILE:HD13	13	0.58
(1,1745)	1:333:A:ASN:HD21	1:338:A:ILE:HD11	15	0.58
(1,1745)	1:333:A:ASN:HD21	1:338:A:ILE:HD12	15	0.58
(1,1745)	1:333:A:ASN:HD21	1:338:A:ILE:HD13	15	0.58
(1,1745)	1:333:A:ASN:HD22	1:338:A:ILE:HD11	15	0.58
(1,1745)	1:333:A:ASN:HD22	1:338:A:ILE:HD12	15	0.58
(1,1745)	1:333:A:ASN:HD22	1:338:A:ILE:HD13	15	0.58
(1,1674)	1:325:A:ILE:HD11	1:327:A:SER:H	15	0.58
(1,1674)	1:325:A:ILE:HD12	1:327:A:SER:H	15	0.58
(1,1674)	1:325:A:ILE:HD13	1:327:A:SER:H	15	0.58
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	12	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	12	0.58
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	12	0.58
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	12	0.58
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	12	0.58
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	12	0.58
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	12	0.58
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	12	0.58
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	12	0.58
(1,1505)	1:315:A:PRO:HD2	1:350:A:ASN:HA	15	0.58
(1,1505)	1:315:A:PRO:HD3	1:350:A:ASN:HA	15	0.58
(1,1334)	1:303:A:ARG:H	1:327:A:SER:H	19	0.58
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	14	0.58
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	14	0.58
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	17	0.58
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	17	0.58
(1,986)	1:287:A:ASP:HB2	1:294:A:LYS:H	9	0.58
(1,986)	1:287:A:ASP:HB3	1:294:A:LYS:H	9	0.58
(1,986)	1:287:A:ASP:HB2	1:294:A:LYS:H	17	0.58
(1,986)	1:287:A:ASP:HB3	1:294:A:LYS:H	17	0.58
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	15	0.58
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	15	0.58
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	15	0.58
(1,525)	1:262:A:THR:HB	1:370:A:LYS:HD2	5	0.58
(1,525)	1:262:A:THR:HB	1:370:A:LYS:HD3	5	0.58
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	11	0.58
(1,440)	1:255:A:HIS:HB2	1:294:A:LYS:HE2	10	0.58
(1,440)	1:255:A:HIS:HB2	1:294:A:LYS:HE3	10	0.58
(1,440)	1:255:A:HIS:HB3	1:294:A:LYS:HE2	10	0.58
(1,440)	1:255:A:HIS:HB3	1:294:A:LYS:HE3	10	0.58
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	5	0.58
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	7	0.58
(1,123)	1:236:A:ARG:HB2	1:240:A:GLU:H	2	0.58
(1,123)	1:236:A:ARG:HB3	1:240:A:GLU:H	2	0.58
(1,102)	1:234:A:TRP:HE1	1:235:A:THR:HB	19	0.58
(1,88)	1:234:A:TRP:HB2	1:265:A:HIS:HD2	7	0.58
(1,88)	1:234:A:TRP:HB3	1:265:A:HIS:HD2	7	0.58
(1,37)	1:233:A:LEU:HD11	1:249:A:PHE:H	8	0.58
(1,37)	1:233:A:LEU:HD12	1:249:A:PHE:H	8	0.58
(1,37)	1:233:A:LEU:HD13	1:249:A:PHE:H	8	0.58
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	8	0.57
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	8	0.57
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	8	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	8	0.57
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	8	0.57
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	8	0.57
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	8	0.57
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	8	0.57
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	8	0.57
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG11	13	0.57
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG12	13	0.57
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG13	13	0.57
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG11	13	0.57
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG12	13	0.57
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG13	13	0.57
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG11	13	0.57
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG12	13	0.57
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG13	13	0.57
(1,3972)	1:318:A:LEU:HD11	2:622:B:TYR:HE1	1	0.57
(1,3972)	1:318:A:LEU:HD12	2:622:B:TYR:HE1	1	0.57
(1,3972)	1:318:A:LEU:HD13	2:622:B:TYR:HE1	1	0.57
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	8	0.57
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	8	0.57
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	8	0.57
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	8	0.57
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	8	0.57
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	8	0.57
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	8	0.57
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	8	0.57
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	8	0.57
(1,3896)	1:486:A:VAL:HA	1:489:A:SER:HB2	2	0.57
(1,3896)	1:486:A:VAL:HA	1:489:A:SER:HB3	2	0.57
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	11	0.57
(1,3882)	1:485:A:LYS:HB2	1:487:A:ASP:HB3	3	0.57
(1,3536)	1:449:A:LEU:HA	1:453:A:LYS:H	8	0.57
(1,3482)	1:446:A:HIS:HA	1:483:A:VAL:HB	13	0.57
(1,3479)	1:446:A:HIS:HD2	1:484:A:SER:H	17	0.57
(1,3271)	1:433:A:ILE:H	1:459:A:LEU:HD21	16	0.57
(1,3271)	1:433:A:ILE:H	1:459:A:LEU:HD22	16	0.57
(1,3271)	1:433:A:ILE:H	1:459:A:LEU:HD23	16	0.57
(1,3245)	1:432:A:TYR:HB2	1:458:A:LEU:H	17	0.57
(1,3245)	1:432:A:TYR:HB3	1:458:A:LEU:H	17	0.57
(1,3178)	1:430:A:ILE:HD11	1:479:A:PRO:HA	12	0.57
(1,3178)	1:430:A:ILE:HD12	1:479:A:PRO:HA	12	0.57
(1,3178)	1:430:A:ILE:HD13	1:479:A:PRO:HA	12	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3110)	1:426:A:GLY:HA2	1:492:A:LYS:HD3	4	0.57
(1,3110)	1:426:A:GLY:HA3	1:492:A:LYS:HD3	4	0.57
(1,3084)	1:423:A:MET:HE1	1:427:A:GLN:HG2	10	0.57
(1,3084)	1:423:A:MET:HE1	1:427:A:GLN:HG3	10	0.57
(1,3084)	1:423:A:MET:HE2	1:427:A:GLN:HG2	10	0.57
(1,3084)	1:423:A:MET:HE2	1:427:A:GLN:HG3	10	0.57
(1,3084)	1:423:A:MET:HE3	1:427:A:GLN:HG2	10	0.57
(1,3084)	1:423:A:MET:HE3	1:427:A:GLN:HG3	10	0.57
(1,2937)	1:414:A:VAL:HG21	1:419:A:TYR:HA	16	0.57
(1,2937)	1:414:A:VAL:HG22	1:419:A:TYR:HA	16	0.57
(1,2937)	1:414:A:VAL:HG23	1:419:A:TYR:HA	16	0.57
(1,2889)	1:408:A:ASP:HB3	1:451:A:ARG:HH22	18	0.57
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG11	8	0.57
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG12	8	0.57
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG13	8	0.57
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB2	14	0.57
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB3	14	0.57
(1,2704)	1:398:A:LYS:HA	1:416:A:LEU:HD11	7	0.57
(1,2704)	1:398:A:LYS:HA	1:416:A:LEU:HD12	7	0.57
(1,2704)	1:398:A:LYS:HA	1:416:A:LEU:HD13	7	0.57
(1,2432)	1:380:A:LEU:HA	1:384:A:GLU:H	11	0.57
(1,2382)	1:376:A:GLN:HG2	1:412:A:GLN:HE21	3	0.57
(1,2382)	1:376:A:GLN:HG2	1:412:A:GLN:HE22	3	0.57
(1,2382)	1:376:A:GLN:HG3	1:412:A:GLN:HE21	3	0.57
(1,2382)	1:376:A:GLN:HG3	1:412:A:GLN:HE22	3	0.57
(1,2357)	1:375:A:TRP:HH2	1:383:A:LYS:HE2	17	0.57
(1,2357)	1:375:A:TRP:HH2	1:383:A:LYS:HE3	17	0.57
(1,2317)	1:374:A:PHE:HZ	1:382:A:LEU:H	16	0.57
(1,2288)	1:372:A:GLN:HE21	1:376:A:GLN:H	11	0.57
(1,2288)	1:372:A:GLN:HE22	1:376:A:GLN:H	11	0.57
(1,2122)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	9	0.57
(1,2122)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	16	0.57
(1,1946)	1:351:A:ALA:HA	1:355:A:ARG:HD2	12	0.57
(1,1946)	1:351:A:ALA:HA	1:355:A:ARG:HD3	12	0.57
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD21	11	0.57
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD22	11	0.57
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	19	0.57
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	4	0.57
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	4	0.57
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	4	0.57
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	4	0.57
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	4	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	4	0.57
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	4	0.57
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	4	0.57
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	4	0.57
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	10	0.57
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	10	0.57
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	10	0.57
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	10	0.57
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	10	0.57
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	10	0.57
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	10	0.57
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	10	0.57
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	10	0.57
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	15	0.57
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	15	0.57
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	15	0.57
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	15	0.57
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	15	0.57
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	15	0.57
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	15	0.57
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	15	0.57
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	15	0.57
(1,1638)	1:320:A:PHE:HA	1:322:A:ARG:HG2	2	0.57
(1,1638)	1:320:A:PHE:HA	1:322:A:ARG:HG3	2	0.57
(1,1430)	1:312:A:GLN:HE21	1:336:A:ARG:HA	10	0.57
(1,1430)	1:312:A:GLN:HE22	1:336:A:ARG:HA	10	0.57
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE1	7	0.57
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE2	7	0.57
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD11	18	0.57
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD12	18	0.57
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD13	18	0.57
(1,1060)	1:294:A:LYS:HD2	1:309:A:ASP:HB2	9	0.57
(1,1060)	1:294:A:LYS:HD2	1:309:A:ASP:HB3	9	0.57
(1,1060)	1:294:A:LYS:HD3	1:309:A:ASP:HB2	9	0.57
(1,1060)	1:294:A:LYS:HD3	1:309:A:ASP:HB3	9	0.57
(1,1044)	1:291:A:ARG:HA	1:293:A:HIS:HA	3	0.57
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	4	0.57
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	9	0.57
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	13	0.57
(1,705)	1:273:A:GLU:HG2	1:328:A:SER:H	8	0.57
(1,705)	1:273:A:GLU:HG3	1:328:A:SER:H	8	0.57
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB2	13	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB3	13	0.57
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	3	0.57
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	3	0.57
(1,456)	1:258:A:ASN:HB2	1:283:A:GLN:HB2	1	0.57
(1,456)	1:258:A:ASN:HB2	1:283:A:GLN:HB3	1	0.57
(1,456)	1:258:A:ASN:HB3	1:283:A:GLN:HB2	1	0.57
(1,456)	1:258:A:ASN:HB3	1:283:A:GLN:HB3	1	0.57
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD2	19	0.57
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD3	19	0.57
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	3	0.57
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	6	0.57
(1,150)	1:238:A:LYS:HG2	1:265:A:HIS:HE1	5	0.57
(1,150)	1:238:A:LYS:HG3	1:265:A:HIS:HE1	5	0.57
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	16	0.57
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG11	3	0.56
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG12	3	0.56
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG13	3	0.56
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG11	3	0.56
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG12	3	0.56
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG13	3	0.56
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG11	3	0.56
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG12	3	0.56
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG13	3	0.56
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG21	3	0.56
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG22	3	0.56
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG23	3	0.56
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG21	3	0.56
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG22	3	0.56
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG23	3	0.56
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG21	3	0.56
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG22	3	0.56
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG23	3	0.56
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	15	0.56
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	15	0.56
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	15	0.56
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	15	0.56
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	15	0.56
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	15	0.56
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	15	0.56
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	15	0.56
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	15	0.56
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	12	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	12	0.56
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	12	0.56
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	12	0.56
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	12	0.56
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	12	0.56
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	12	0.56
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	12	0.56
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	12	0.56
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	9	0.56
(1,3891)	1:486:A:VAL:HG11	1:490:A:LEU:H	14	0.56
(1,3891)	1:486:A:VAL:HG12	1:490:A:LEU:H	14	0.56
(1,3891)	1:486:A:VAL:HG13	1:490:A:LEU:H	14	0.56
(1,3848)	1:481:A:GLN:HG2	1:486:A:VAL:HA	3	0.56
(1,3848)	1:481:A:GLN:HG3	1:486:A:VAL:HA	3	0.56
(1,3747)	1:469:A:MET:HE1	1:472:A:LEU:HD11	17	0.56
(1,3747)	1:469:A:MET:HE1	1:472:A:LEU:HD12	17	0.56
(1,3747)	1:469:A:MET:HE1	1:472:A:LEU:HD13	17	0.56
(1,3747)	1:469:A:MET:HE2	1:472:A:LEU:HD11	17	0.56
(1,3747)	1:469:A:MET:HE2	1:472:A:LEU:HD12	17	0.56
(1,3747)	1:469:A:MET:HE2	1:472:A:LEU:HD13	17	0.56
(1,3747)	1:469:A:MET:HE3	1:472:A:LEU:HD11	17	0.56
(1,3747)	1:469:A:MET:HE3	1:472:A:LEU:HD12	17	0.56
(1,3747)	1:469:A:MET:HE3	1:472:A:LEU:HD13	17	0.56
(1,3538)	1:449:A:LEU:HD11	1:453:A:LYS:HB2	8	0.56
(1,3538)	1:449:A:LEU:HD11	1:453:A:LYS:HB3	8	0.56
(1,3538)	1:449:A:LEU:HD12	1:453:A:LYS:HB2	8	0.56
(1,3538)	1:449:A:LEU:HD12	1:453:A:LYS:HB3	8	0.56
(1,3538)	1:449:A:LEU:HD13	1:453:A:LYS:HB2	8	0.56
(1,3538)	1:449:A:LEU:HD13	1:453:A:LYS:HB3	8	0.56
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB2	4	0.56
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB3	4	0.56
(1,3360)	1:437:A:SER:HA	1:462:A:ASP:HA	18	0.56
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB2	4	0.56
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB3	4	0.56
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB2	4	0.56
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB3	4	0.56
(1,3143)	1:429:A:LYS:HD2	1:489:A:SER:H	8	0.56
(1,3143)	1:429:A:LYS:HD3	1:489:A:SER:H	8	0.56
(1,2938)	1:414:A:VAL:HG21	1:418:A:ASP:H	13	0.56
(1,2938)	1:414:A:VAL:HG22	1:418:A:ASP:H	13	0.56
(1,2938)	1:414:A:VAL:HG23	1:418:A:ASP:H	13	0.56
(1,2889)	1:408:A:ASP:HB3	1:451:A:ARG:HH22	8	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2695)	1:398:A:LYS:HD2	1:475:A:PHE:HZ	7	0.56
(1,2695)	1:398:A:LYS:HD3	1:475:A:PHE:HZ	7	0.56
(1,2632)	1:393:A:GLN:HA	1:396:A:ILE:HB	17	0.56
(1,2382)	1:376:A:GLN:HG2	1:412:A:GLN:HE21	4	0.56
(1,2382)	1:376:A:GLN:HG2	1:412:A:GLN:HE22	4	0.56
(1,2382)	1:376:A:GLN:HG3	1:412:A:GLN:HE21	4	0.56
(1,2382)	1:376:A:GLN:HG3	1:412:A:GLN:HE22	4	0.56
(1,2045)	1:357:A:LEU:HD21	1:395:A:ALA:H	8	0.56
(1,2045)	1:357:A:LEU:HD22	1:395:A:ALA:H	8	0.56
(1,2045)	1:357:A:LEU:HD23	1:395:A:ALA:H	8	0.56
(1,1996)	1:354:A:LYS:HA	1:358:A:GLN:HE21	4	0.56
(1,1996)	1:354:A:LYS:HA	1:358:A:GLN:HE22	4	0.56
(1,1989)	1:354:A:LYS:HA	1:392:A:ASN:HD21	10	0.56
(1,1989)	1:354:A:LYS:HA	1:392:A:ASN:HD22	10	0.56
(1,1726)	1:331:A:PRO:HB2	1:338:A:ILE:HB	1	0.56
(1,1726)	1:331:A:PRO:HB3	1:338:A:ILE:HB	1	0.56
(1,1452)	1:313:A:PHE:HZ	1:345:A:THR:HA	3	0.56
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE1	8	0.56
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE2	8	0.56
(1,1072)	1:295:A:HIS:HE1	1:311:A:GLU:HA	15	0.56
(1,1072)	1:295:A:HIS:HE1	1:311:A:GLU:HA	18	0.56
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	11	0.56
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	11	0.56
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD2	12	0.56
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD3	12	0.56
(1,1030)	1:289:A:TRP:HZ2	1:380:A:LEU:HD11	13	0.56
(1,1030)	1:289:A:TRP:HZ2	1:380:A:LEU:HD12	13	0.56
(1,1030)	1:289:A:TRP:HZ2	1:380:A:LEU:HD13	13	0.56
(1,986)	1:287:A:ASP:HB2	1:294:A:LYS:H	1	0.56
(1,986)	1:287:A:ASP:HB3	1:294:A:LYS:H	1	0.56
(1,986)	1:287:A:ASP:HB2	1:294:A:LYS:H	7	0.56
(1,986)	1:287:A:ASP:HB3	1:294:A:LYS:H	7	0.56
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	16	0.56
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	16	0.56
(1,868)	1:280:A:ILE:HD11	1:360:A:LEU:H	18	0.56
(1,868)	1:280:A:ILE:HD12	1:360:A:LEU:H	18	0.56
(1,868)	1:280:A:ILE:HD13	1:360:A:LEU:H	18	0.56
(1,719)	1:274:A:TYR:HD1	1:348:A:LEU:HD21	9	0.56
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB2	16	0.56
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB3	16	0.56
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	11	0.56
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	11	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	11	0.56
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	10	0.56
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	10	0.56
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	8	0.56
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	15	0.56
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB2	10	0.56
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB3	10	0.56
(1,102)	1:234:A:TRP:HE1	1:235:A:THR:HB	2	0.56
(1,37)	1:233:A:LEU:HD11	1:249:A:PHE:H	19	0.56
(1,37)	1:233:A:LEU:HD12	1:249:A:PHE:H	19	0.56
(1,37)	1:233:A:LEU:HD13	1:249:A:PHE:H	19	0.56
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	9	0.55
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	9	0.55
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	9	0.55
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	9	0.55
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	9	0.55
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	9	0.55
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	9	0.55
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	9	0.55
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	9	0.55
(1,3927)	1:489:A:SER:HB2	1:493:A:LEU:HD11	3	0.55
(1,3927)	1:489:A:SER:HB2	1:493:A:LEU:HD12	3	0.55
(1,3927)	1:489:A:SER:HB2	1:493:A:LEU:HD13	3	0.55
(1,3927)	1:489:A:SER:HB3	1:493:A:LEU:HD11	3	0.55
(1,3927)	1:489:A:SER:HB3	1:493:A:LEU:HD12	3	0.55
(1,3927)	1:489:A:SER:HB3	1:493:A:LEU:HD13	3	0.55
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	1	0.55
(1,3891)	1:486:A:VAL:HG11	1:490:A:LEU:H	16	0.55
(1,3891)	1:486:A:VAL:HG12	1:490:A:LEU:H	16	0.55
(1,3891)	1:486:A:VAL:HG13	1:490:A:LEU:H	16	0.55
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE2	5	0.55
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE3	5	0.55
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE2	5	0.55
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE3	5	0.55
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE2	16	0.55
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE3	16	0.55
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE2	16	0.55
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE3	16	0.55
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB2	9	0.55
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB3	9	0.55
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB2	9	0.55
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB3	9	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3848)	1:481:A:GLN:HG2	1:486:A:VAL:HA	8	0.55
(1,3848)	1:481:A:GLN:HG3	1:486:A:VAL:HA	8	0.55
(1,3772)	1:472:A:LEU:HD21	1:474:A:GLU:HA	10	0.55
(1,3772)	1:472:A:LEU:HD22	1:474:A:GLU:HA	10	0.55
(1,3772)	1:472:A:LEU:HD23	1:474:A:GLU:HA	10	0.55
(1,3671)	1:462:A:ASP:H	1:465:A:ASP:HB2	4	0.55
(1,3671)	1:462:A:ASP:H	1:465:A:ASP:HB3	4	0.55
(1,3178)	1:430:A:ILE:HD11	1:479:A:PRO:HA	18	0.55
(1,3178)	1:430:A:ILE:HD12	1:479:A:PRO:HA	18	0.55
(1,3178)	1:430:A:ILE:HD13	1:479:A:PRO:HA	18	0.55
(1,3155)	1:429:A:LYS:HB2	1:480:A:PHE:HA	20	0.55
(1,3155)	1:429:A:LYS:HB3	1:480:A:PHE:HA	20	0.55
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB2	18	0.55
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB3	18	0.55
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB2	18	0.55
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB3	18	0.55
(1,3135)	1:428:A:GLU:HA	1:478:A:LYS:HA	15	0.55
(1,3037)	1:420:A:VAL:HG11	1:478:A:LYS:HE2	14	0.55
(1,3037)	1:420:A:VAL:HG11	1:478:A:LYS:HE3	14	0.55
(1,3037)	1:420:A:VAL:HG12	1:478:A:LYS:HE2	14	0.55
(1,3037)	1:420:A:VAL:HG12	1:478:A:LYS:HE3	14	0.55
(1,3037)	1:420:A:VAL:HG13	1:478:A:LYS:HE2	14	0.55
(1,3037)	1:420:A:VAL:HG13	1:478:A:LYS:HE3	14	0.55
(1,2938)	1:414:A:VAL:HG21	1:418:A:ASP:H	6	0.55
(1,2938)	1:414:A:VAL:HG22	1:418:A:ASP:H	6	0.55
(1,2938)	1:414:A:VAL:HG23	1:418:A:ASP:H	6	0.55
(1,2764)	1:402:A:PHE:H	1:414:A:VAL:HB	10	0.55
(1,2699)	1:398:A:LYS:HE2	1:417:A:GLU:HG2	10	0.55
(1,2699)	1:398:A:LYS:HE2	1:417:A:GLU:HG3	10	0.55
(1,2699)	1:398:A:LYS:HE3	1:417:A:GLU:HG2	10	0.55
(1,2699)	1:398:A:LYS:HE3	1:417:A:GLU:HG3	10	0.55
(1,2643)	1:394:A:GLU:HG2	1:398:A:LYS:H	8	0.55
(1,2643)	1:394:A:GLU:HG3	1:398:A:LYS:H	8	0.55
(1,2595)	1:390:A:PHE:HE1	1:393:A:GLN:HE21	18	0.55
(1,2595)	1:390:A:PHE:HE1	1:393:A:GLN:HE22	18	0.55
(1,2595)	1:390:A:PHE:HE2	1:393:A:GLN:HE21	18	0.55
(1,2595)	1:390:A:PHE:HE2	1:393:A:GLN:HE22	18	0.55
(1,2427)	1:380:A:LEU:HD11	1:463:A:ARG:H	16	0.55
(1,2427)	1:380:A:LEU:HD12	1:463:A:ARG:H	16	0.55
(1,2427)	1:380:A:LEU:HD13	1:463:A:ARG:H	16	0.55
(1,2426)	1:380:A:LEU:HD22	1:464:A:ILE:H	14	0.55
(1,2380)	1:376:A:GLN:HE21	1:412:A:GLN:H	8	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2380)	1:376:A:GLN:HE22	1:412:A:GLN:H	8	0.55
(1,2281)	1:372:A:GLN:HE21	1:412:A:GLN:H	17	0.55
(1,2281)	1:372:A:GLN:HE22	1:412:A:GLN:H	17	0.55
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG2	8	0.55
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG3	8	0.55
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG2	8	0.55
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG3	8	0.55
(1,2083)	1:359:A:MET:HA	1:362:A:LYS:HD2	10	0.55
(1,2083)	1:359:A:MET:HA	1:362:A:LYS:HD3	10	0.55
(1,1933)	1:350:A:ASN:HA	1:354:A:LYS:H	1	0.55
(1,1859)	1:344:A:VAL:HB	1:348:A:LEU:H	19	0.55
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	13	0.55
(1,1745)	1:333:A:ASN:HD21	1:338:A:ILE:HD11	19	0.55
(1,1745)	1:333:A:ASN:HD21	1:338:A:ILE:HD12	19	0.55
(1,1745)	1:333:A:ASN:HD21	1:338:A:ILE:HD13	19	0.55
(1,1745)	1:333:A:ASN:HD22	1:338:A:ILE:HD11	19	0.55
(1,1745)	1:333:A:ASN:HD22	1:338:A:ILE:HD12	19	0.55
(1,1745)	1:333:A:ASN:HD22	1:338:A:ILE:HD13	19	0.55
(1,1725)	1:331:A:PRO:HD2	1:339:A:LEU:HD21	14	0.55
(1,1725)	1:331:A:PRO:HD2	1:339:A:LEU:HD22	14	0.55
(1,1725)	1:331:A:PRO:HD2	1:339:A:LEU:HD23	14	0.55
(1,1725)	1:331:A:PRO:HD3	1:339:A:LEU:HD21	14	0.55
(1,1725)	1:331:A:PRO:HD3	1:339:A:LEU:HD22	14	0.55
(1,1725)	1:331:A:PRO:HD3	1:339:A:LEU:HD23	14	0.55
(1,1525)	1:316:A:ASN:H	1:388:A:GLU:HG2	10	0.55
(1,1525)	1:316:A:ASN:H	1:388:A:GLU:HG3	10	0.55
(1,1452)	1:313:A:PHE:HZ	1:345:A:THR:HA	18	0.55
(1,1428)	1:312:A:GLN:H	1:339:A:LEU:HD11	14	0.55
(1,1428)	1:312:A:GLN:H	1:339:A:LEU:HD12	14	0.55
(1,1428)	1:312:A:GLN:H	1:339:A:LEU:HD13	14	0.55
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	14	0.55
(1,897)	1:281:A:PRO:HG2	1:322:A:ARG:HG2	4	0.55
(1,897)	1:281:A:PRO:HG2	1:322:A:ARG:HG3	4	0.55
(1,897)	1:281:A:PRO:HG3	1:322:A:ARG:HG2	4	0.55
(1,897)	1:281:A:PRO:HG3	1:322:A:ARG:HG3	4	0.55
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB2	20	0.55
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB3	20	0.55
(1,564)	1:263:A:TRP:HE1	1:265:A:HIS:H	2	0.55
(1,564)	1:263:A:TRP:HE1	1:265:A:HIS:H	15	0.55
(1,352)	1:250:A:TYR:HE1	1:256:A:ASP:H	18	0.55
(1,352)	1:250:A:TYR:HE2	1:256:A:ASP:H	18	0.55
(1,110)	1:235:A:THR:HG1	1:267:A:ARG:HD2	8	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,110)	1:235:A:THR:HG1	1:267:A:ARG:HD3	8	0.55
(1,103)	1:235:A:THR:H	1:303:A:ARG:HD2	3	0.55
(1,103)	1:235:A:THR:H	1:303:A:ARG:HD3	3	0.55
(1,102)	1:234:A:TRP:HE1	1:235:A:THR:HB	14	0.55
(1,102)	1:234:A:TRP:HE1	1:235:A:THR:HB	18	0.55
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	13	0.55
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	7	0.55
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG21	5	0.55
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG22	5	0.55
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG23	5	0.55
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG21	15	0.54
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG22	15	0.54
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG23	15	0.54
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG21	15	0.54
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG22	15	0.54
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG23	15	0.54
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG21	15	0.54
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG22	15	0.54
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG23	15	0.54
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE1	4	0.54
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE2	4	0.54
(1,3974)	1:472:A:LEU:HD11	2:629:B:MET:HE3	4	0.54
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE1	4	0.54
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE2	4	0.54
(1,3974)	1:472:A:LEU:HD12	2:629:B:MET:HE3	4	0.54
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE1	4	0.54
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE2	4	0.54
(1,3974)	1:472:A:LEU:HD13	2:629:B:MET:HE3	4	0.54
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	6	0.54
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	6	0.54
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	6	0.54
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	6	0.54
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	6	0.54
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	6	0.54
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	6	0.54
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	6	0.54
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	6	0.54
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	15	0.54
(1,3841)	1:481:A:GLN:HG2	1:489:A:SER:HA	1	0.54
(1,3841)	1:481:A:GLN:HG3	1:489:A:SER:HA	1	0.54
(1,3772)	1:472:A:LEU:HD21	1:474:A:GLU:HA	9	0.54
(1,3772)	1:472:A:LEU:HD22	1:474:A:GLU:HA	9	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3772)	1:472:A:LEU:HD23	1:474:A:GLU:HA	9	0.54
(1,3536)	1:449:A:LEU:HA	1:453:A:LYS:H	1	0.54
(1,3482)	1:446:A:HIS:HA	1:483:A:VAL:HB	3	0.54
(1,3315)	1:434:A:THR:HA	1:461:A:SER:HA	17	0.54
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	13	0.54
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	13	0.54
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	13	0.54
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	13	0.54
(1,3178)	1:430:A:ILE:HD11	1:479:A:PRO:HA	3	0.54
(1,3178)	1:430:A:ILE:HD12	1:479:A:PRO:HA	3	0.54
(1,3178)	1:430:A:ILE:HD13	1:479:A:PRO:HA	3	0.54
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD11	16	0.54
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD12	16	0.54
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD13	16	0.54
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD11	16	0.54
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD12	16	0.54
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD13	16	0.54
(1,2927)	1:412:A:GLN:HA	1:414:A:VAL:HB	10	0.54
(1,2824)	1:404:A:SER:H	1:414:A:VAL:HB	11	0.54
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG11	17	0.54
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG12	17	0.54
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG13	17	0.54
(1,2619)	1:393:A:GLN:HE21	1:474:A:GLU:H	5	0.54
(1,2619)	1:393:A:GLN:HE22	1:474:A:GLU:H	5	0.54
(1,2575)	1:388:A:GLU:HA	1:390:A:PHE:H	15	0.54
(1,2566)	1:387:A:ALA:H	1:468:A:MET:HA	10	0.54
(1,2488)	1:383:A:LYS:HE2	1:402:A:PHE:HZ	7	0.54
(1,2488)	1:383:A:LYS:HE3	1:402:A:PHE:HZ	7	0.54
(1,2484)	1:383:A:LYS:HB2	1:464:A:ILE:HD11	5	0.54
(1,2484)	1:383:A:LYS:HB2	1:464:A:ILE:HD12	5	0.54
(1,2484)	1:383:A:LYS:HB2	1:464:A:ILE:HD13	5	0.54
(1,2484)	1:383:A:LYS:HB3	1:464:A:ILE:HD11	5	0.54
(1,2484)	1:383:A:LYS:HB3	1:464:A:ILE:HD12	5	0.54
(1,2484)	1:383:A:LYS:HB3	1:464:A:ILE:HD13	5	0.54
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	2	0.54
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	2	0.54
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	2	0.54
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	2	0.54
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	13	0.54
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	13	0.54
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	13	0.54
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	13	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	18	0.54
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	18	0.54
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	18	0.54
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	18	0.54
(1,2135)	1:361:A:GLU:HG2	1:365:A:LYS:HG2	9	0.54
(1,2135)	1:361:A:GLU:HG2	1:365:A:LYS:HG3	9	0.54
(1,2135)	1:361:A:GLU:HG3	1:365:A:LYS:HG2	9	0.54
(1,2135)	1:361:A:GLU:HG3	1:365:A:LYS:HG3	9	0.54
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD21	15	0.54
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD22	15	0.54
(1,1858)	1:344:A:VAL:HA	1:348:A:LEU:H	19	0.54
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	3	0.54
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	8	0.54
(1,1778)	1:336:A:ARG:HA	1:340:A:GLN:HB2	18	0.54
(1,1778)	1:336:A:ARG:HA	1:340:A:GLN:HB3	18	0.54
(1,1726)	1:331:A:PRO:HB2	1:338:A:ILE:HB	13	0.54
(1,1726)	1:331:A:PRO:HB3	1:338:A:ILE:HB	13	0.54
(1,1505)	1:315:A:PRO:HD2	1:350:A:ASN:HA	5	0.54
(1,1505)	1:315:A:PRO:HD3	1:350:A:ASN:HA	5	0.54
(1,1505)	1:315:A:PRO:HD2	1:350:A:ASN:HA	12	0.54
(1,1505)	1:315:A:PRO:HD3	1:350:A:ASN:HA	12	0.54
(1,1486)	1:314:A:MET:HB2	1:319:A:ARG:H	3	0.54
(1,1486)	1:314:A:MET:HB3	1:319:A:ARG:H	3	0.54
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG21	18	0.54
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG22	18	0.54
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG23	18	0.54
(1,1367)	1:307:A:MET:HE1	1:339:A:LEU:H	10	0.54
(1,1367)	1:307:A:MET:HE2	1:339:A:LEU:H	10	0.54
(1,1367)	1:307:A:MET:HE3	1:339:A:LEU:H	10	0.54
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE1	10	0.54
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE2	10	0.54
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD11	1	0.54
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD12	1	0.54
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD13	1	0.54
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD11	17	0.54
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD12	17	0.54
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD13	17	0.54
(1,1090)	1:296:A:GLY:H	1:311:A:GLU:HA	15	0.54
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	10	0.54
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	10	0.54
(1,1044)	1:291:A:ARG:HA	1:293:A:HIS:HA	15	0.54
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	6	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE1	1	0.54
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE2	1	0.54
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE3	1	0.54
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE1	1	0.54
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE2	1	0.54
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE3	1	0.54
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE1	2	0.54
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE2	2	0.54
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE3	2	0.54
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE1	2	0.54
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE2	2	0.54
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE3	2	0.54
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE1	7	0.54
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE2	7	0.54
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE3	7	0.54
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE1	7	0.54
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE2	7	0.54
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE3	7	0.54
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	10	0.54
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	10	0.54
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	12	0.54
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB2	4	0.54
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB3	4	0.54
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD21	3	0.54
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD22	3	0.54
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	16	0.54
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	12	0.54
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	7	0.54
(1,21)	1:232:A:ALA:H	1:235:A:THR:H	11	0.54
(1,5)	1:231:A:GLN:HG2	1:236:A:ARG:H	6	0.54
(1,5)	1:231:A:GLN:HG3	1:236:A:ARG:H	6	0.54
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	20	0.53
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	14	0.53
(1,3848)	1:481:A:GLN:HG2	1:486:A:VAL:HA	7	0.53
(1,3848)	1:481:A:GLN:HG3	1:486:A:VAL:HA	7	0.53
(1,3848)	1:481:A:GLN:HG2	1:486:A:VAL:HA	18	0.53
(1,3848)	1:481:A:GLN:HG3	1:486:A:VAL:HA	18	0.53
(1,3561)	1:450:A:LEU:HD11	1:456:A:GLU:H	18	0.53
(1,3561)	1:450:A:LEU:HD12	1:456:A:GLU:H	18	0.53
(1,3561)	1:450:A:LEU:HD13	1:456:A:GLU:H	18	0.53
(1,3471)	1:445:A:PRO:HA	1:448:A:GLU:HG2	13	0.53
(1,3471)	1:445:A:PRO:HA	1:448:A:GLU:HG3	13	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3315)	1:434:A:THR:HA	1:461:A:SER:HA	7	0.53
(1,3294)	1:433:A:ILE:HB	1:441:A:ALA:HA	10	0.53
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	19	0.53
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	19	0.53
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	19	0.53
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	19	0.53
(1,3245)	1:432:A:TYR:HB2	1:458:A:LEU:H	4	0.53
(1,3245)	1:432:A:TYR:HB3	1:458:A:LEU:H	4	0.53
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD11	6	0.53
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD12	6	0.53
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD13	6	0.53
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG2	8	0.53
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG3	8	0.53
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG2	8	0.53
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG3	8	0.53
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD11	7	0.53
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD12	7	0.53
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD13	7	0.53
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD11	7	0.53
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD12	7	0.53
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD13	7	0.53
(1,3084)	1:423:A:MET:HE1	1:427:A:GLN:HG2	6	0.53
(1,3084)	1:423:A:MET:HE1	1:427:A:GLN:HG3	6	0.53
(1,3084)	1:423:A:MET:HE2	1:427:A:GLN:HG2	6	0.53
(1,3084)	1:423:A:MET:HE2	1:427:A:GLN:HG3	6	0.53
(1,3084)	1:423:A:MET:HE3	1:427:A:GLN:HG2	6	0.53
(1,3084)	1:423:A:MET:HE3	1:427:A:GLN:HG3	6	0.53
(1,3070)	1:423:A:MET:HA	1:456:A:GLU:H	18	0.53
(1,3060)	1:422:A:ARG:HB2	1:456:A:GLU:HB2	2	0.53
(1,3060)	1:422:A:ARG:HB2	1:456:A:GLU:HB3	2	0.53
(1,3060)	1:422:A:ARG:HB3	1:456:A:GLU:HB2	2	0.53
(1,3060)	1:422:A:ARG:HB3	1:456:A:GLU:HB3	2	0.53
(1,2984)	1:417:A:GLU:HA	1:421:A:SER:H	5	0.53
(1,2875)	1:406:A:HIS:HB2	1:414:A:VAL:HB	20	0.53
(1,2875)	1:406:A:HIS:HB3	1:414:A:VAL:HB	20	0.53
(1,2849)	1:405:A:THR:HG21	1:457:A:VAL:HB	5	0.53
(1,2849)	1:405:A:THR:HG22	1:457:A:VAL:HB	5	0.53
(1,2849)	1:405:A:THR:HG23	1:457:A:VAL:HB	5	0.53
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG11	2	0.53
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG12	2	0.53
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG13	2	0.53
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG11	8	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG12	8	0.53
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG13	8	0.53
(1,2538)	1:386:A:PRO:HA	1:471:A:TYR:HB2	14	0.53
(1,2538)	1:386:A:PRO:HA	1:471:A:TYR:HB3	14	0.53
(1,2487)	1:383:A:LYS:HE2	1:402:A:PHE:HA	2	0.53
(1,2487)	1:383:A:LYS:HE3	1:402:A:PHE:HA	2	0.53
(1,2357)	1:375:A:TRP:HH2	1:383:A:LYS:HE2	10	0.53
(1,2357)	1:375:A:TRP:HH2	1:383:A:LYS:HE3	10	0.53
(1,1859)	1:344:A:VAL:HB	1:348:A:LEU:H	10	0.53
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	2	0.53
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	6	0.53
(1,1847)	1:343:A:THR:HG21	1:347:A:ASN:HD21	2	0.53
(1,1847)	1:343:A:THR:HG21	1:347:A:ASN:HD22	2	0.53
(1,1847)	1:343:A:THR:HG22	1:347:A:ASN:HD21	2	0.53
(1,1847)	1:343:A:THR:HG22	1:347:A:ASN:HD22	2	0.53
(1,1847)	1:343:A:THR:HG23	1:347:A:ASN:HD21	2	0.53
(1,1847)	1:343:A:THR:HG23	1:347:A:ASN:HD22	2	0.53
(1,1658)	1:322:A:ARG:HD2	1:323:A:GLY:H	19	0.53
(1,1658)	1:322:A:ARG:HD3	1:323:A:GLY:H	19	0.53
(1,1324)	1:302:A:GLN:H	1:327:A:SER:H	16	0.53
(1,1051)	1:293:A:HIS:HE1	1:309:A:ASP:HB2	16	0.53
(1,1051)	1:293:A:HIS:HE1	1:309:A:ASP:HB3	16	0.53
(1,1010)	1:288:A:MET:HA	1:319:A:ARG:HD2	2	0.53
(1,1010)	1:288:A:MET:HA	1:319:A:ARG:HD3	2	0.53
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE1	10	0.53
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE2	10	0.53
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE3	10	0.53
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE1	10	0.53
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE2	10	0.53
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE3	10	0.53
(1,961)	1:285:A:PRO:HG2	1:294:A:LYS:HB2	15	0.53
(1,961)	1:285:A:PRO:HG2	1:294:A:LYS:HB3	15	0.53
(1,961)	1:285:A:PRO:HG3	1:294:A:LYS:HB2	15	0.53
(1,961)	1:285:A:PRO:HG3	1:294:A:LYS:HB3	15	0.53
(1,927)	1:283:A:GLN:HA	1:377:A:GLN:HA	8	0.53
(1,574)	1:264:A:SER:HB2	1:358:A:GLN:HB2	13	0.53
(1,574)	1:264:A:SER:HB2	1:358:A:GLN:HB3	13	0.53
(1,574)	1:264:A:SER:HB3	1:358:A:GLN:HB2	13	0.53
(1,574)	1:264:A:SER:HB3	1:358:A:GLN:HB3	13	0.53
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	4	0.53
(1,352)	1:250:A:TYR:HE1	1:256:A:ASP:H	1	0.53
(1,352)	1:250:A:TYR:HE2	1:256:A:ASP:H	1	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	11	0.53
(1,144)	1:237:A:ASN:HD21	1:238:A:LYS:H	7	0.53
(1,144)	1:237:A:ASN:HD22	1:238:A:LYS:H	7	0.53
(1,102)	1:234:A:TRP:HE1	1:235:A:THR:HB	5	0.53
(1,102)	1:234:A:TRP:HE1	1:235:A:THR:HB	17	0.53
(2,9)	1:338:A:ILE:HD11	1:342:A:SER:H	14	0.52
(2,9)	1:338:A:ILE:HD12	1:342:A:SER:H	14	0.52
(2,9)	1:338:A:ILE:HD13	1:342:A:SER:H	14	0.52
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG21	18	0.52
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG22	18	0.52
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG23	18	0.52
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG21	18	0.52
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG22	18	0.52
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG23	18	0.52
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG21	18	0.52
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG22	18	0.52
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG23	18	0.52
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB1	20	0.52
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB2	20	0.52
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB3	20	0.52
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB1	20	0.52
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB2	20	0.52
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB3	20	0.52
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB1	20	0.52
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB2	20	0.52
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB3	20	0.52
(1,3936)	1:490:A:LEU:HB2	1:494:A:ALA:H	7	0.52
(1,3936)	1:490:A:LEU:HB3	1:494:A:ALA:H	7	0.52
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB2	3	0.52
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB3	3	0.52
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB2	3	0.52
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB3	3	0.52
(1,3845)	1:481:A:GLN:HG2	1:487:A:ASP:H	8	0.52
(1,3845)	1:481:A:GLN:HG3	1:487:A:ASP:H	8	0.52
(1,3294)	1:433:A:ILE:HB	1:441:A:ALA:HA	11	0.52
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD21	1	0.52
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD22	1	0.52
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD23	1	0.52
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	1	0.52
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	1	0.52
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	1	0.52
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	1	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD11	14	0.52
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD12	14	0.52
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD13	14	0.52
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD11	14	0.52
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD12	14	0.52
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD13	14	0.52
(1,3081)	1:423:A:MET:HE1	1:427:A:GLN:HB2	5	0.52
(1,3081)	1:423:A:MET:HE1	1:427:A:GLN:HB3	5	0.52
(1,3081)	1:423:A:MET:HE2	1:427:A:GLN:HB2	5	0.52
(1,3081)	1:423:A:MET:HE2	1:427:A:GLN:HB3	5	0.52
(1,3081)	1:423:A:MET:HE3	1:427:A:GLN:HB2	5	0.52
(1,3081)	1:423:A:MET:HE3	1:427:A:GLN:HB3	5	0.52
(1,2984)	1:417:A:GLU:HA	1:421:A:SER:H	19	0.52
(1,2875)	1:406:A:HIS:HB2	1:414:A:VAL:HB	4	0.52
(1,2875)	1:406:A:HIS:HB3	1:414:A:VAL:HB	4	0.52
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	3	0.52
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	3	0.52
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	3	0.52
(1,2694)	1:398:A:LYS:HA	1:475:A:PHE:HZ	7	0.52
(1,2632)	1:393:A:GLN:HA	1:396:A:ILE:HB	18	0.52
(1,2619)	1:393:A:GLN:HE21	1:474:A:GLU:H	7	0.52
(1,2619)	1:393:A:GLN:HE22	1:474:A:GLU:H	7	0.52
(1,2619)	1:393:A:GLN:HE21	1:474:A:GLU:H	8	0.52
(1,2619)	1:393:A:GLN:HE22	1:474:A:GLU:H	8	0.52
(1,2575)	1:388:A:GLU:HA	1:390:A:PHE:H	8	0.52
(1,2563)	1:387:A:ALA:HA	1:471:A:TYR:HE1	14	0.52
(1,2563)	1:387:A:ALA:HA	1:471:A:TYR:HE2	14	0.52
(1,2426)	1:380:A:LEU:HD22	1:464:A:ILE:H	8	0.52
(1,2290)	1:372:A:GLN:HG2	1:376:A:GLN:HE21	4	0.52
(1,2290)	1:372:A:GLN:HG2	1:376:A:GLN:HE22	4	0.52
(1,2290)	1:372:A:GLN:HG3	1:376:A:GLN:HE21	4	0.52
(1,2290)	1:372:A:GLN:HG3	1:376:A:GLN:HE22	4	0.52
(1,2077)	1:359:A:MET:HG2	1:363:A:LEU:H	19	0.52
(1,2077)	1:359:A:MET:HG3	1:363:A:LEU:H	19	0.52
(1,1790)	1:337:A:GLU:HG2	1:341:A:ASP:HB2	5	0.52
(1,1790)	1:337:A:GLU:HG2	1:341:A:ASP:HB3	5	0.52
(1,1790)	1:337:A:GLU:HG3	1:341:A:ASP:HB2	5	0.52
(1,1790)	1:337:A:GLU:HG3	1:341:A:ASP:HB3	5	0.52
(1,1727)	1:331:A:PRO:HB2	1:338:A:ILE:HD11	19	0.52
(1,1727)	1:331:A:PRO:HB2	1:338:A:ILE:HD12	19	0.52
(1,1727)	1:331:A:PRO:HB2	1:338:A:ILE:HD13	19	0.52
(1,1727)	1:331:A:PRO:HB3	1:338:A:ILE:HD11	19	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1727)	1:331:A:PRO:HB3	1:338:A:ILE:HD12	19	0.52
(1,1727)	1:331:A:PRO:HB3	1:338:A:ILE:HD13	19	0.52
(1,1570)	1:317:A:TYR:HA	1:320:A:PHE:HE1	13	0.52
(1,1570)	1:317:A:TYR:HA	1:320:A:PHE:HE2	13	0.52
(1,1543)	1:317:A:TYR:HD1	1:389:A:ASP:HB2	1	0.52
(1,1543)	1:317:A:TYR:HD1	1:389:A:ASP:HB3	1	0.52
(1,1543)	1:317:A:TYR:HD2	1:389:A:ASP:HB2	1	0.52
(1,1543)	1:317:A:TYR:HD2	1:389:A:ASP:HB3	1	0.52
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD11	13	0.52
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD12	13	0.52
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD13	13	0.52
(1,1081)	1:296:A:GLY:H	1:319:A:ARG:HA	13	0.52
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	5	0.52
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	5	0.52
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD2	16	0.52
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD3	16	0.52
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	3	0.52
(1,684)	1:272:A:GLN:HE21	1:351:A:ALA:H	1	0.52
(1,684)	1:272:A:GLN:HE22	1:351:A:ALA:H	1	0.52
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	4	0.52
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	4	0.52
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	4	0.52
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	5	0.52
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	5	0.52
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	12	0.52
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	12	0.52
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	12	0.52
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	12	0.52
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	12	0.52
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	12	0.52
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	9	0.51
(1,3772)	1:472:A:LEU:HD21	1:474:A:GLU:HA	20	0.51
(1,3772)	1:472:A:LEU:HD22	1:474:A:GLU:HA	20	0.51
(1,3772)	1:472:A:LEU:HD23	1:474:A:GLU:HA	20	0.51
(1,3730)	1:468:A:MET:HA	1:471:A:TYR:HD1	8	0.51
(1,3730)	1:468:A:MET:HA	1:471:A:TYR:HD2	8	0.51
(1,3657)	1:460:A:LEU:HA	1:465:A:ASP:HB2	18	0.51
(1,3657)	1:460:A:LEU:HA	1:465:A:ASP:HB3	18	0.51
(1,3601)	1:453:A:LYS:HG2	1:493:A:LEU:HD21	4	0.51
(1,3601)	1:453:A:LYS:HG2	1:493:A:LEU:HD22	4	0.51
(1,3601)	1:453:A:LYS:HG2	1:493:A:LEU:HD23	4	0.51
(1,3601)	1:453:A:LYS:HG3	1:493:A:LEU:HD21	4	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3601)	1:453:A:LYS:HG3	1:493:A:LEU:HD22	4	0.51
(1,3601)	1:453:A:LYS:HG3	1:493:A:LEU:HD23	4	0.51
(1,3530)	1:449:A:LEU:HD11	1:494:A:ALA:HA	16	0.51
(1,3530)	1:449:A:LEU:HD12	1:494:A:ALA:HA	16	0.51
(1,3530)	1:449:A:LEU:HD13	1:494:A:ALA:HA	16	0.51
(1,3530)	1:449:A:LEU:HD21	1:494:A:ALA:HA	16	0.51
(1,3530)	1:449:A:LEU:HD22	1:494:A:ALA:HA	16	0.51
(1,3530)	1:449:A:LEU:HD23	1:494:A:ALA:HA	16	0.51
(1,3480)	1:446:A:HIS:HE1	1:484:A:SER:HA	3	0.51
(1,3406)	1:439:A:ALA:HA	1:442:A:LYS:HD2	6	0.51
(1,3406)	1:439:A:ALA:HA	1:442:A:LYS:HD3	6	0.51
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD21	6	0.51
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD22	6	0.51
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD23	6	0.51
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	17	0.51
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	17	0.51
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	17	0.51
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	17	0.51
(1,3170)	1:430:A:ILE:H	1:481:A:GLN:H	7	0.51
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD11	2	0.51
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD12	2	0.51
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD13	2	0.51
(1,3154)	1:429:A:LYS:HA	1:480:A:PHE:HA	7	0.51
(1,3143)	1:429:A:LYS:HD2	1:489:A:SER:H	4	0.51
(1,3143)	1:429:A:LYS:HD3	1:489:A:SER:H	4	0.51
(1,3143)	1:429:A:LYS:HD2	1:489:A:SER:H	18	0.51
(1,3143)	1:429:A:LYS:HD3	1:489:A:SER:H	18	0.51
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD11	10	0.51
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD12	10	0.51
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD13	10	0.51
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD11	10	0.51
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD12	10	0.51
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD13	10	0.51
(1,3028)	1:419:A:TYR:HA	1:422:A:ARG:HD2	5	0.51
(1,3028)	1:419:A:TYR:HA	1:422:A:ARG:HD3	5	0.51
(1,2875)	1:406:A:HIS:HB2	1:414:A:VAL:HB	3	0.51
(1,2875)	1:406:A:HIS:HB3	1:414:A:VAL:HB	3	0.51
(1,2704)	1:398:A:LYS:HA	1:416:A:LEU:HD11	10	0.51
(1,2704)	1:398:A:LYS:HA	1:416:A:LEU:HD12	10	0.51
(1,2704)	1:398:A:LYS:HA	1:416:A:LEU:HD13	10	0.51
(1,2487)	1:383:A:LYS:HE2	1:402:A:PHE:HA	7	0.51
(1,2487)	1:383:A:LYS:HE3	1:402:A:PHE:HA	7	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2344)	1:375:A:TRP:HZ2	1:402:A:PHE:HA	1	0.51
(1,2288)	1:372:A:GLN:HE21	1:376:A:GLN:H	19	0.51
(1,2288)	1:372:A:GLN:HE22	1:376:A:GLN:H	19	0.51
(1,2236)	1:369:A:GLU:HG2	1:373:A:THR:H	20	0.51
(1,2236)	1:369:A:GLU:HG3	1:373:A:THR:H	20	0.51
(1,2166)	1:363:A:LEU:HA	1:367:A:ASP:HB2	10	0.51
(1,2166)	1:363:A:LEU:HA	1:367:A:ASP:HB3	10	0.51
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG2	19	0.51
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG3	19	0.51
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG2	19	0.51
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG3	19	0.51
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD21	11	0.51
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD22	11	0.51
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD21	11	0.51
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD22	11	0.51
(1,1959)	1:352:A:LEU:HD21	1:356:A:VAL:H	6	0.51
(1,1959)	1:352:A:LEU:HD22	1:356:A:VAL:H	6	0.51
(1,1959)	1:352:A:LEU:HD23	1:356:A:VAL:H	6	0.51
(1,1886)	1:346:A:ARG:HG2	1:350:A:ASN:HD21	15	0.51
(1,1886)	1:346:A:ARG:HG2	1:350:A:ASN:HD22	15	0.51
(1,1886)	1:346:A:ARG:HG3	1:350:A:ASN:HD21	15	0.51
(1,1886)	1:346:A:ARG:HG3	1:350:A:ASN:HD22	15	0.51
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	16	0.51
(1,1762)	1:335:A:SER:H	1:339:A:LEU:H	14	0.51
(1,1658)	1:322:A:ARG:HD2	1:323:A:GLY:H	4	0.51
(1,1658)	1:322:A:ARG:HD3	1:323:A:GLY:H	4	0.51
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE1	11	0.51
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE2	11	0.51
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE3	11	0.51
(1,1374)	1:307:A:MET:HE1	1:335:A:SER:HA	7	0.51
(1,1374)	1:307:A:MET:HE2	1:335:A:SER:HA	7	0.51
(1,1374)	1:307:A:MET:HE3	1:335:A:SER:HA	7	0.51
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD11	6	0.51
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD12	6	0.51
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD13	6	0.51
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD11	9	0.51
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD12	9	0.51
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD13	9	0.51
(1,1072)	1:295:A:HIS:HE1	1:311:A:GLU:HA	5	0.51
(1,1060)	1:294:A:LYS:HD2	1:309:A:ASP:HB2	14	0.51
(1,1060)	1:294:A:LYS:HD2	1:309:A:ASP:HB3	14	0.51
(1,1060)	1:294:A:LYS:HD3	1:309:A:ASP:HB2	14	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1060)	1:294:A:LYS:HD3	1:309:A:ASP:HB3	14	0.51
(1,1060)	1:294:A:LYS:HD2	1:309:A:ASP:HB2	20	0.51
(1,1060)	1:294:A:LYS:HD2	1:309:A:ASP:HB3	20	0.51
(1,1060)	1:294:A:LYS:HD3	1:309:A:ASP:HB2	20	0.51
(1,1060)	1:294:A:LYS:HD3	1:309:A:ASP:HB3	20	0.51
(1,1044)	1:291:A:ARG:HA	1:293:A:HIS:HA	1	0.51
(1,784)	1:277:A:LEU:H	1:324:A:LEU:HD21	2	0.51
(1,784)	1:277:A:LEU:H	1:324:A:LEU:HD22	2	0.51
(1,784)	1:277:A:LEU:H	1:324:A:LEU:HD23	2	0.51
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	2	0.51
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	2	0.51
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	9	0.51
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	17	0.51
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	2	0.51
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	18	0.51
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	18	0.51
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	18	0.51
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	18	0.51
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	18	0.51
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	18	0.51
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG21	12	0.5
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG22	12	0.5
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG23	12	0.5
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG21	12	0.5
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG22	12	0.5
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG23	12	0.5
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG21	12	0.5
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG22	12	0.5
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG23	12	0.5
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG21	17	0.5
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG22	17	0.5
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG23	17	0.5
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG21	17	0.5
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG22	17	0.5
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG23	17	0.5
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG21	17	0.5
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG22	17	0.5
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG23	17	0.5
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	19	0.5
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	19	0.5
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	19	0.5
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	19	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	19	0.5
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	19	0.5
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	19	0.5
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	19	0.5
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	19	0.5
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	13	0.5
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	13	0.5
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	13	0.5
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	13	0.5
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	13	0.5
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	13	0.5
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	13	0.5
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	13	0.5
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	13	0.5
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	16	0.5
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	12	0.5
(1,3848)	1:481:A:GLN:HG2	1:486:A:VAL:HA	4	0.5
(1,3848)	1:481:A:GLN:HG3	1:486:A:VAL:HA	4	0.5
(1,3840)	1:481:A:GLN:HG2	1:489:A:SER:H	3	0.5
(1,3840)	1:481:A:GLN:HG3	1:489:A:SER:H	3	0.5
(1,3740)	1:469:A:MET:HE1	1:473:A:THR:H	17	0.5
(1,3740)	1:469:A:MET:HE2	1:473:A:THR:H	17	0.5
(1,3740)	1:469:A:MET:HE3	1:473:A:THR:H	17	0.5
(1,3726)	1:468:A:MET:HG2	1:472:A:LEU:HB2	16	0.5
(1,3726)	1:468:A:MET:HG2	1:472:A:LEU:HB3	16	0.5
(1,3726)	1:468:A:MET:HG3	1:472:A:LEU:HB2	16	0.5
(1,3726)	1:468:A:MET:HG3	1:472:A:LEU:HB3	16	0.5
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	13	0.5
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	13	0.5
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	13	0.5
(1,3477)	1:446:A:HIS:HD2	1:490:A:LEU:HD11	14	0.5
(1,3477)	1:446:A:HIS:HD2	1:490:A:LEU:HD12	14	0.5
(1,3477)	1:446:A:HIS:HD2	1:490:A:LEU:HD13	14	0.5
(1,3406)	1:439:A:ALA:HA	1:442:A:LYS:HD2	1	0.5
(1,3406)	1:439:A:ALA:HA	1:442:A:LYS:HD3	1	0.5
(1,3199)	1:431:A:TYR:HE1	1:489:A:SER:HA	1	0.5
(1,3199)	1:431:A:TYR:HE2	1:489:A:SER:HA	1	0.5
(1,3187)	1:430:A:ILE:HD11	1:474:A:GLU:HA	12	0.5
(1,3187)	1:430:A:ILE:HD12	1:474:A:GLU:HA	12	0.5
(1,3187)	1:430:A:ILE:HD13	1:474:A:GLU:HA	12	0.5
(1,3090)	1:424:A:LYS:HE2	1:455:A:ILE:HA	20	0.5
(1,3090)	1:424:A:LYS:HE3	1:455:A:ILE:HA	20	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3063)	1:422:A:ARG:HB2	1:427:A:GLN:HE21	20	0.5
(1,3063)	1:422:A:ARG:HB2	1:427:A:GLN:HE22	20	0.5
(1,3063)	1:422:A:ARG:HB3	1:427:A:GLN:HE21	20	0.5
(1,3063)	1:422:A:ARG:HB3	1:427:A:GLN:HE22	20	0.5
(1,3027)	1:419:A:TYR:HA	1:422:A:ARG:HB2	7	0.5
(1,3027)	1:419:A:TYR:HA	1:422:A:ARG:HB3	7	0.5
(1,2889)	1:408:A:ASP:HB3	1:451:A:ARG:HH22	3	0.5
(1,2887)	1:407:A:THR:HG21	1:408:A:ASP:H	6	0.5
(1,2887)	1:407:A:THR:HG22	1:408:A:ASP:H	6	0.5
(1,2887)	1:407:A:THR:HG23	1:408:A:ASP:H	6	0.5
(1,2790)	1:403:A:ALA:HA	1:414:A:VAL:HB	15	0.5
(1,2699)	1:398:A:LYS:HE2	1:417:A:GLU:HG2	17	0.5
(1,2699)	1:398:A:LYS:HE2	1:417:A:GLU:HG3	17	0.5
(1,2699)	1:398:A:LYS:HE3	1:417:A:GLU:HG2	17	0.5
(1,2699)	1:398:A:LYS:HE3	1:417:A:GLU:HG3	17	0.5
(1,2461)	1:382:A:LEU:HD11	1:399:A:LEU:H	19	0.5
(1,2461)	1:382:A:LEU:HD12	1:399:A:LEU:H	19	0.5
(1,2461)	1:382:A:LEU:HD13	1:399:A:LEU:H	19	0.5
(1,2196)	1:365:A:LYS:HE2	1:398:A:LYS:HE2	14	0.5
(1,2196)	1:365:A:LYS:HE2	1:398:A:LYS:HE3	14	0.5
(1,2196)	1:365:A:LYS:HE3	1:398:A:LYS:HE2	14	0.5
(1,2196)	1:365:A:LYS:HE3	1:398:A:LYS:HE3	14	0.5
(1,2135)	1:361:A:GLU:HG2	1:365:A:LYS:HG2	7	0.5
(1,2135)	1:361:A:GLU:HG2	1:365:A:LYS:HG3	7	0.5
(1,2135)	1:361:A:GLU:HG3	1:365:A:LYS:HG2	7	0.5
(1,2135)	1:361:A:GLU:HG3	1:365:A:LYS:HG3	7	0.5
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB1	7	0.5
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB2	7	0.5
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB3	7	0.5
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB1	7	0.5
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB2	7	0.5
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB3	7	0.5
(1,1674)	1:325:A:ILE:HD11	1:327:A:SER:H	13	0.5
(1,1674)	1:325:A:ILE:HD12	1:327:A:SER:H	13	0.5
(1,1674)	1:325:A:ILE:HD13	1:327:A:SER:H	13	0.5
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	2	0.5
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	2	0.5
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	2	0.5
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	2	0.5
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	2	0.5
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	2	0.5
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	2	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	2	0.5
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	2	0.5
(1,1490)	1:314:A:MET:HB2	1:318:A:LEU:H	10	0.5
(1,1490)	1:314:A:MET:HB3	1:318:A:LEU:H	10	0.5
(1,1317)	1:302:A:GLN:HE21	1:332:A:LEU:HD21	2	0.5
(1,1317)	1:302:A:GLN:HE21	1:332:A:LEU:HD22	2	0.5
(1,1317)	1:302:A:GLN:HE21	1:332:A:LEU:HD23	2	0.5
(1,1317)	1:302:A:GLN:HE22	1:332:A:LEU:HD21	2	0.5
(1,1317)	1:302:A:GLN:HE22	1:332:A:LEU:HD22	2	0.5
(1,1317)	1:302:A:GLN:HE22	1:332:A:LEU:HD23	2	0.5
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE1	6	0.5
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE2	6	0.5
(1,1223)	1:299:A:LEU:H	1:305:A:PHE:HA	18	0.5
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	2	0.5
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	2	0.5
(1,1029)	1:289:A:TRP:HZ2	1:380:A:LEU:HB2	9	0.5
(1,1029)	1:289:A:TRP:HZ2	1:380:A:LEU:HB3	9	0.5
(1,1020)	1:289:A:TRP:HH2	1:384:A:GLU:HG2	4	0.5
(1,1020)	1:289:A:TRP:HH2	1:384:A:GLU:HG3	4	0.5
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	4	0.5
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	4	0.5
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	11	0.5
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	11	0.5
(1,574)	1:264:A:SER:HB2	1:358:A:GLN:HB2	7	0.5
(1,574)	1:264:A:SER:HB2	1:358:A:GLN:HB3	7	0.5
(1,574)	1:264:A:SER:HB3	1:358:A:GLN:HB2	7	0.5
(1,574)	1:264:A:SER:HB3	1:358:A:GLN:HB3	7	0.5
(1,570)	1:264:A:SER:HB2	1:359:A:MET:HA	13	0.5
(1,570)	1:264:A:SER:HB3	1:359:A:MET:HA	13	0.5
(1,549)	1:263:A:TRP:H	1:359:A:MET:HG2	14	0.5
(1,549)	1:263:A:TRP:H	1:359:A:MET:HG3	14	0.5
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD2	3	0.5
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD3	3	0.5
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB2	4	0.5
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB3	4	0.5
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB2	4	0.5
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB3	4	0.5
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB2	4	0.5
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB3	4	0.5
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	11	0.5
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	2	0.5
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	4	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,153)	1:238:A:LYS:HE2	1:264:A:SER:HA	6	0.5
(1,153)	1:238:A:LYS:HE3	1:264:A:SER:HA	6	0.5
(1,102)	1:234:A:TRP:HE1	1:235:A:THR:HB	20	0.5
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	19	0.5
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD2	10	0.5
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD3	10	0.5
(2,9)	1:338:A:ILE:HD11	1:342:A:SER:H	4	0.49
(2,9)	1:338:A:ILE:HD12	1:342:A:SER:H	4	0.49
(2,9)	1:338:A:ILE:HD13	1:342:A:SER:H	4	0.49
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD11	1	0.49
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD12	1	0.49
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD13	1	0.49
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD11	1	0.49
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD12	1	0.49
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD13	1	0.49
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD11	1	0.49
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD12	1	0.49
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD13	1	0.49
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	11	0.49
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	13	0.49
(1,3882)	1:485:A:LYS:HB2	1:487:A:ASP:HB3	17	0.49
(1,3846)	1:481:A:GLN:HE21	1:486:A:VAL:H	8	0.49
(1,3846)	1:481:A:GLN:HE22	1:486:A:VAL:H	8	0.49
(1,3655)	1:460:A:LEU:HD21	1:466:A:GLU:H	18	0.49
(1,3655)	1:460:A:LEU:HD22	1:466:A:GLU:H	18	0.49
(1,3655)	1:460:A:LEU:HD23	1:466:A:GLU:H	18	0.49
(1,3634)	1:458:A:LEU:HD11	1:480:A:PHE:HE1	4	0.49
(1,3634)	1:458:A:LEU:HD11	1:480:A:PHE:HE2	4	0.49
(1,3634)	1:458:A:LEU:HD12	1:480:A:PHE:HE1	4	0.49
(1,3634)	1:458:A:LEU:HD12	1:480:A:PHE:HE2	4	0.49
(1,3634)	1:458:A:LEU:HD13	1:480:A:PHE:HE1	4	0.49
(1,3634)	1:458:A:LEU:HD13	1:480:A:PHE:HE2	4	0.49
(1,3567)	1:450:A:LEU:HA	1:454:A:GLY:H	13	0.49
(1,3529)	1:449:A:LEU:HD21	1:494:A:ALA:H	11	0.49
(1,3529)	1:449:A:LEU:HD22	1:494:A:ALA:H	11	0.49
(1,3529)	1:449:A:LEU:HD23	1:494:A:ALA:H	11	0.49
(1,3422)	1:441:A:ALA:H	1:461:A:SER:HB2	8	0.49
(1,3422)	1:441:A:ALA:H	1:461:A:SER:HB3	8	0.49
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB2	14	0.49
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB3	14	0.49
(1,3362)	1:437:A:SER:HA	1:461:A:SER:HA	11	0.49
(1,3333)	1:435:A:ALA:HB1	1:460:A:LEU:H	20	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3333)	1:435:A:ALA:HB2	1:460:A:LEU:H	20	0.49
(1,3333)	1:435:A:ALA:HB3	1:460:A:LEU:H	20	0.49
(1,3170)	1:430:A:ILE:H	1:481:A:GLN:H	2	0.49
(1,3154)	1:429:A:LYS:HA	1:480:A:PHE:HA	8	0.49
(1,3137)	1:428:A:GLU:HA	1:478:A:LYS:HG2	2	0.49
(1,3137)	1:428:A:GLU:HA	1:478:A:LYS:HG3	2	0.49
(1,3137)	1:428:A:GLU:HA	1:478:A:LYS:HG2	15	0.49
(1,3137)	1:428:A:GLU:HA	1:478:A:LYS:HG3	15	0.49
(1,3083)	1:423:A:MET:HB2	1:427:A:GLN:HE21	2	0.49
(1,3083)	1:423:A:MET:HB2	1:427:A:GLN:HE22	2	0.49
(1,3083)	1:423:A:MET:HB3	1:427:A:GLN:HE21	2	0.49
(1,3083)	1:423:A:MET:HB3	1:427:A:GLN:HE22	2	0.49
(1,3081)	1:423:A:MET:HE1	1:427:A:GLN:HB2	9	0.49
(1,3081)	1:423:A:MET:HE1	1:427:A:GLN:HB3	9	0.49
(1,3081)	1:423:A:MET:HE2	1:427:A:GLN:HB2	9	0.49
(1,3081)	1:423:A:MET:HE2	1:427:A:GLN:HB3	9	0.49
(1,3081)	1:423:A:MET:HE3	1:427:A:GLN:HB2	9	0.49
(1,3081)	1:423:A:MET:HE3	1:427:A:GLN:HB3	9	0.49
(1,2608)	1:392:A:ASN:HB2	1:396:A:ILE:H	1	0.49
(1,2608)	1:392:A:ASN:HB3	1:396:A:ILE:H	1	0.49
(1,2563)	1:387:A:ALA:HA	1:471:A:TYR:HE1	17	0.49
(1,2563)	1:387:A:ALA:HA	1:471:A:TYR:HE2	17	0.49
(1,2445)	1:381:A:VAL:HA	1:385:A:GLY:H	9	0.49
(1,2381)	1:376:A:GLN:HA	1:412:A:GLN:HE21	3	0.49
(1,2381)	1:376:A:GLN:HA	1:412:A:GLN:HE22	3	0.49
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	9	0.49
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	9	0.49
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	9	0.49
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	9	0.49
(1,2196)	1:365:A:LYS:HE2	1:398:A:LYS:HE2	18	0.49
(1,2196)	1:365:A:LYS:HE2	1:398:A:LYS:HE3	18	0.49
(1,2196)	1:365:A:LYS:HE3	1:398:A:LYS:HE2	18	0.49
(1,2196)	1:365:A:LYS:HE3	1:398:A:LYS:HE3	18	0.49
(1,2133)	1:361:A:GLU:HA	1:365:A:LYS:H	14	0.49
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB1	1	0.49
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB2	1	0.49
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB3	1	0.49
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB1	1	0.49
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB2	1	0.49
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB3	1	0.49
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD21	13	0.49
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD22	13	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD21	13	0.49
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD22	13	0.49
(1,1935)	1:350:A:ASN:HA	1:354:A:LYS:HG2	20	0.49
(1,1935)	1:350:A:ASN:HA	1:354:A:LYS:HG3	20	0.49
(1,1933)	1:350:A:ASN:HA	1:354:A:LYS:H	3	0.49
(1,1776)	1:336:A:ARG:HA	1:340:A:GLN:H	14	0.49
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD11	16	0.49
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD12	16	0.49
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD13	16	0.49
(1,1674)	1:325:A:ILE:HD11	1:327:A:SER:H	1	0.49
(1,1674)	1:325:A:ILE:HD12	1:327:A:SER:H	1	0.49
(1,1674)	1:325:A:ILE:HD13	1:327:A:SER:H	1	0.49
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	9	0.49
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	9	0.49
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	9	0.49
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	9	0.49
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	9	0.49
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	9	0.49
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	9	0.49
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	9	0.49
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	9	0.49
(1,1487)	1:314:A:MET:HB2	1:319:A:ARG:HA	8	0.49
(1,1487)	1:314:A:MET:HB3	1:319:A:ARG:HA	8	0.49
(1,1422)	1:312:A:GLN:HE21	1:340:A:GLN:HA	2	0.49
(1,1422)	1:312:A:GLN:HE22	1:340:A:GLN:HA	2	0.49
(1,1422)	1:312:A:GLN:HE21	1:340:A:GLN:HA	18	0.49
(1,1422)	1:312:A:GLN:HE22	1:340:A:GLN:HA	18	0.49
(1,1219)	1:299:A:LEU:H	1:306:A:ILE:H	18	0.49
(1,1118)	1:297:A:LEU:HA	1:322:A:ARG:HD2	4	0.49
(1,1118)	1:297:A:LEU:HA	1:322:A:ARG:HD3	4	0.49
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	16	0.49
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	16	0.49
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD2	3	0.49
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD3	3	0.49
(1,1029)	1:289:A:TRP:HZ2	1:380:A:LEU:HB2	4	0.49
(1,1029)	1:289:A:TRP:HZ2	1:380:A:LEU:HB3	4	0.49
(1,1020)	1:289:A:TRP:HH2	1:384:A:GLU:HG2	7	0.49
(1,1020)	1:289:A:TRP:HH2	1:384:A:GLU:HG3	7	0.49
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE1	12	0.49
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE2	12	0.49
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE3	12	0.49
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE1	12	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE2	12	0.49
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE3	12	0.49
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	20	0.49
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	20	0.49
(1,719)	1:274:A:TYR:HD2	1:348:A:LEU:HD22	19	0.49
(1,705)	1:273:A:GLU:HG2	1:328:A:SER:H	19	0.49
(1,705)	1:273:A:GLU:HG3	1:328:A:SER:H	19	0.49
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	8	0.49
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	16	0.49
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	16	0.49
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	16	0.49
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD2	5	0.49
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD3	5	0.49
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD2	5	0.49
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD3	5	0.49
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD2	5	0.49
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD3	5	0.49
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	18	0.49
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	20	0.49
(1,123)	1:236:A:ARG:HB2	1:240:A:GLU:H	7	0.49
(1,123)	1:236:A:ARG:HB3	1:240:A:GLU:H	7	0.49
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	5	0.49
(1,3890)	1:486:A:VAL:HA	1:490:A:LEU:H	14	0.48
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE2	12	0.48
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE3	12	0.48
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE2	12	0.48
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE3	12	0.48
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE2	13	0.48
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE3	13	0.48
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE2	13	0.48
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE3	13	0.48
(1,3848)	1:481:A:GLN:HG2	1:486:A:VAL:HA	20	0.48
(1,3848)	1:481:A:GLN:HG3	1:486:A:VAL:HA	20	0.48
(1,3784)	1:474:A:GLU:H	1:480:A:PHE:H	13	0.48
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB2	14	0.48
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB3	14	0.48
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB2	14	0.48
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB3	14	0.48
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB2	14	0.48
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB3	14	0.48
(1,3730)	1:468:A:MET:HA	1:471:A:TYR:HD1	12	0.48
(1,3730)	1:468:A:MET:HA	1:471:A:TYR:HD2	12	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3674)	1:462:A:ASP:HB2	1:464:A:ILE:H	7	0.48
(1,3674)	1:462:A:ASP:HB3	1:464:A:ILE:H	7	0.48
(1,3635)	1:458:A:LEU:HD13	1:480:A:PHE:HE1	17	0.48
(1,3567)	1:450:A:LEU:HA	1:454:A:GLY:H	8	0.48
(1,3567)	1:450:A:LEU:HA	1:454:A:GLY:H	15	0.48
(1,3245)	1:432:A:TYR:HB2	1:458:A:LEU:H	16	0.48
(1,3245)	1:432:A:TYR:HB3	1:458:A:LEU:H	16	0.48
(1,3235)	1:432:A:TYR:H	1:482:A:SER:HA	18	0.48
(1,3208)	1:431:A:TYR:HB2	1:482:A:SER:HA	18	0.48
(1,3208)	1:431:A:TYR:HB3	1:482:A:SER:HA	18	0.48
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG2	2	0.48
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG3	2	0.48
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG2	2	0.48
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG3	2	0.48
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG2	15	0.48
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG3	15	0.48
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG2	15	0.48
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG3	15	0.48
(1,3128)	1:427:A:GLN:HG2	1:429:A:LYS:H	11	0.48
(1,3128)	1:427:A:GLN:HG3	1:429:A:LYS:H	11	0.48
(1,3121)	1:427:A:GLN:HE21	1:455:A:ILE:HA	11	0.48
(1,3121)	1:427:A:GLN:HE22	1:455:A:ILE:HA	11	0.48
(1,3007)	1:419:A:TYR:HE2	1:478:A:LYS:HG2	3	0.48
(1,3007)	1:419:A:TYR:HE2	1:478:A:LYS:HG3	3	0.48
(1,2737)	1:401:A:ARG:HD2	1:414:A:VAL:HA	15	0.48
(1,2737)	1:401:A:ARG:HD3	1:414:A:VAL:HA	15	0.48
(1,2430)	1:380:A:LEU:HD21	1:462:A:ASP:HB2	4	0.48
(1,2430)	1:380:A:LEU:HD21	1:462:A:ASP:HB3	4	0.48
(1,2430)	1:380:A:LEU:HD22	1:462:A:ASP:HB2	4	0.48
(1,2430)	1:380:A:LEU:HD22	1:462:A:ASP:HB3	4	0.48
(1,2430)	1:380:A:LEU:HD23	1:462:A:ASP:HB2	4	0.48
(1,2430)	1:380:A:LEU:HD23	1:462:A:ASP:HB3	4	0.48
(1,2425)	1:380:A:LEU:HB2	1:464:A:ILE:H	16	0.48
(1,2425)	1:380:A:LEU:HB3	1:464:A:ILE:H	16	0.48
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA2	9	0.48
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA3	9	0.48
(1,2123)	1:361:A:GLU:HA	1:399:A:LEU:HA	10	0.48
(1,1997)	1:354:A:LYS:HB2	1:358:A:GLN:HE21	4	0.48
(1,1997)	1:354:A:LYS:HB2	1:358:A:GLN:HE22	4	0.48
(1,1997)	1:354:A:LYS:HB3	1:358:A:GLN:HE21	4	0.48
(1,1997)	1:354:A:LYS:HB3	1:358:A:GLN:HE22	4	0.48
(1,1933)	1:350:A:ASN:HA	1:354:A:LYS:H	7	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1886)	1:346:A:ARG:HG2	1:350:A:ASN:HD21	12	0.48
(1,1886)	1:346:A:ARG:HG2	1:350:A:ASN:HD22	12	0.48
(1,1886)	1:346:A:ARG:HG3	1:350:A:ASN:HD21	12	0.48
(1,1886)	1:346:A:ARG:HG3	1:350:A:ASN:HD22	12	0.48
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD11	1	0.48
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD12	1	0.48
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD13	1	0.48
(1,1745)	1:333:A:ASN:HD21	1:338:A:ILE:HD11	3	0.48
(1,1745)	1:333:A:ASN:HD21	1:338:A:ILE:HD12	3	0.48
(1,1745)	1:333:A:ASN:HD21	1:338:A:ILE:HD13	3	0.48
(1,1745)	1:333:A:ASN:HD22	1:338:A:ILE:HD11	3	0.48
(1,1745)	1:333:A:ASN:HD22	1:338:A:ILE:HD12	3	0.48
(1,1745)	1:333:A:ASN:HD22	1:338:A:ILE:HD13	3	0.48
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE1	13	0.48
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE2	13	0.48
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE3	13	0.48
(1,1511)	1:315:A:PRO:HG2	1:319:A:ARG:H	18	0.48
(1,1511)	1:315:A:PRO:HG3	1:319:A:ARG:H	18	0.48
(1,1490)	1:314:A:MET:HB2	1:318:A:LEU:H	8	0.48
(1,1490)	1:314:A:MET:HB3	1:318:A:LEU:H	8	0.48
(1,1374)	1:307:A:MET:HE1	1:335:A:SER:HA	19	0.48
(1,1374)	1:307:A:MET:HE2	1:335:A:SER:HA	19	0.48
(1,1374)	1:307:A:MET:HE3	1:335:A:SER:HA	19	0.48
(1,1321)	1:302:A:GLN:HA	1:328:A:SER:HA	18	0.48
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	6	0.48
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	6	0.48
(1,1060)	1:294:A:LYS:HD2	1:309:A:ASP:HB2	5	0.48
(1,1060)	1:294:A:LYS:HD2	1:309:A:ASP:HB3	5	0.48
(1,1060)	1:294:A:LYS:HD3	1:309:A:ASP:HB2	5	0.48
(1,1060)	1:294:A:LYS:HD3	1:309:A:ASP:HB3	5	0.48
(1,1044)	1:291:A:ARG:HA	1:293:A:HIS:HA	14	0.48
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	8	0.48
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE1	6	0.48
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE2	6	0.48
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE3	6	0.48
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE1	6	0.48
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE2	6	0.48
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE3	6	0.48
(1,927)	1:283:A:GLN:HA	1:377:A:GLN:HA	2	0.48
(1,673)	1:270:A:GLY:H	1:273:A:GLU:HA	1	0.48
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	14	0.48
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	14	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	14	0.48
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	14	0.48
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	14	0.48
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	14	0.48
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	4	0.48
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	1	0.48
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG21	14	0.48
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG22	14	0.48
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG23	14	0.48
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	11	0.47
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	15	0.47
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	16	0.47
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	16	0.47
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	16	0.47
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	16	0.47
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	16	0.47
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	16	0.47
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	16	0.47
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	16	0.47
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	16	0.47
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	19	0.47
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	19	0.47
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	19	0.47
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	19	0.47
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	19	0.47
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	19	0.47
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	19	0.47
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	19	0.47
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	19	0.47
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	5	0.47
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	14	0.47
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	4	0.47
(1,3846)	1:481:A:GLN:HE21	1:486:A:VAL:H	18	0.47
(1,3846)	1:481:A:GLN:HE22	1:486:A:VAL:H	18	0.47
(1,3845)	1:481:A:GLN:HG2	1:487:A:ASP:H	10	0.47
(1,3845)	1:481:A:GLN:HG3	1:487:A:ASP:H	10	0.47
(1,3634)	1:458:A:LEU:HD11	1:480:A:PHE:HE1	3	0.47
(1,3634)	1:458:A:LEU:HD11	1:480:A:PHE:HE2	3	0.47
(1,3634)	1:458:A:LEU:HD12	1:480:A:PHE:HE1	3	0.47
(1,3634)	1:458:A:LEU:HD12	1:480:A:PHE:HE2	3	0.47
(1,3634)	1:458:A:LEU:HD13	1:480:A:PHE:HE1	3	0.47
(1,3634)	1:458:A:LEU:HD13	1:480:A:PHE:HE2	3	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3548)	1:450:A:LEU:HD21	1:493:A:LEU:HB2	14	0.47
(1,3548)	1:450:A:LEU:HD21	1:493:A:LEU:HB3	14	0.47
(1,3548)	1:450:A:LEU:HD22	1:493:A:LEU:HB2	14	0.47
(1,3548)	1:450:A:LEU:HD22	1:493:A:LEU:HB3	14	0.47
(1,3548)	1:450:A:LEU:HD23	1:493:A:LEU:HB2	14	0.47
(1,3548)	1:450:A:LEU:HD23	1:493:A:LEU:HB3	14	0.47
(1,3329)	1:435:A:ALA:H	1:461:A:SER:HA	13	0.47
(1,3309)	1:434:A:THR:HB	1:466:A:GLU:H	7	0.47
(1,3245)	1:432:A:TYR:HB2	1:458:A:LEU:H	18	0.47
(1,3245)	1:432:A:TYR:HB3	1:458:A:LEU:H	18	0.47
(1,3187)	1:430:A:ILE:HD11	1:474:A:GLU:HA	19	0.47
(1,3187)	1:430:A:ILE:HD12	1:474:A:GLU:HA	19	0.47
(1,3187)	1:430:A:ILE:HD13	1:474:A:GLU:HA	19	0.47
(1,3178)	1:430:A:ILE:HD11	1:479:A:PRO:HA	7	0.47
(1,3178)	1:430:A:ILE:HD12	1:479:A:PRO:HA	7	0.47
(1,3178)	1:430:A:ILE:HD13	1:479:A:PRO:HA	7	0.47
(1,3178)	1:430:A:ILE:HD11	1:479:A:PRO:HA	16	0.47
(1,3178)	1:430:A:ILE:HD12	1:479:A:PRO:HA	16	0.47
(1,3178)	1:430:A:ILE:HD13	1:479:A:PRO:HA	16	0.47
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD11	11	0.47
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD12	11	0.47
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD13	11	0.47
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB2	20	0.47
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB3	20	0.47
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB2	20	0.47
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB3	20	0.47
(1,3128)	1:427:A:GLN:HG2	1:429:A:LYS:H	10	0.47
(1,3128)	1:427:A:GLN:HG3	1:429:A:LYS:H	10	0.47
(1,3110)	1:426:A:GLY:HA2	1:492:A:LYS:HD3	7	0.47
(1,3110)	1:426:A:GLY:HA3	1:492:A:LYS:HD3	7	0.47
(1,3079)	1:423:A:MET:HE1	1:428:A:GLU:HA	6	0.47
(1,3079)	1:423:A:MET:HE2	1:428:A:GLU:HA	6	0.47
(1,3079)	1:423:A:MET:HE3	1:428:A:GLU:HA	6	0.47
(1,2984)	1:417:A:GLU:HA	1:421:A:SER:H	17	0.47
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB2	13	0.47
(1,2787)	1:403:A:ALA:H	1:458:A:LEU:HB3	13	0.47
(1,2777)	1:403:A:ALA:H	1:461:A:SER:H	5	0.47
(1,2755)	1:402:A:PHE:HD1	1:460:A:LEU:HD13	10	0.47
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	6	0.47
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	6	0.47
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	6	0.47
(1,2699)	1:398:A:LYS:HE2	1:417:A:GLU:HG2	9	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2699)	1:398:A:LYS:HE2	1:417:A:GLU:HG3	9	0.47
(1,2699)	1:398:A:LYS:HE3	1:417:A:GLU:HG2	9	0.47
(1,2699)	1:398:A:LYS:HE3	1:417:A:GLU:HG3	9	0.47
(1,2696)	1:398:A:LYS:HA	1:475:A:PHE:HE1	7	0.47
(1,2696)	1:398:A:LYS:HA	1:475:A:PHE:HE2	7	0.47
(1,2621)	1:393:A:GLN:HE21	1:473:A:THR:H	8	0.47
(1,2621)	1:393:A:GLN:HE22	1:473:A:THR:H	8	0.47
(1,2538)	1:386:A:PRO:HA	1:471:A:TYR:HB2	6	0.47
(1,2538)	1:386:A:PRO:HA	1:471:A:TYR:HB3	6	0.47
(1,2337)	1:375:A:TRP:HD1	1:413:A:THR:HA	10	0.47
(1,2335)	1:375:A:TRP:HH2	1:468:A:MET:HE1	12	0.47
(1,2335)	1:375:A:TRP:HH2	1:468:A:MET:HE2	12	0.47
(1,2335)	1:375:A:TRP:HH2	1:468:A:MET:HE3	12	0.47
(1,2123)	1:361:A:GLU:HA	1:399:A:LEU:HA	9	0.47
(1,2041)	1:357:A:LEU:HD21	1:396:A:ILE:H	15	0.47
(1,2041)	1:357:A:LEU:HD22	1:396:A:ILE:H	15	0.47
(1,2041)	1:357:A:LEU:HD23	1:396:A:ILE:H	15	0.47
(1,1886)	1:346:A:ARG:HG2	1:350:A:ASN:HD21	6	0.47
(1,1886)	1:346:A:ARG:HG2	1:350:A:ASN:HD22	6	0.47
(1,1886)	1:346:A:ARG:HG3	1:350:A:ASN:HD21	6	0.47
(1,1886)	1:346:A:ARG:HG3	1:350:A:ASN:HD22	6	0.47
(1,1884)	1:346:A:ARG:HA	1:350:A:ASN:H	8	0.47
(1,1776)	1:336:A:ARG:HA	1:340:A:GLN:H	18	0.47
(1,1776)	1:336:A:ARG:HA	1:340:A:GLN:H	19	0.47
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD11	19	0.47
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD12	19	0.47
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD13	19	0.47
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD11	20	0.47
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD12	20	0.47
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD13	20	0.47
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE1	18	0.47
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE2	18	0.47
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE3	18	0.47
(1,1519)	1:315:A:PRO:HG2	1:317:A:TYR:HE1	15	0.47
(1,1519)	1:315:A:PRO:HG2	1:317:A:TYR:HE2	15	0.47
(1,1519)	1:315:A:PRO:HG3	1:317:A:TYR:HE1	15	0.47
(1,1519)	1:315:A:PRO:HG3	1:317:A:TYR:HE2	15	0.47
(1,1422)	1:312:A:GLN:HE21	1:340:A:GLN:HA	19	0.47
(1,1422)	1:312:A:GLN:HE22	1:340:A:GLN:HA	19	0.47
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG21	19	0.47
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG22	19	0.47
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG23	19	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1374)	1:307:A:MET:HE1	1:335:A:SER:HA	2	0.47
(1,1374)	1:307:A:MET:HE2	1:335:A:SER:HA	2	0.47
(1,1374)	1:307:A:MET:HE3	1:335:A:SER:HA	2	0.47
(1,1318)	1:302:A:GLN:H	1:329:A:ASP:H	18	0.47
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD11	19	0.47
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD12	19	0.47
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD13	19	0.47
(1,1166)	1:298:A:LYS:HG2	1:309:A:ASP:H	5	0.47
(1,1166)	1:298:A:LYS:HG3	1:309:A:ASP:H	5	0.47
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	2	0.47
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	13	0.47
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	13	0.47
(1,869)	1:280:A:ILE:HD11	1:360:A:LEU:HA	18	0.47
(1,869)	1:280:A:ILE:HD12	1:360:A:LEU:HA	18	0.47
(1,869)	1:280:A:ILE:HD13	1:360:A:LEU:HA	18	0.47
(1,608)	1:266:A:ASN:HB2	1:355:A:ARG:HG2	7	0.47
(1,608)	1:266:A:ASN:HB2	1:355:A:ARG:HG3	7	0.47
(1,608)	1:266:A:ASN:HB3	1:355:A:ARG:HG2	7	0.47
(1,608)	1:266:A:ASN:HB3	1:355:A:ARG:HG3	7	0.47
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	12	0.47
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	9	0.47
(1,222)	1:244:A:GLU:H	1:247:A:LYS:H	12	0.47
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	10	0.47
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	10	0.47
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	11	0.47
(1,153)	1:238:A:LYS:HE2	1:264:A:SER:HA	16	0.47
(1,153)	1:238:A:LYS:HE3	1:264:A:SER:HA	16	0.47
(1,139)	1:237:A:ASN:HD21	1:239:A:SER:H	6	0.47
(1,139)	1:237:A:ASN:HD22	1:239:A:SER:H	6	0.47
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD2	3	0.47
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD3	3	0.47
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	13	0.47
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD2	18	0.47
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD3	18	0.47
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG21	14	0.47
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG22	14	0.47
(1,53)	1:233:A:LEU:H	1:235:A:THR:HG23	14	0.47
(1,21)	1:232:A:ALA:H	1:235:A:THR:H	15	0.47
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG21	2	0.46
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG22	2	0.46
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG23	2	0.46
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG21	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG22	2	0.46
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG23	2	0.46
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG21	2	0.46
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG22	2	0.46
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG23	2	0.46
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	13	0.46
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	13	0.46
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	13	0.46
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	13	0.46
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	13	0.46
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	13	0.46
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	13	0.46
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	13	0.46
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	13	0.46
(1,3942)	1:490:A:LEU:H	1:492:A:LYS:H	8	0.46
(1,3936)	1:490:A:LEU:HB2	1:494:A:ALA:H	11	0.46
(1,3936)	1:490:A:LEU:HB3	1:494:A:ALA:H	11	0.46
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	3	0.46
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	16	0.46
(1,3882)	1:485:A:LYS:HB2	1:487:A:ASP:HB3	9	0.46
(1,3848)	1:481:A:GLN:HG2	1:486:A:VAL:HA	17	0.46
(1,3848)	1:481:A:GLN:HG3	1:486:A:VAL:HA	17	0.46
(1,3772)	1:472:A:LEU:HD21	1:474:A:GLU:HA	18	0.46
(1,3772)	1:472:A:LEU:HD22	1:474:A:GLU:HA	18	0.46
(1,3772)	1:472:A:LEU:HD23	1:474:A:GLU:HA	18	0.46
(1,3726)	1:468:A:MET:HG2	1:472:A:LEU:HB2	8	0.46
(1,3726)	1:468:A:MET:HG2	1:472:A:LEU:HB3	8	0.46
(1,3726)	1:468:A:MET:HG3	1:472:A:LEU:HB2	8	0.46
(1,3726)	1:468:A:MET:HG3	1:472:A:LEU:HB3	8	0.46
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	5	0.46
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	5	0.46
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	5	0.46
(1,3635)	1:458:A:LEU:HD13	1:480:A:PHE:HE1	10	0.46
(1,3561)	1:450:A:LEU:HD11	1:456:A:GLU:H	4	0.46
(1,3561)	1:450:A:LEU:HD12	1:456:A:GLU:H	4	0.46
(1,3561)	1:450:A:LEU:HD13	1:456:A:GLU:H	4	0.46
(1,3301)	1:434:A:THR:H	1:484:A:SER:H	14	0.46
(1,3222)	1:431:A:TYR:HD1	1:456:A:GLU:H	7	0.46
(1,3222)	1:431:A:TYR:HD2	1:456:A:GLU:H	7	0.46
(1,3170)	1:430:A:ILE:H	1:481:A:GLN:H	13	0.46
(1,3155)	1:429:A:LYS:HB2	1:480:A:PHE:HA	8	0.46
(1,3155)	1:429:A:LYS:HB3	1:480:A:PHE:HA	8	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3121)	1:427:A:GLN:HE21	1:455:A:ILE:HA	16	0.46
(1,3121)	1:427:A:GLN:HE22	1:455:A:ILE:HA	16	0.46
(1,2937)	1:414:A:VAL:HG21	1:419:A:TYR:HA	13	0.46
(1,2937)	1:414:A:VAL:HG22	1:419:A:TYR:HA	13	0.46
(1,2937)	1:414:A:VAL:HG23	1:419:A:TYR:HA	13	0.46
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG11	1	0.46
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG12	1	0.46
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG13	1	0.46
(1,2632)	1:393:A:GLN:HA	1:396:A:ILE:HB	20	0.46
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB2	14	0.46
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB3	14	0.46
(1,2525)	1:385:A:GLY:HA2	1:389:A:ASP:HB2	1	0.46
(1,2525)	1:385:A:GLY:HA2	1:389:A:ASP:HB3	1	0.46
(1,2525)	1:385:A:GLY:HA3	1:389:A:ASP:HB2	1	0.46
(1,2525)	1:385:A:GLY:HA3	1:389:A:ASP:HB3	1	0.46
(1,2359)	1:375:A:TRP:HH2	1:383:A:LYS:HG2	8	0.46
(1,2359)	1:375:A:TRP:HH2	1:383:A:LYS:HG3	8	0.46
(1,2135)	1:361:A:GLU:HG2	1:365:A:LYS:HG2	16	0.46
(1,2135)	1:361:A:GLU:HG2	1:365:A:LYS:HG3	16	0.46
(1,2135)	1:361:A:GLU:HG3	1:365:A:LYS:HG2	16	0.46
(1,2135)	1:361:A:GLU:HG3	1:365:A:LYS:HG3	16	0.46
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG2	1	0.46
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG3	1	0.46
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG2	1	0.46
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG3	1	0.46
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	15	0.46
(1,1814)	1:339:A:LEU:HD21	1:344:A:VAL:HG21	14	0.46
(1,1814)	1:339:A:LEU:HD21	1:344:A:VAL:HG22	14	0.46
(1,1814)	1:339:A:LEU:HD21	1:344:A:VAL:HG23	14	0.46
(1,1814)	1:339:A:LEU:HD22	1:344:A:VAL:HG21	14	0.46
(1,1814)	1:339:A:LEU:HD22	1:344:A:VAL:HG22	14	0.46
(1,1814)	1:339:A:LEU:HD22	1:344:A:VAL:HG23	14	0.46
(1,1814)	1:339:A:LEU:HD23	1:344:A:VAL:HG21	14	0.46
(1,1814)	1:339:A:LEU:HD23	1:344:A:VAL:HG22	14	0.46
(1,1814)	1:339:A:LEU:HD23	1:344:A:VAL:HG23	14	0.46
(1,1570)	1:317:A:TYR:HA	1:320:A:PHE:HE1	8	0.46
(1,1570)	1:317:A:TYR:HA	1:320:A:PHE:HE2	8	0.46
(1,1430)	1:312:A:GLN:HE21	1:336:A:ARG:HA	9	0.46
(1,1430)	1:312:A:GLN:HE22	1:336:A:ARG:HA	9	0.46
(1,1321)	1:302:A:GLN:HA	1:328:A:SER:HA	4	0.46
(1,1298)	1:301:A:VAL:H	1:306:A:ILE:HB	19	0.46
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD11	13	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD12	13	0.46
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD13	13	0.46
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD11	13	0.46
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD12	13	0.46
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD13	13	0.46
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD11	13	0.46
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD12	13	0.46
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD13	13	0.46
(1,1166)	1:298:A:LYS:HG2	1:309:A:ASP:H	15	0.46
(1,1166)	1:298:A:LYS:HG3	1:309:A:ASP:H	15	0.46
(1,1029)	1:289:A:TRP:HZ2	1:380:A:LEU:HB2	7	0.46
(1,1029)	1:289:A:TRP:HZ2	1:380:A:LEU:HB3	7	0.46
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE1	11	0.46
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE2	11	0.46
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE3	11	0.46
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE1	11	0.46
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE2	11	0.46
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE3	11	0.46
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	5	0.46
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	5	0.46
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	14	0.46
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	14	0.46
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	19	0.46
(1,454)	1:257:A:PHE:H	1:258:A:ASN:HD21	16	0.46
(1,454)	1:257:A:PHE:H	1:258:A:ASN:HD22	16	0.46
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	15	0.46
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	15	0.46
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	15	0.46
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	15	0.46
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	6	0.46
(1,291)	1:248:A:GLU:HA	1:252:A:HIS:H	5	0.46
(1,219)	1:244:A:GLU:HA	1:248:A:GLU:H	12	0.46
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	9	0.46
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	11	0.46
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG21	20	0.46
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG22	20	0.46
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG23	20	0.46
(1,3938)	1:490:A:LEU:HA	1:493:A:LEU:H	1	0.45
(1,3882)	1:485:A:LYS:HB2	1:487:A:ASP:HB3	10	0.45
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB2	16	0.45
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB3	16	0.45
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB2	16	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB3	16	0.45
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB2	16	0.45
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB3	16	0.45
(1,3726)	1:468:A:MET:HG2	1:472:A:LEU:HB2	17	0.45
(1,3726)	1:468:A:MET:HG2	1:472:A:LEU:HB3	17	0.45
(1,3726)	1:468:A:MET:HG3	1:472:A:LEU:HB2	17	0.45
(1,3726)	1:468:A:MET:HG3	1:472:A:LEU:HB3	17	0.45
(1,3726)	1:468:A:MET:HG2	1:472:A:LEU:HB2	20	0.45
(1,3726)	1:468:A:MET:HG2	1:472:A:LEU:HB3	20	0.45
(1,3726)	1:468:A:MET:HG3	1:472:A:LEU:HB2	20	0.45
(1,3726)	1:468:A:MET:HG3	1:472:A:LEU:HB3	20	0.45
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	20	0.45
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	20	0.45
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	20	0.45
(1,3674)	1:462:A:ASP:HB2	1:464:A:ILE:H	2	0.45
(1,3674)	1:462:A:ASP:HB3	1:464:A:ILE:H	2	0.45
(1,3674)	1:462:A:ASP:HB2	1:464:A:ILE:H	6	0.45
(1,3674)	1:462:A:ASP:HB3	1:464:A:ILE:H	6	0.45
(1,3422)	1:441:A:ALA:H	1:461:A:SER:HB2	3	0.45
(1,3422)	1:441:A:ALA:H	1:461:A:SER:HB3	3	0.45
(1,3406)	1:439:A:ALA:HA	1:442:A:LYS:HD2	19	0.45
(1,3406)	1:439:A:ALA:HA	1:442:A:LYS:HD3	19	0.45
(1,3361)	1:437:A:SER:H	1:461:A:SER:HA	20	0.45
(1,3311)	1:434:A:THR:HB	1:466:A:GLU:HA	20	0.45
(1,3245)	1:432:A:TYR:HB2	1:458:A:LEU:H	10	0.45
(1,3245)	1:432:A:TYR:HB3	1:458:A:LEU:H	10	0.45
(1,3245)	1:432:A:TYR:HB2	1:458:A:LEU:H	13	0.45
(1,3245)	1:432:A:TYR:HB3	1:458:A:LEU:H	13	0.45
(1,3245)	1:432:A:TYR:HB2	1:458:A:LEU:H	14	0.45
(1,3245)	1:432:A:TYR:HB3	1:458:A:LEU:H	14	0.45
(1,3245)	1:432:A:TYR:HB2	1:458:A:LEU:H	19	0.45
(1,3245)	1:432:A:TYR:HB3	1:458:A:LEU:H	19	0.45
(1,3170)	1:430:A:ILE:H	1:481:A:GLN:H	9	0.45
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD11	16	0.45
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD12	16	0.45
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD13	16	0.45
(1,3154)	1:429:A:LYS:HA	1:480:A:PHE:HA	17	0.45
(1,3154)	1:429:A:LYS:HA	1:480:A:PHE:HA	20	0.45
(1,3147)	1:429:A:LYS:HD2	1:488:A:GLU:HG2	5	0.45
(1,3147)	1:429:A:LYS:HD2	1:488:A:GLU:HG3	5	0.45
(1,3147)	1:429:A:LYS:HD3	1:488:A:GLU:HG2	5	0.45
(1,3147)	1:429:A:LYS:HD3	1:488:A:GLU:HG3	5	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3144)	1:429:A:LYS:HD2	1:489:A:SER:HA	4	0.45
(1,3144)	1:429:A:LYS:HD3	1:489:A:SER:HA	4	0.45
(1,3112)	1:426:A:GLY:HA2	1:428:A:GLU:HA	18	0.45
(1,3112)	1:426:A:GLY:HA3	1:428:A:GLU:HA	18	0.45
(1,3096)	1:424:A:LYS:H	1:427:A:GLN:HB2	6	0.45
(1,3096)	1:424:A:LYS:H	1:427:A:GLN:HB3	6	0.45
(1,3071)	1:423:A:MET:HE1	1:431:A:TYR:H	18	0.45
(1,3071)	1:423:A:MET:HE2	1:431:A:TYR:H	18	0.45
(1,3071)	1:423:A:MET:HE3	1:431:A:TYR:H	18	0.45
(1,2984)	1:417:A:GLU:HA	1:421:A:SER:H	15	0.45
(1,2982)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	14	0.45
(1,2982)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	14	0.45
(1,2937)	1:414:A:VAL:HG21	1:419:A:TYR:HA	9	0.45
(1,2937)	1:414:A:VAL:HG22	1:419:A:TYR:HA	9	0.45
(1,2937)	1:414:A:VAL:HG23	1:419:A:TYR:HA	9	0.45
(1,2562)	1:387:A:ALA:HB1	1:471:A:TYR:HD1	14	0.45
(1,2562)	1:387:A:ALA:HB1	1:471:A:TYR:HD2	14	0.45
(1,2562)	1:387:A:ALA:HB2	1:471:A:TYR:HD1	14	0.45
(1,2562)	1:387:A:ALA:HB2	1:471:A:TYR:HD2	14	0.45
(1,2562)	1:387:A:ALA:HB3	1:471:A:TYR:HD1	14	0.45
(1,2562)	1:387:A:ALA:HB3	1:471:A:TYR:HD2	14	0.45
(1,2436)	1:380:A:LEU:HA	1:383:A:LYS:HD2	19	0.45
(1,2436)	1:380:A:LEU:HA	1:383:A:LYS:HD3	19	0.45
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	3	0.45
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	3	0.45
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	3	0.45
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	3	0.45
(1,2041)	1:357:A:LEU:HD21	1:396:A:ILE:H	10	0.45
(1,2041)	1:357:A:LEU:HD22	1:396:A:ILE:H	10	0.45
(1,2041)	1:357:A:LEU:HD23	1:396:A:ILE:H	10	0.45
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE21	15	0.45
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE22	15	0.45
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD21	4	0.45
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD22	4	0.45
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD21	4	0.45
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD22	4	0.45
(1,1951)	1:351:A:ALA:HA	1:354:A:LYS:HD2	17	0.45
(1,1951)	1:351:A:ALA:HA	1:354:A:LYS:HD3	17	0.45
(1,1793)	1:337:A:GLU:HA	1:340:A:GLN:HB2	15	0.45
(1,1793)	1:337:A:GLU:HA	1:340:A:GLN:HB3	15	0.45
(1,1506)	1:315:A:PRO:HA	1:349:A:ARG:HD2	15	0.45
(1,1506)	1:315:A:PRO:HA	1:349:A:ARG:HD3	15	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1420)	1:312:A:GLN:HE21	1:340:A:GLN:H	11	0.45
(1,1420)	1:312:A:GLN:HE22	1:340:A:GLN:H	11	0.45
(1,1390)	1:309:A:ASP:HA	1:311:A:GLU:HB2	18	0.45
(1,1390)	1:309:A:ASP:HA	1:311:A:GLU:HB3	18	0.45
(1,1321)	1:302:A:GLN:HA	1:328:A:SER:HA	11	0.45
(1,1318)	1:302:A:GLN:H	1:329:A:ASP:H	15	0.45
(1,1172)	1:298:A:LYS:HA	1:307:A:MET:H	18	0.45
(1,1140)	1:297:A:LEU:HA	1:309:A:ASP:HA	7	0.45
(1,1140)	1:297:A:LEU:HA	1:309:A:ASP:HA	11	0.45
(1,1023)	1:289:A:TRP:HZ2	1:381:A:VAL:H	9	0.45
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	15	0.45
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	19	0.45
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	19	0.45
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	19	0.45
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	7	0.45
(1,705)	1:273:A:GLU:HG2	1:328:A:SER:H	18	0.45
(1,705)	1:273:A:GLU:HG3	1:328:A:SER:H	18	0.45
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB2	5	0.45
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB3	5	0.45
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	9	0.45
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	9	0.45
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	9	0.45
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	16	0.45
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	16	0.45
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	12	0.45
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	12	0.45
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	12	0.45
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	12	0.45
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	12	0.45
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	7	0.45
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	10	0.45
(1,153)	1:238:A:LYS:HE2	1:264:A:SER:HA	11	0.45
(1,153)	1:238:A:LYS:HE3	1:264:A:SER:HA	11	0.45
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	20	0.44
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	20	0.44
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	20	0.44
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	20	0.44
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	20	0.44
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	20	0.44
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	20	0.44
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	20	0.44
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	20	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG11	18	0.44
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG12	18	0.44
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG13	18	0.44
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG11	18	0.44
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG12	18	0.44
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG13	18	0.44
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG11	18	0.44
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG12	18	0.44
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG13	18	0.44
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	2	0.44
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	2	0.44
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	2	0.44
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	2	0.44
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	2	0.44
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	2	0.44
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	2	0.44
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	2	0.44
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	2	0.44
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	16	0.44
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	16	0.44
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	16	0.44
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	16	0.44
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	16	0.44
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	16	0.44
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	16	0.44
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	16	0.44
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	16	0.44
(1,3943)	1:490:A:LEU:HA	1:492:A:LYS:H	13	0.44
(1,3938)	1:490:A:LEU:HA	1:493:A:LEU:H	17	0.44
(1,3936)	1:490:A:LEU:HB2	1:494:A:ALA:H	2	0.44
(1,3936)	1:490:A:LEU:HB3	1:494:A:ALA:H	2	0.44
(1,3936)	1:490:A:LEU:HB2	1:494:A:ALA:H	5	0.44
(1,3936)	1:490:A:LEU:HB3	1:494:A:ALA:H	5	0.44
(1,3926)	1:489:A:SER:HA	1:493:A:LEU:HD11	3	0.44
(1,3926)	1:489:A:SER:HA	1:493:A:LEU:HD12	3	0.44
(1,3926)	1:489:A:SER:HA	1:493:A:LEU:HD13	3	0.44
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	1	0.44
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	3	0.44
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	15	0.44
(1,3896)	1:486:A:VAL:HA	1:489:A:SER:HB2	11	0.44
(1,3896)	1:486:A:VAL:HA	1:489:A:SER:HB3	11	0.44
(1,3891)	1:486:A:VAL:HG11	1:490:A:LEU:H	12	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3891)	1:486:A:VAL:HG12	1:490:A:LEU:H	12	0.44
(1,3891)	1:486:A:VAL:HG13	1:490:A:LEU:H	12	0.44
(1,3872)	1:483:A:VAL:HA	1:486:A:VAL:HG21	11	0.44
(1,3872)	1:483:A:VAL:HA	1:486:A:VAL:HG22	11	0.44
(1,3872)	1:483:A:VAL:HA	1:486:A:VAL:HG23	11	0.44
(1,3848)	1:481:A:GLN:HG2	1:486:A:VAL:HA	10	0.44
(1,3848)	1:481:A:GLN:HG3	1:486:A:VAL:HA	10	0.44
(1,3674)	1:462:A:ASP:HB2	1:464:A:ILE:H	14	0.44
(1,3674)	1:462:A:ASP:HB3	1:464:A:ILE:H	14	0.44
(1,3674)	1:462:A:ASP:HB2	1:464:A:ILE:H	17	0.44
(1,3674)	1:462:A:ASP:HB3	1:464:A:ILE:H	17	0.44
(1,3536)	1:449:A:LEU:HA	1:453:A:LYS:H	13	0.44
(1,3329)	1:435:A:ALA:H	1:461:A:SER:HA	19	0.44
(1,3311)	1:434:A:THR:HB	1:466:A:GLU:HA	3	0.44
(1,3170)	1:430:A:ILE:H	1:481:A:GLN:H	1	0.44
(1,3079)	1:423:A:MET:HE1	1:428:A:GLU:HA	14	0.44
(1,3079)	1:423:A:MET:HE2	1:428:A:GLU:HA	14	0.44
(1,3079)	1:423:A:MET:HE3	1:428:A:GLU:HA	14	0.44
(1,2910)	1:410:A:SER:HA	1:459:A:LEU:HD11	16	0.44
(1,2910)	1:410:A:SER:HA	1:459:A:LEU:HD12	16	0.44
(1,2910)	1:410:A:SER:HA	1:459:A:LEU:HD13	16	0.44
(1,2887)	1:407:A:THR:HG21	1:408:A:ASP:H	16	0.44
(1,2887)	1:407:A:THR:HG22	1:408:A:ASP:H	16	0.44
(1,2887)	1:407:A:THR:HG23	1:408:A:ASP:H	16	0.44
(1,2855)	1:405:A:THR:HB	1:451:A:ARG:HA	17	0.44
(1,2849)	1:405:A:THR:HG21	1:457:A:VAL:HB	9	0.44
(1,2849)	1:405:A:THR:HG22	1:457:A:VAL:HB	9	0.44
(1,2849)	1:405:A:THR:HG23	1:457:A:VAL:HB	9	0.44
(1,2763)	1:402:A:PHE:H	1:414:A:VAL:H	14	0.44
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	5	0.44
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	5	0.44
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	5	0.44
(1,2582)	1:389:A:ASP:HA	1:392:A:ASN:H	10	0.44
(1,2562)	1:387:A:ALA:HB1	1:471:A:TYR:HD1	10	0.44
(1,2562)	1:387:A:ALA:HB1	1:471:A:TYR:HD2	10	0.44
(1,2562)	1:387:A:ALA:HB2	1:471:A:TYR:HD1	10	0.44
(1,2562)	1:387:A:ALA:HB2	1:471:A:TYR:HD2	10	0.44
(1,2562)	1:387:A:ALA:HB3	1:471:A:TYR:HD1	10	0.44
(1,2562)	1:387:A:ALA:HB3	1:471:A:TYR:HD2	10	0.44
(1,2288)	1:372:A:GLN:HE21	1:376:A:GLN:H	2	0.44
(1,2288)	1:372:A:GLN:HE22	1:376:A:GLN:H	2	0.44
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG2	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG3	4	0.44
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG2	4	0.44
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG3	4	0.44
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG2	15	0.44
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG3	15	0.44
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG2	15	0.44
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG3	15	0.44
(1,1992)	1:354:A:LYS:HG2	1:392:A:ASN:HD21	2	0.44
(1,1992)	1:354:A:LYS:HG2	1:392:A:ASN:HD22	2	0.44
(1,1992)	1:354:A:LYS:HG3	1:392:A:ASN:HD21	2	0.44
(1,1992)	1:354:A:LYS:HG3	1:392:A:ASN:HD22	2	0.44
(1,1992)	1:354:A:LYS:HG2	1:392:A:ASN:HD21	18	0.44
(1,1992)	1:354:A:LYS:HG2	1:392:A:ASN:HD22	18	0.44
(1,1992)	1:354:A:LYS:HG3	1:392:A:ASN:HD21	18	0.44
(1,1992)	1:354:A:LYS:HG3	1:392:A:ASN:HD22	18	0.44
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD21	7	0.44
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD22	7	0.44
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD21	7	0.44
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD22	7	0.44
(1,1989)	1:354:A:LYS:HA	1:392:A:ASN:HD21	18	0.44
(1,1989)	1:354:A:LYS:HA	1:392:A:ASN:HD22	18	0.44
(1,1933)	1:350:A:ASN:HA	1:354:A:LYS:H	12	0.44
(1,1768)	1:335:A:SER:H	1:338:A:ILE:HD11	20	0.44
(1,1768)	1:335:A:SER:H	1:338:A:ILE:HD12	20	0.44
(1,1768)	1:335:A:SER:H	1:338:A:ILE:HD13	20	0.44
(1,1726)	1:331:A:PRO:HB2	1:338:A:ILE:HB	7	0.44
(1,1726)	1:331:A:PRO:HB3	1:338:A:ILE:HB	7	0.44
(1,1726)	1:331:A:PRO:HB2	1:338:A:ILE:HB	20	0.44
(1,1726)	1:331:A:PRO:HB3	1:338:A:ILE:HB	20	0.44
(1,1490)	1:314:A:MET:HB2	1:318:A:LEU:H	11	0.44
(1,1490)	1:314:A:MET:HB3	1:318:A:LEU:H	11	0.44
(1,1354)	1:305:A:PHE:HE2	1:307:A:MET:HA	20	0.44
(1,1352)	1:305:A:PHE:HZ	1:307:A:MET:HA	20	0.44
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE1	1	0.44
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE2	1	0.44
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HA	2	0.44
(1,1053)	1:293:A:HIS:HB2	1:295:A:HIS:H	15	0.44
(1,1053)	1:293:A:HIS:HB3	1:295:A:HIS:H	15	0.44
(1,1022)	1:289:A:TRP:HH2	1:381:A:VAL:H	5	0.44
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	6	0.44
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	20	0.44
(1,963)	1:285:A:PRO:HG2	1:288:A:MET:H	14	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:285:A:PRO:HG3	1:288:A:MET:H	14	0.44
(1,960)	1:285:A:PRO:HB2	1:294:A:LYS:HB2	9	0.44
(1,960)	1:285:A:PRO:HB2	1:294:A:LYS:HB3	9	0.44
(1,960)	1:285:A:PRO:HB3	1:294:A:LYS:HB2	9	0.44
(1,960)	1:285:A:PRO:HB3	1:294:A:LYS:HB3	9	0.44
(1,869)	1:280:A:ILE:HD11	1:360:A:LEU:HA	11	0.44
(1,869)	1:280:A:ILE:HD12	1:360:A:LEU:HA	11	0.44
(1,869)	1:280:A:ILE:HD13	1:360:A:LEU:HA	11	0.44
(1,864)	1:280:A:ILE:HD11	1:371:A:TYR:HE1	5	0.44
(1,864)	1:280:A:ILE:HD11	1:371:A:TYR:HE2	5	0.44
(1,864)	1:280:A:ILE:HD12	1:371:A:TYR:HE1	5	0.44
(1,864)	1:280:A:ILE:HD12	1:371:A:TYR:HE2	5	0.44
(1,864)	1:280:A:ILE:HD13	1:371:A:TYR:HE1	5	0.44
(1,864)	1:280:A:ILE:HD13	1:371:A:TYR:HE2	5	0.44
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	16	0.44
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	16	0.44
(1,473)	1:260:A:PRO:HA	1:281:A:PRO:HA	15	0.44
(1,447)	1:256:A:ASP:HA	1:258:A:ASN:HD21	20	0.44
(1,447)	1:256:A:ASP:HA	1:258:A:ASN:HD22	20	0.44
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD2	10	0.44
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD3	10	0.44
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	10	0.44
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	10	0.44
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	10	0.44
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	10	0.44
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	18	0.44
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	4	0.44
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	9	0.44
(1,145)	1:238:A:LYS:HD2	1:267:A:ARG:H	16	0.44
(1,145)	1:238:A:LYS:HD3	1:267:A:ARG:H	16	0.44
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	6	0.44
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	5	0.44
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	5	0.44
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	5	0.44
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	5	0.44
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	5	0.44
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	5	0.44
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG21	5	0.44
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG22	5	0.44
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG23	5	0.44
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	9	0.43
(1,3940)	1:490:A:LEU:HD21	1:493:A:LEU:HB2	19	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3940)	1:490:A:LEU:HD21	1:493:A:LEU:HB3	19	0.43
(1,3940)	1:490:A:LEU:HD22	1:493:A:LEU:HB2	19	0.43
(1,3940)	1:490:A:LEU:HD22	1:493:A:LEU:HB3	19	0.43
(1,3940)	1:490:A:LEU:HD23	1:493:A:LEU:HB2	19	0.43
(1,3940)	1:490:A:LEU:HD23	1:493:A:LEU:HB3	19	0.43
(1,3936)	1:490:A:LEU:HB2	1:494:A:ALA:H	1	0.43
(1,3936)	1:490:A:LEU:HB3	1:494:A:ALA:H	1	0.43
(1,3936)	1:490:A:LEU:HB2	1:494:A:ALA:H	17	0.43
(1,3936)	1:490:A:LEU:HB3	1:494:A:ALA:H	17	0.43
(1,3918)	1:488:A:GLU:HA	1:491:A:GLU:HA	19	0.43
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	12	0.43
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	17	0.43
(1,3891)	1:486:A:VAL:HG11	1:490:A:LEU:H	11	0.43
(1,3891)	1:486:A:VAL:HG12	1:490:A:LEU:H	11	0.43
(1,3891)	1:486:A:VAL:HG13	1:490:A:LEU:H	11	0.43
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE2	15	0.43
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE3	15	0.43
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE2	15	0.43
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE3	15	0.43
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB2	15	0.43
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB3	15	0.43
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB2	15	0.43
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB3	15	0.43
(1,3845)	1:481:A:GLN:HG2	1:487:A:ASP:H	3	0.43
(1,3845)	1:481:A:GLN:HG3	1:487:A:ASP:H	3	0.43
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB2	5	0.43
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB3	5	0.43
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB2	5	0.43
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB3	5	0.43
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB2	5	0.43
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB3	5	0.43
(1,3725)	1:468:A:MET:HA	1:472:A:LEU:H	2	0.43
(1,3329)	1:435:A:ALA:H	1:461:A:SER:HA	9	0.43
(1,3311)	1:434:A:THR:HB	1:466:A:GLU:HA	14	0.43
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	10	0.43
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	10	0.43
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	10	0.43
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	10	0.43
(1,3170)	1:430:A:ILE:H	1:481:A:GLN:H	12	0.43
(1,3170)	1:430:A:ILE:H	1:481:A:GLN:H	15	0.43
(1,3113)	1:426:A:GLY:HA2	1:428:A:GLU:HB2	18	0.43
(1,3113)	1:426:A:GLY:HA2	1:428:A:GLU:HB3	18	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3113)	1:426:A:GLY:HA3	1:428:A:GLU:HB2	18	0.43
(1,3113)	1:426:A:GLY:HA3	1:428:A:GLU:HB3	18	0.43
(1,3071)	1:423:A:MET:HE1	1:431:A:TYR:H	2	0.43
(1,3071)	1:423:A:MET:HE2	1:431:A:TYR:H	2	0.43
(1,3071)	1:423:A:MET:HE3	1:431:A:TYR:H	2	0.43
(1,2915)	1:410:A:SER:HB3	1:438:A:TYR:HD2	15	0.43
(1,2889)	1:408:A:ASP:HB3	1:451:A:ARG:HH22	19	0.43
(1,2882)	1:407:A:THR:HG21	1:409:A:SER:H	6	0.43
(1,2882)	1:407:A:THR:HG22	1:409:A:SER:H	6	0.43
(1,2882)	1:407:A:THR:HG23	1:409:A:SER:H	6	0.43
(1,2790)	1:403:A:ALA:HA	1:414:A:VAL:HB	11	0.43
(1,2621)	1:393:A:GLN:HE21	1:473:A:THR:H	19	0.43
(1,2621)	1:393:A:GLN:HE22	1:473:A:THR:H	19	0.43
(1,2597)	1:390:A:PHE:HA	1:392:A:ASN:H	5	0.43
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD1	18	0.43
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD2	18	0.43
(1,2436)	1:380:A:LEU:HA	1:383:A:LYS:HD2	5	0.43
(1,2436)	1:380:A:LEU:HA	1:383:A:LYS:HD3	5	0.43
(1,2379)	1:376:A:GLN:HE21	1:413:A:THR:HG21	3	0.43
(1,2379)	1:376:A:GLN:HE21	1:413:A:THR:HG22	3	0.43
(1,2379)	1:376:A:GLN:HE21	1:413:A:THR:HG23	3	0.43
(1,2379)	1:376:A:GLN:HE22	1:413:A:THR:HG21	3	0.43
(1,2379)	1:376:A:GLN:HE22	1:413:A:THR:HG22	3	0.43
(1,2379)	1:376:A:GLN:HE22	1:413:A:THR:HG23	3	0.43
(1,2335)	1:375:A:TRP:HH2	1:468:A:MET:HE1	13	0.43
(1,2335)	1:375:A:TRP:HH2	1:468:A:MET:HE2	13	0.43
(1,2335)	1:375:A:TRP:HH2	1:468:A:MET:HE3	13	0.43
(1,2169)	1:363:A:LEU:HA	1:366:A:ASP:H	3	0.43
(1,2045)	1:357:A:LEU:HD21	1:395:A:ALA:H	17	0.43
(1,2045)	1:357:A:LEU:HD22	1:395:A:ALA:H	17	0.43
(1,2045)	1:357:A:LEU:HD23	1:395:A:ALA:H	17	0.43
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE21	10	0.43
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE22	10	0.43
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD11	4	0.43
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD12	4	0.43
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD13	4	0.43
(1,1871)	1:345:A:THR:HA	1:349:A:ARG:H	19	0.43
(1,1762)	1:335:A:SER:H	1:339:A:LEU:H	19	0.43
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE1	12	0.43
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE2	12	0.43
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE3	12	0.43
(1,1487)	1:314:A:MET:HB2	1:319:A:ARG:HA	3	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1487)	1:314:A:MET:HB3	1:319:A:ARG:HA	3	0.43
(1,1373)	1:307:A:MET:HE1	1:335:A:SER:H	12	0.43
(1,1373)	1:307:A:MET:HE2	1:335:A:SER:H	12	0.43
(1,1373)	1:307:A:MET:HE3	1:335:A:SER:H	12	0.43
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD11	13	0.43
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD12	13	0.43
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD13	13	0.43
(1,1024)	1:289:A:TRP:HH2	1:381:A:VAL:HA	4	0.43
(1,1023)	1:289:A:TRP:HZ2	1:381:A:VAL:H	10	0.43
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	13	0.43
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD21	17	0.43
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD22	17	0.43
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	5	0.43
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	5	0.43
(1,706)	1:273:A:GLU:HB2	1:328:A:SER:HB2	8	0.43
(1,706)	1:273:A:GLU:HB2	1:328:A:SER:HB3	8	0.43
(1,706)	1:273:A:GLU:HB3	1:328:A:SER:HB2	8	0.43
(1,706)	1:273:A:GLU:HB3	1:328:A:SER:HB3	8	0.43
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD2	15	0.43
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD3	15	0.43
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	9	0.43
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	9	0.43
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	9	0.43
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	9	0.43
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	11	0.43
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	11	0.43
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	11	0.43
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	11	0.43
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	10	0.43
(1,291)	1:248:A:GLU:HA	1:252:A:HIS:H	1	0.43
(1,290)	1:248:A:GLU:HA	1:260:A:PRO:HD2	20	0.43
(1,290)	1:248:A:GLU:HA	1:260:A:PRO:HD3	20	0.43
(1,223)	1:244:A:GLU:HA	1:247:A:LYS:H	12	0.43
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	19	0.43
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	4	0.43
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	17	0.43
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	19	0.43
(1,153)	1:238:A:LYS:HE2	1:264:A:SER:HA	7	0.43
(1,153)	1:238:A:LYS:HE3	1:264:A:SER:HA	7	0.43
(1,123)	1:236:A:ARG:HB2	1:240:A:GLU:H	12	0.43
(1,123)	1:236:A:ARG:HB3	1:240:A:GLU:H	12	0.43
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD2	10	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD3	10	0.43
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	16	0.43
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	17	0.43
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD2	12	0.43
(1,70)	1:234:A:TRP:HE1	1:303:A:ARG:HD3	12	0.43
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	20	0.43
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	20	0.43
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	20	0.43
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	20	0.43
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	20	0.43
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	20	0.43
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	5	0.42
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	4	0.42
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	4	0.42
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	4	0.42
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	4	0.42
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	4	0.42
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	4	0.42
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	4	0.42
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	4	0.42
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	4	0.42
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB1	18	0.42
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB2	18	0.42
(1,3973)	1:464:A:ILE:HD11	2:625:B:ALA:HB3	18	0.42
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB1	18	0.42
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB2	18	0.42
(1,3973)	1:464:A:ILE:HD12	2:625:B:ALA:HB3	18	0.42
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB1	18	0.42
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB2	18	0.42
(1,3973)	1:464:A:ILE:HD13	2:625:B:ALA:HB3	18	0.42
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD11	19	0.42
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD12	19	0.42
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD13	19	0.42
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD11	19	0.42
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD12	19	0.42
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD13	19	0.42
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD11	19	0.42
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD12	19	0.42
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD13	19	0.42
(1,3917)	1:488:A:GLU:HA	1:491:A:GLU:H	19	0.42
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	4	0.42
(1,3772)	1:472:A:LEU:HD21	1:474:A:GLU:HA	2	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3772)	1:472:A:LEU:HD22	1:474:A:GLU:HA	2	0.42
(1,3772)	1:472:A:LEU:HD23	1:474:A:GLU:HA	2	0.42
(1,3767)	1:472:A:LEU:HD21	1:480:A:PHE:HE1	2	0.42
(1,3767)	1:472:A:LEU:HD23	1:480:A:PHE:HE2	20	0.42
(1,3749)	1:469:A:MET:HA	1:471:A:TYR:H	4	0.42
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	6	0.42
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	6	0.42
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	6	0.42
(1,3522)	1:448:A:GLU:HA	1:451:A:ARG:H	14	0.42
(1,3492)	1:447:A:LEU:HA	1:483:A:VAL:HB	17	0.42
(1,3309)	1:434:A:THR:HB	1:466:A:GLU:H	12	0.42
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	18	0.42
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	18	0.42
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	18	0.42
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	18	0.42
(1,3188)	1:430:A:ILE:HB	1:469:A:MET:HE1	16	0.42
(1,3188)	1:430:A:ILE:HB	1:469:A:MET:HE2	16	0.42
(1,3188)	1:430:A:ILE:HB	1:469:A:MET:HE3	16	0.42
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG2	5	0.42
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG3	5	0.42
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG2	5	0.42
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG3	5	0.42
(1,3147)	1:429:A:LYS:HD2	1:488:A:GLU:HG2	17	0.42
(1,3147)	1:429:A:LYS:HD2	1:488:A:GLU:HG3	17	0.42
(1,3147)	1:429:A:LYS:HD3	1:488:A:GLU:HG2	17	0.42
(1,3147)	1:429:A:LYS:HD3	1:488:A:GLU:HG3	17	0.42
(1,3074)	1:423:A:MET:HE1	1:430:A:ILE:HA	18	0.42
(1,3074)	1:423:A:MET:HE2	1:430:A:ILE:HA	18	0.42
(1,3074)	1:423:A:MET:HE3	1:430:A:ILE:HA	18	0.42
(1,3070)	1:423:A:MET:HA	1:456:A:GLU:H	1	0.42
(1,2982)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	9	0.42
(1,2982)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	9	0.42
(1,2980)	1:417:A:GLU:H	1:475:A:PHE:HZ	1	0.42
(1,2828)	1:404:A:SER:H	1:412:A:GLN:HA	11	0.42
(1,2827)	1:404:A:SER:H	1:413:A:THR:H	14	0.42
(1,2824)	1:404:A:SER:H	1:414:A:VAL:HB	18	0.42
(1,2823)	1:404:A:SER:H	1:414:A:VAL:H	18	0.42
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG11	5	0.42
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG12	5	0.42
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG13	5	0.42
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG11	3	0.42
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG12	3	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG13	3	0.42
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG11	7	0.42
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG12	7	0.42
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG13	7	0.42
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	19	0.42
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	19	0.42
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	19	0.42
(1,2562)	1:387:A:ALA:HB1	1:471:A:TYR:HD1	4	0.42
(1,2562)	1:387:A:ALA:HB1	1:471:A:TYR:HD2	4	0.42
(1,2562)	1:387:A:ALA:HB2	1:471:A:TYR:HD1	4	0.42
(1,2562)	1:387:A:ALA:HB2	1:471:A:TYR:HD2	4	0.42
(1,2562)	1:387:A:ALA:HB3	1:471:A:TYR:HD1	4	0.42
(1,2562)	1:387:A:ALA:HB3	1:471:A:TYR:HD2	4	0.42
(1,2359)	1:375:A:TRP:HH2	1:383:A:LYS:HG2	19	0.42
(1,2359)	1:375:A:TRP:HH2	1:383:A:LYS:HG3	19	0.42
(1,2133)	1:361:A:GLU:HA	1:365:A:LYS:H	19	0.42
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE21	13	0.42
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE22	13	0.42
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD11	7	0.42
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD12	7	0.42
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD13	7	0.42
(1,1937)	1:350:A:ASN:HA	1:353:A:THR:H	14	0.42
(1,1886)	1:346:A:ARG:HG2	1:350:A:ASN:HD21	2	0.42
(1,1886)	1:346:A:ARG:HG2	1:350:A:ASN:HD22	2	0.42
(1,1886)	1:346:A:ARG:HG3	1:350:A:ASN:HD21	2	0.42
(1,1886)	1:346:A:ARG:HG3	1:350:A:ASN:HD22	2	0.42
(1,1816)	1:339:A:LEU:HA	1:342:A:SER:H	13	0.42
(1,1726)	1:331:A:PRO:HB2	1:338:A:ILE:HB	14	0.42
(1,1726)	1:331:A:PRO:HB3	1:338:A:ILE:HB	14	0.42
(1,1674)	1:325:A:ILE:HD11	1:327:A:SER:H	12	0.42
(1,1674)	1:325:A:ILE:HD12	1:327:A:SER:H	12	0.42
(1,1674)	1:325:A:ILE:HD13	1:327:A:SER:H	12	0.42
(1,1578)	1:318:A:LEU:HA	1:382:A:LEU:HA	20	0.42
(1,1353)	1:305:A:PHE:HE1	1:307:A:MET:HA	20	0.42
(1,1353)	1:305:A:PHE:HE2	1:307:A:MET:HA	20	0.42
(1,1324)	1:302:A:GLN:H	1:327:A:SER:H	9	0.42
(1,1321)	1:302:A:GLN:HA	1:328:A:SER:HA	14	0.42
(1,1314)	1:302:A:GLN:HB2	1:332:A:LEU:HD11	4	0.42
(1,1314)	1:302:A:GLN:HB2	1:332:A:LEU:HD12	4	0.42
(1,1314)	1:302:A:GLN:HB2	1:332:A:LEU:HD13	4	0.42
(1,1314)	1:302:A:GLN:HB3	1:332:A:LEU:HD11	4	0.42
(1,1314)	1:302:A:GLN:HB3	1:332:A:LEU:HD12	4	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1314)	1:302:A:GLN:HB3	1:332:A:LEU:HD13	4	0.42
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD11	3	0.42
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD12	3	0.42
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD13	3	0.42
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD11	15	0.42
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD12	15	0.42
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD13	15	0.42
(1,1077)	1:295:A:HIS:HB2	1:296:A:GLY:H	9	0.42
(1,1077)	1:295:A:HIS:HB3	1:296:A:GLY:H	9	0.42
(1,1044)	1:291:A:ARG:HA	1:293:A:HIS:HA	11	0.42
(1,1029)	1:289:A:TRP:HZ2	1:380:A:LEU:HB2	12	0.42
(1,1029)	1:289:A:TRP:HZ2	1:380:A:LEU:HB3	12	0.42
(1,1024)	1:289:A:TRP:HH2	1:381:A:VAL:HA	9	0.42
(1,1022)	1:289:A:TRP:HH2	1:381:A:VAL:H	19	0.42
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	1	0.42
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD21	8	0.42
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD22	8	0.42
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	8	0.42
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	8	0.42
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	12	0.42
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	12	0.42
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	2	0.42
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	2	0.42
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	2	0.42
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	2	0.42
(1,684)	1:272:A:GLN:HE21	1:351:A:ALA:H	2	0.42
(1,684)	1:272:A:GLN:HE22	1:351:A:ALA:H	2	0.42
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	14	0.42
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	14	0.42
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	14	0.42
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	18	0.42
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	18	0.42
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	18	0.42
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	14	0.42
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	15	0.42
(1,454)	1:257:A:PHE:H	1:258:A:ASN:HD21	20	0.42
(1,454)	1:257:A:PHE:H	1:258:A:ASN:HD22	20	0.42
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD2	1	0.42
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD3	1	0.42
(1,219)	1:244:A:GLU:HA	1:248:A:GLU:H	4	0.42
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	13	0.42
(1,139)	1:237:A:ASN:HD21	1:239:A:SER:H	18	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,139)	1:237:A:ASN:HD22	1:239:A:SER:H	18	0.42
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	20	0.42
(1,3938)	1:490:A:LEU:HA	1:493:A:LEU:H	8	0.41
(1,3936)	1:490:A:LEU:HB2	1:494:A:ALA:H	3	0.41
(1,3936)	1:490:A:LEU:HB3	1:494:A:ALA:H	3	0.41
(1,3936)	1:490:A:LEU:HB2	1:494:A:ALA:H	13	0.41
(1,3936)	1:490:A:LEU:HB3	1:494:A:ALA:H	13	0.41
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB2	20	0.41
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB3	20	0.41
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB2	20	0.41
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB3	20	0.41
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB2	20	0.41
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB3	20	0.41
(1,3726)	1:468:A:MET:HG2	1:472:A:LEU:HB2	18	0.41
(1,3726)	1:468:A:MET:HG2	1:472:A:LEU:HB3	18	0.41
(1,3726)	1:468:A:MET:HG3	1:472:A:LEU:HB2	18	0.41
(1,3726)	1:468:A:MET:HG3	1:472:A:LEU:HB3	18	0.41
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	8	0.41
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	8	0.41
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	8	0.41
(1,3633)	1:458:A:LEU:HD11	1:480:A:PHE:HD1	18	0.41
(1,3633)	1:458:A:LEU:HD11	1:480:A:PHE:HD2	18	0.41
(1,3633)	1:458:A:LEU:HD12	1:480:A:PHE:HD1	18	0.41
(1,3633)	1:458:A:LEU:HD12	1:480:A:PHE:HD2	18	0.41
(1,3633)	1:458:A:LEU:HD13	1:480:A:PHE:HD1	18	0.41
(1,3633)	1:458:A:LEU:HD13	1:480:A:PHE:HD2	18	0.41
(1,3567)	1:450:A:LEU:HA	1:454:A:GLY:H	4	0.41
(1,3476)	1:445:A:PRO:HG2	1:446:A:HIS:H	5	0.41
(1,3476)	1:445:A:PRO:HG3	1:446:A:HIS:H	5	0.41
(1,3476)	1:445:A:PRO:HG2	1:446:A:HIS:H	9	0.41
(1,3476)	1:445:A:PRO:HG3	1:446:A:HIS:H	9	0.41
(1,3476)	1:445:A:PRO:HG2	1:446:A:HIS:H	10	0.41
(1,3476)	1:445:A:PRO:HG3	1:446:A:HIS:H	10	0.41
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD11	19	0.41
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD12	19	0.41
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD13	19	0.41
(1,3329)	1:435:A:ALA:H	1:461:A:SER:HA	12	0.41
(1,3222)	1:431:A:TYR:HD1	1:456:A:GLU:H	18	0.41
(1,3222)	1:431:A:TYR:HD2	1:456:A:GLU:H	18	0.41
(1,3214)	1:431:A:TYR:H	1:458:A:LEU:H	11	0.41
(1,3170)	1:430:A:ILE:H	1:481:A:GLN:H	8	0.41
(1,3150)	1:429:A:LYS:HD2	1:481:A:GLN:HB2	11	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3150)	1:429:A:LYS:HD2	1:481:A:GLN:HB3	11	0.41
(1,3150)	1:429:A:LYS:HD3	1:481:A:GLN:HB2	11	0.41
(1,3150)	1:429:A:LYS:HD3	1:481:A:GLN:HB3	11	0.41
(1,3135)	1:428:A:GLU:HA	1:478:A:LYS:HA	9	0.41
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD11	5	0.41
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD12	5	0.41
(1,3122)	1:427:A:GLN:HE21	1:455:A:ILE:HD13	5	0.41
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD11	5	0.41
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD12	5	0.41
(1,3122)	1:427:A:GLN:HE22	1:455:A:ILE:HD13	5	0.41
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD11	7	0.41
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD12	7	0.41
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD13	7	0.41
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD11	7	0.41
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD12	7	0.41
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD13	7	0.41
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD11	17	0.41
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD12	17	0.41
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD13	17	0.41
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD11	17	0.41
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD12	17	0.41
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD13	17	0.41
(1,3082)	1:423:A:MET:HA	1:427:A:GLN:HE21	18	0.41
(1,3082)	1:423:A:MET:HA	1:427:A:GLN:HE22	18	0.41
(1,3039)	1:420:A:VAL:HB	1:475:A:PHE:HZ	4	0.41
(1,2982)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	2	0.41
(1,2982)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	2	0.41
(1,2889)	1:408:A:ASP:HB3	1:451:A:ARG:HH22	9	0.41
(1,2861)	1:405:A:THR:HA	1:408:A:ASP:HA	9	0.41
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG11	1	0.41
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG12	1	0.41
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG13	1	0.41
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG11	1	0.41
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG12	1	0.41
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG13	1	0.41
(1,2563)	1:387:A:ALA:HA	1:471:A:TYR:HE1	10	0.41
(1,2563)	1:387:A:ALA:HA	1:471:A:TYR:HE2	10	0.41
(1,2538)	1:386:A:PRO:HA	1:471:A:TYR:HB2	3	0.41
(1,2538)	1:386:A:PRO:HA	1:471:A:TYR:HB3	3	0.41
(1,2506)	1:384:A:GLU:HA	1:468:A:MET:HB2	13	0.41
(1,2506)	1:384:A:GLU:HA	1:468:A:MET:HB3	13	0.41
(1,2359)	1:375:A:TRP:HH2	1:383:A:LYS:HG2	14	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2359)	1:375:A:TRP:HH2	1:383:A:LYS:HG3	14	0.41
(1,2348)	1:375:A:TRP:HZ3	1:401:A:ARG:H	9	0.41
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA2	8	0.41
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA3	8	0.41
(1,2314)	1:374:A:PHE:HZ	1:399:A:LEU:HD11	17	0.41
(1,2314)	1:374:A:PHE:HZ	1:399:A:LEU:HD12	17	0.41
(1,2314)	1:374:A:PHE:HZ	1:399:A:LEU:HD13	17	0.41
(1,2290)	1:372:A:GLN:HG2	1:376:A:GLN:HE21	1	0.41
(1,2290)	1:372:A:GLN:HG2	1:376:A:GLN:HE22	1	0.41
(1,2290)	1:372:A:GLN:HG3	1:376:A:GLN:HE21	1	0.41
(1,2290)	1:372:A:GLN:HG3	1:376:A:GLN:HE22	1	0.41
(1,2288)	1:372:A:GLN:HE21	1:376:A:GLN:H	17	0.41
(1,2288)	1:372:A:GLN:HE22	1:376:A:GLN:H	17	0.41
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD11	13	0.41
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD12	13	0.41
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD13	13	0.41
(1,1994)	1:354:A:LYS:HA	1:358:A:GLN:H	20	0.41
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD21	8	0.41
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD22	8	0.41
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD21	8	0.41
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD22	8	0.41
(1,1951)	1:351:A:ALA:HA	1:354:A:LYS:HD2	14	0.41
(1,1951)	1:351:A:ALA:HA	1:354:A:LYS:HD3	14	0.41
(1,1858)	1:344:A:VAL:HA	1:348:A:LEU:H	13	0.41
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	10	0.41
(1,1726)	1:331:A:PRO:HB2	1:338:A:ILE:HB	12	0.41
(1,1726)	1:331:A:PRO:HB3	1:338:A:ILE:HB	12	0.41
(1,1511)	1:315:A:PRO:HG2	1:319:A:ARG:H	1	0.41
(1,1511)	1:315:A:PRO:HG3	1:319:A:ARG:H	1	0.41
(1,1416)	1:312:A:GLN:HB2	1:349:A:ARG:HD2	20	0.41
(1,1416)	1:312:A:GLN:HB2	1:349:A:ARG:HD3	20	0.41
(1,1416)	1:312:A:GLN:HB3	1:349:A:ARG:HD2	20	0.41
(1,1416)	1:312:A:GLN:HB3	1:349:A:ARG:HD3	20	0.41
(1,1374)	1:307:A:MET:HE1	1:335:A:SER:HA	12	0.41
(1,1374)	1:307:A:MET:HE2	1:335:A:SER:HA	12	0.41
(1,1374)	1:307:A:MET:HE3	1:335:A:SER:HA	12	0.41
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE1	4	0.41
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE2	4	0.41
(1,1140)	1:297:A:LEU:HA	1:309:A:ASP:HA	15	0.41
(1,960)	1:285:A:PRO:HB2	1:294:A:LYS:HB2	3	0.41
(1,960)	1:285:A:PRO:HB2	1:294:A:LYS:HB3	3	0.41
(1,960)	1:285:A:PRO:HB3	1:294:A:LYS:HB2	3	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,960)	1:285:A:PRO:HB3	1:294:A:LYS:HB3	3	0.41
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	16	0.41
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	10	0.41
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	10	0.41
(1,764)	1:276:A:SER:HB2	1:326:A:ASP:H	2	0.41
(1,764)	1:276:A:SER:HB3	1:326:A:ASP:H	2	0.41
(1,447)	1:256:A:ASP:HA	1:258:A:ASN:HD21	18	0.41
(1,447)	1:256:A:ASP:HA	1:258:A:ASN:HD22	18	0.41
(1,403)	1:253:A:ILE:HB	1:323:A:GLY:HA2	3	0.41
(1,403)	1:253:A:ILE:HB	1:323:A:GLY:HA3	3	0.41
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	4	0.41
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	4	0.41
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	4	0.41
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	4	0.41
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	5	0.41
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	11	0.41
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	20	0.4
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	20	0.4
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	20	0.4
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	20	0.4
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	20	0.4
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	20	0.4
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	20	0.4
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	20	0.4
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	20	0.4
(1,3840)	1:481:A:GLN:HG2	1:489:A:SER:H	1	0.4
(1,3840)	1:481:A:GLN:HG3	1:489:A:SER:H	1	0.4
(1,3816)	1:475:A:PHE:HE1	1:476:A:ASP:HB2	16	0.4
(1,3816)	1:475:A:PHE:HE1	1:476:A:ASP:HB3	16	0.4
(1,3816)	1:475:A:PHE:HE2	1:476:A:ASP:HB2	16	0.4
(1,3816)	1:475:A:PHE:HE2	1:476:A:ASP:HB3	16	0.4
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	9	0.4
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	9	0.4
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	9	0.4
(1,3633)	1:458:A:LEU:HD11	1:480:A:PHE:HD1	4	0.4
(1,3633)	1:458:A:LEU:HD11	1:480:A:PHE:HD2	4	0.4
(1,3633)	1:458:A:LEU:HD12	1:480:A:PHE:HD1	4	0.4
(1,3633)	1:458:A:LEU:HD12	1:480:A:PHE:HD2	4	0.4
(1,3633)	1:458:A:LEU:HD13	1:480:A:PHE:HD1	4	0.4
(1,3633)	1:458:A:LEU:HD13	1:480:A:PHE:HD2	4	0.4
(1,3567)	1:450:A:LEU:HA	1:454:A:GLY:H	3	0.4
(1,3368)	1:437:A:SER:H	1:440:A:ALA:H	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3248)	1:432:A:TYR:HA	1:457:A:VAL:HA	17	0.4
(1,3207)	1:431:A:TYR:HA	1:482:A:SER:HA	17	0.4
(1,3188)	1:430:A:ILE:HB	1:469:A:MET:HE1	14	0.4
(1,3188)	1:430:A:ILE:HB	1:469:A:MET:HE2	14	0.4
(1,3188)	1:430:A:ILE:HB	1:469:A:MET:HE3	14	0.4
(1,3152)	1:429:A:LYS:HD2	1:481:A:GLN:HG2	11	0.4
(1,3152)	1:429:A:LYS:HD2	1:481:A:GLN:HG3	11	0.4
(1,3152)	1:429:A:LYS:HD3	1:481:A:GLN:HG2	11	0.4
(1,3152)	1:429:A:LYS:HD3	1:481:A:GLN:HG3	11	0.4
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD11	20	0.4
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD12	20	0.4
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD13	20	0.4
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD11	20	0.4
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD12	20	0.4
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD13	20	0.4
(1,2984)	1:417:A:GLU:HA	1:421:A:SER:H	14	0.4
(1,2839)	1:405:A:THR:HA	1:459:A:LEU:HD11	8	0.4
(1,2839)	1:405:A:THR:HA	1:459:A:LEU:HD12	8	0.4
(1,2839)	1:405:A:THR:HA	1:459:A:LEU:HD13	8	0.4
(1,2813)	1:404:A:SER:HB2	1:458:A:LEU:HA	3	0.4
(1,2813)	1:404:A:SER:HB3	1:458:A:LEU:HA	3	0.4
(1,2794)	1:403:A:ALA:HA	1:413:A:THR:H	14	0.4
(1,2762)	1:402:A:PHE:HB2	1:415:A:SER:HA	18	0.4
(1,2762)	1:402:A:PHE:HB3	1:415:A:SER:HA	18	0.4
(1,2642)	1:394:A:GLU:HA	1:398:A:LYS:H	5	0.4
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB2	19	0.4
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB3	19	0.4
(1,2429)	1:380:A:LEU:HA	1:462:A:ASP:HB2	2	0.4
(1,2429)	1:380:A:LEU:HA	1:462:A:ASP:HB3	2	0.4
(1,2359)	1:375:A:TRP:HH2	1:383:A:LYS:HG2	7	0.4
(1,2359)	1:375:A:TRP:HH2	1:383:A:LYS:HG3	7	0.4
(1,2077)	1:359:A:MET:HG2	1:363:A:LEU:H	6	0.4
(1,2077)	1:359:A:MET:HG3	1:363:A:LEU:H	6	0.4
(1,2045)	1:357:A:LEU:HD21	1:395:A:ALA:H	2	0.4
(1,2045)	1:357:A:LEU:HD22	1:395:A:ALA:H	2	0.4
(1,2045)	1:357:A:LEU:HD23	1:395:A:ALA:H	2	0.4
(1,2041)	1:357:A:LEU:HD21	1:396:A:ILE:H	8	0.4
(1,2041)	1:357:A:LEU:HD22	1:396:A:ILE:H	8	0.4
(1,2041)	1:357:A:LEU:HD23	1:396:A:ILE:H	8	0.4
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE21	6	0.4
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE22	6	0.4
(1,1958)	1:352:A:LEU:HA	1:356:A:VAL:H	12	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1946)	1:351:A:ALA:HA	1:355:A:ARG:HD2	7	0.4
(1,1946)	1:351:A:ALA:HA	1:355:A:ARG:HD3	7	0.4
(1,1909)	1:348:A:LEU:HA	1:352:A:LEU:H	5	0.4
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD11	8	0.4
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD12	8	0.4
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD13	8	0.4
(1,1726)	1:331:A:PRO:HB2	1:338:A:ILE:HB	5	0.4
(1,1726)	1:331:A:PRO:HB3	1:338:A:ILE:HB	5	0.4
(1,1194)	1:299:A:LEU:HA	1:326:A:ASP:HA	11	0.4
(1,1140)	1:297:A:LEU:HA	1:309:A:ASP:HA	14	0.4
(1,1051)	1:293:A:HIS:HE1	1:309:A:ASP:HB2	3	0.4
(1,1051)	1:293:A:HIS:HE1	1:309:A:ASP:HB3	3	0.4
(1,1023)	1:289:A:TRP:HZ2	1:381:A:VAL:H	12	0.4
(1,1003)	1:288:A:MET:HG2	1:381:A:VAL:HG21	4	0.4
(1,1003)	1:288:A:MET:HG2	1:381:A:VAL:HG22	4	0.4
(1,1003)	1:288:A:MET:HG2	1:381:A:VAL:HG23	4	0.4
(1,1003)	1:288:A:MET:HG3	1:381:A:VAL:HG21	4	0.4
(1,1003)	1:288:A:MET:HG3	1:381:A:VAL:HG22	4	0.4
(1,1003)	1:288:A:MET:HG3	1:381:A:VAL:HG23	4	0.4
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	17	0.4
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD21	1	0.4
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD22	1	0.4
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD21	3	0.4
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD22	3	0.4
(1,975)	1:286:A:TRP:HZ3	1:290:A:ASN:HA	9	0.4
(1,757)	1:276:A:SER:HB2	1:355:A:ARG:HG2	19	0.4
(1,757)	1:276:A:SER:HB3	1:355:A:ARG:HG2	19	0.4
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	18	0.4
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	18	0.4
(1,631)	1:267:A:ARG:HG2	1:275:A:THR:HA	14	0.4
(1,631)	1:267:A:ARG:HG3	1:275:A:THR:HA	14	0.4
(1,550)	1:263:A:TRP:HA	1:359:A:MET:HG2	5	0.4
(1,550)	1:263:A:TRP:HA	1:359:A:MET:HG3	5	0.4
(1,550)	1:263:A:TRP:HA	1:359:A:MET:HG2	14	0.4
(1,550)	1:263:A:TRP:HA	1:359:A:MET:HG3	14	0.4
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	20	0.4
(1,382)	1:251:A:LYS:HA	1:255:A:HIS:HA	2	0.4
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	8	0.4
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	8	0.4
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	8	0.4
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	8	0.4
(1,347)	1:250:A:TYR:HE1	1:260:A:PRO:HA	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:250:A:TYR:HE2	1:260:A:PRO:HA	4	0.4
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	4	0.4
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	7	0.4
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	12	0.4
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	9	0.4
(1,95)	1:234:A:TRP:HA	1:246:A:TYR:HE2	11	0.4
(2,9)	1:338:A:ILE:HD11	1:342:A:SER:H	6	0.39
(2,9)	1:338:A:ILE:HD12	1:342:A:SER:H	6	0.39
(2,9)	1:338:A:ILE:HD13	1:342:A:SER:H	6	0.39
(2,5)	1:290:A:ASN:HB2	1:293:A:HIS:HA	3	0.39
(2,5)	1:290:A:ASN:HB3	1:293:A:HIS:HA	3	0.39
(1,3959)	1:492:A:LYS:HA	1:494:A:ALA:H	9	0.39
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD11	15	0.39
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD12	15	0.39
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD13	15	0.39
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD11	15	0.39
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD12	15	0.39
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD13	15	0.39
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD11	15	0.39
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD12	15	0.39
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD13	15	0.39
(1,3940)	1:490:A:LEU:HD21	1:493:A:LEU:HB2	1	0.39
(1,3940)	1:490:A:LEU:HD21	1:493:A:LEU:HB3	1	0.39
(1,3940)	1:490:A:LEU:HD22	1:493:A:LEU:HB2	1	0.39
(1,3940)	1:490:A:LEU:HD22	1:493:A:LEU:HB3	1	0.39
(1,3940)	1:490:A:LEU:HD23	1:493:A:LEU:HB2	1	0.39
(1,3940)	1:490:A:LEU:HD23	1:493:A:LEU:HB3	1	0.39
(1,3936)	1:490:A:LEU:HB2	1:494:A:ALA:H	16	0.39
(1,3936)	1:490:A:LEU:HB3	1:494:A:ALA:H	16	0.39
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	17	0.39
(1,3848)	1:481:A:GLN:HG2	1:486:A:VAL:HA	12	0.39
(1,3848)	1:481:A:GLN:HG3	1:486:A:VAL:HA	12	0.39
(1,3845)	1:481:A:GLN:HG2	1:487:A:ASP:H	18	0.39
(1,3845)	1:481:A:GLN:HG3	1:487:A:ASP:H	18	0.39
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	10	0.39
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	10	0.39
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	10	0.39
(1,3254)	1:433:A:ILE:HA	1:484:A:SER:H	11	0.39
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB2	7	0.39
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB3	7	0.39
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB2	7	0.39
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB3	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3144)	1:429:A:LYS:HD2	1:489:A:SER:HA	2	0.39
(1,3144)	1:429:A:LYS:HD3	1:489:A:SER:HA	2	0.39
(1,3143)	1:429:A:LYS:HD2	1:489:A:SER:H	12	0.39
(1,3143)	1:429:A:LYS:HD3	1:489:A:SER:H	12	0.39
(1,3135)	1:428:A:GLU:HA	1:478:A:LYS:HA	7	0.39
(1,3121)	1:427:A:GLN:HE21	1:455:A:ILE:HA	9	0.39
(1,3121)	1:427:A:GLN:HE22	1:455:A:ILE:HA	9	0.39
(1,3095)	1:424:A:LYS:H	1:427:A:GLN:H	11	0.39
(1,3091)	1:424:A:LYS:HG2	1:455:A:ILE:HA	17	0.39
(1,3091)	1:424:A:LYS:HG3	1:455:A:ILE:HA	17	0.39
(1,2989)	1:417:A:GLU:HA	1:420:A:VAL:HB	14	0.39
(1,2984)	1:417:A:GLU:HA	1:421:A:SER:H	8	0.39
(1,2984)	1:417:A:GLU:HA	1:421:A:SER:H	11	0.39
(1,2982)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	5	0.39
(1,2982)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	5	0.39
(1,2915)	1:410:A:SER:HB3	1:438:A:TYR:HD2	17	0.39
(1,2887)	1:407:A:THR:HG21	1:408:A:ASP:H	13	0.39
(1,2887)	1:407:A:THR:HG22	1:408:A:ASP:H	13	0.39
(1,2887)	1:407:A:THR:HG23	1:408:A:ASP:H	13	0.39
(1,2861)	1:405:A:THR:HA	1:408:A:ASP:HA	7	0.39
(1,2859)	1:405:A:THR:HG21	1:442:A:LYS:HA	12	0.39
(1,2859)	1:405:A:THR:HG22	1:442:A:LYS:HA	12	0.39
(1,2859)	1:405:A:THR:HG23	1:442:A:LYS:HA	12	0.39
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	8	0.39
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	8	0.39
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	8	0.39
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD1	4	0.39
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD2	4	0.39
(1,2488)	1:383:A:LYS:HE2	1:402:A:PHE:HZ	6	0.39
(1,2488)	1:383:A:LYS:HE3	1:402:A:PHE:HZ	6	0.39
(1,2360)	1:375:A:TRP:HZ2	1:383:A:LYS:HG2	9	0.39
(1,2360)	1:375:A:TRP:HZ2	1:383:A:LYS:HG3	9	0.39
(1,2359)	1:375:A:TRP:HH2	1:383:A:LYS:HG2	9	0.39
(1,2359)	1:375:A:TRP:HH2	1:383:A:LYS:HG3	9	0.39
(1,2353)	1:375:A:TRP:HZ3	1:400:A:LEU:HA	8	0.39
(1,2317)	1:374:A:PHE:HZ	1:382:A:LEU:H	1	0.39
(1,2048)	1:357:A:LEU:HD11	1:392:A:ASN:H	12	0.39
(1,2048)	1:357:A:LEU:HD12	1:392:A:ASN:H	12	0.39
(1,2048)	1:357:A:LEU:HD13	1:392:A:ASN:H	12	0.39
(1,1973)	1:353:A:THR:HG21	1:392:A:ASN:HB2	10	0.39
(1,1973)	1:353:A:THR:HG21	1:392:A:ASN:HB3	10	0.39
(1,1973)	1:353:A:THR:HG22	1:392:A:ASN:HB2	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1973)	1:353:A:THR:HG22	1:392:A:ASN:HB3	10	0.39
(1,1973)	1:353:A:THR:HG23	1:392:A:ASN:HB2	10	0.39
(1,1973)	1:353:A:THR:HG23	1:392:A:ASN:HB3	10	0.39
(1,1889)	1:346:A:ARG:HA	1:349:A:ARG:HG2	16	0.39
(1,1859)	1:344:A:VAL:HB	1:348:A:LEU:H	13	0.39
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	20	0.39
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD11	3	0.39
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD12	3	0.39
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD13	3	0.39
(1,1710)	1:330:A:LEU:HD11	1:344:A:VAL:HB	7	0.39
(1,1710)	1:330:A:LEU:HD12	1:344:A:VAL:HB	7	0.39
(1,1710)	1:330:A:LEU:HD13	1:344:A:VAL:HB	7	0.39
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD21	7	0.39
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD22	7	0.39
(1,1647)	1:321:A:VAL:HG21	1:352:A:LEU:HD23	7	0.39
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD21	7	0.39
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD22	7	0.39
(1,1647)	1:321:A:VAL:HG22	1:352:A:LEU:HD23	7	0.39
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD21	7	0.39
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD22	7	0.39
(1,1647)	1:321:A:VAL:HG23	1:352:A:LEU:HD23	7	0.39
(1,1486)	1:314:A:MET:HB2	1:319:A:ARG:H	10	0.39
(1,1486)	1:314:A:MET:HB3	1:319:A:ARG:H	10	0.39
(1,1422)	1:312:A:GLN:HE21	1:340:A:GLN:HA	11	0.39
(1,1422)	1:312:A:GLN:HE22	1:340:A:GLN:HA	11	0.39
(1,1159)	1:298:A:LYS:H	1:322:A:ARG:HD2	1	0.39
(1,1159)	1:298:A:LYS:H	1:322:A:ARG:HD3	1	0.39
(1,1097)	1:296:A:GLY:H	1:309:A:ASP:HA	11	0.39
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	5	0.39
(1,975)	1:286:A:TRP:HZ3	1:290:A:ASN:HA	14	0.39
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	9	0.39
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	17	0.39
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	17	0.39
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	2	0.39
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	14	0.39
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	14	0.39
(1,757)	1:276:A:SER:HB2	1:355:A:ARG:HG2	8	0.39
(1,757)	1:276:A:SER:HB3	1:355:A:ARG:HG2	8	0.39
(1,690)	1:272:A:GLN:HG2	1:344:A:VAL:HG11	19	0.39
(1,690)	1:272:A:GLN:HG2	1:344:A:VAL:HG12	19	0.39
(1,690)	1:272:A:GLN:HG2	1:344:A:VAL:HG13	19	0.39
(1,690)	1:272:A:GLN:HG3	1:344:A:VAL:HG11	19	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:272:A:GLN:HG3	1:344:A:VAL:HG12	19	0.39
(1,690)	1:272:A:GLN:HG3	1:344:A:VAL:HG13	19	0.39
(1,685)	1:272:A:GLN:HE21	1:351:A:ALA:HB1	4	0.39
(1,685)	1:272:A:GLN:HE21	1:351:A:ALA:HB2	4	0.39
(1,685)	1:272:A:GLN:HE21	1:351:A:ALA:HB3	4	0.39
(1,685)	1:272:A:GLN:HE22	1:351:A:ALA:HB1	4	0.39
(1,685)	1:272:A:GLN:HE22	1:351:A:ALA:HB2	4	0.39
(1,685)	1:272:A:GLN:HE22	1:351:A:ALA:HB3	4	0.39
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB2	11	0.39
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB3	11	0.39
(1,219)	1:244:A:GLU:HA	1:248:A:GLU:H	10	0.39
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	2	0.39
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	17	0.39
(1,139)	1:237:A:ASN:HD21	1:239:A:SER:H	7	0.39
(1,139)	1:237:A:ASN:HD22	1:239:A:SER:H	7	0.39
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	1	0.39
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	2	0.39
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	5	0.39
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	10	0.39
(1,36)	1:233:A:LEU:HD21	1:265:A:HIS:HB2	5	0.39
(1,36)	1:233:A:LEU:HD21	1:265:A:HIS:HB3	5	0.39
(1,36)	1:233:A:LEU:HD22	1:265:A:HIS:HB2	5	0.39
(1,36)	1:233:A:LEU:HD22	1:265:A:HIS:HB3	5	0.39
(1,36)	1:233:A:LEU:HD23	1:265:A:HIS:HB2	5	0.39
(1,36)	1:233:A:LEU:HD23	1:265:A:HIS:HB3	5	0.39
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	11	0.39
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	11	0.39
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	11	0.39
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	11	0.39
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	11	0.39
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	11	0.39
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	15	0.39
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	15	0.39
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	15	0.39
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	15	0.39
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	15	0.39
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	15	0.39
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	18	0.39
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	19	0.39
(1,3891)	1:486:A:VAL:HG11	1:490:A:LEU:H	4	0.38
(1,3891)	1:486:A:VAL:HG12	1:490:A:LEU:H	4	0.38
(1,3891)	1:486:A:VAL:HG13	1:490:A:LEU:H	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB2	2	0.38
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB3	2	0.38
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB2	2	0.38
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB3	2	0.38
(1,3848)	1:481:A:GLN:HG2	1:486:A:VAL:HA	13	0.38
(1,3848)	1:481:A:GLN:HG3	1:486:A:VAL:HA	13	0.38
(1,3740)	1:469:A:MET:HE1	1:473:A:THR:H	15	0.38
(1,3740)	1:469:A:MET:HE2	1:473:A:THR:H	15	0.38
(1,3740)	1:469:A:MET:HE3	1:473:A:THR:H	15	0.38
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	12	0.38
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	12	0.38
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	12	0.38
(1,3540)	1:449:A:LEU:HA	1:452:A:LYS:H	12	0.38
(1,3406)	1:439:A:ALA:HA	1:442:A:LYS:HD2	12	0.38
(1,3406)	1:439:A:ALA:HA	1:442:A:LYS:HD3	12	0.38
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB2	19	0.38
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB3	19	0.38
(1,3329)	1:435:A:ALA:H	1:461:A:SER:HA	1	0.38
(1,3245)	1:432:A:TYR:HB2	1:458:A:LEU:H	12	0.38
(1,3245)	1:432:A:TYR:HB3	1:458:A:LEU:H	12	0.38
(1,3235)	1:432:A:TYR:H	1:482:A:SER:HA	11	0.38
(1,3231)	1:432:A:TYR:H	1:483:A:VAL:H	1	0.38
(1,3187)	1:430:A:ILE:HD11	1:474:A:GLU:HA	18	0.38
(1,3187)	1:430:A:ILE:HD12	1:474:A:GLU:HA	18	0.38
(1,3187)	1:430:A:ILE:HD13	1:474:A:GLU:HA	18	0.38
(1,3082)	1:423:A:MET:HA	1:427:A:GLN:HE21	2	0.38
(1,3082)	1:423:A:MET:HA	1:427:A:GLN:HE22	2	0.38
(1,3082)	1:423:A:MET:HA	1:427:A:GLN:HE21	20	0.38
(1,3082)	1:423:A:MET:HA	1:427:A:GLN:HE22	20	0.38
(1,2984)	1:417:A:GLU:HA	1:421:A:SER:H	10	0.38
(1,2915)	1:410:A:SER:HB2	1:438:A:TYR:HD1	18	0.38
(1,2912)	1:410:A:SER:HB2	1:438:A:TYR:HD1	7	0.38
(1,2912)	1:410:A:SER:HB2	1:438:A:TYR:HD2	7	0.38
(1,2912)	1:410:A:SER:HB3	1:438:A:TYR:HD1	7	0.38
(1,2912)	1:410:A:SER:HB3	1:438:A:TYR:HD2	7	0.38
(1,2892)	1:408:A:ASP:HA	1:442:A:LYS:HE2	10	0.38
(1,2892)	1:408:A:ASP:HA	1:442:A:LYS:HE3	10	0.38
(1,2839)	1:405:A:THR:HA	1:459:A:LEU:HD11	6	0.38
(1,2839)	1:405:A:THR:HA	1:459:A:LEU:HD12	6	0.38
(1,2839)	1:405:A:THR:HA	1:459:A:LEU:HD13	6	0.38
(1,2736)	1:401:A:ARG:HD2	1:414:A:VAL:H	15	0.38
(1,2736)	1:401:A:ARG:HD3	1:414:A:VAL:H	15	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	1:392:A:ASN:HA	1:396:A:ILE:H	1	0.38
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD1	17	0.38
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD2	17	0.38
(1,2380)	1:376:A:GLN:HE21	1:412:A:GLN:H	7	0.38
(1,2380)	1:376:A:GLN:HE22	1:412:A:GLN:H	7	0.38
(1,2317)	1:374:A:PHE:HZ	1:382:A:LEU:H	18	0.38
(1,2289)	1:372:A:GLN:HE21	1:376:A:GLN:HE21	12	0.38
(1,2289)	1:372:A:GLN:HE21	1:376:A:GLN:HE22	12	0.38
(1,2289)	1:372:A:GLN:HE22	1:376:A:GLN:HE21	12	0.38
(1,2289)	1:372:A:GLN:HE22	1:376:A:GLN:HE22	12	0.38
(1,2042)	1:357:A:LEU:HD21	1:396:A:ILE:HA	8	0.38
(1,2042)	1:357:A:LEU:HD22	1:396:A:ILE:HA	8	0.38
(1,2042)	1:357:A:LEU:HD23	1:396:A:ILE:HA	8	0.38
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE21	7	0.38
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE22	7	0.38
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD11	1	0.38
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD12	1	0.38
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD13	1	0.38
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB1	3	0.38
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB2	3	0.38
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB3	3	0.38
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB1	3	0.38
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB2	3	0.38
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB3	3	0.38
(1,1992)	1:354:A:LYS:HG2	1:392:A:ASN:HD21	10	0.38
(1,1992)	1:354:A:LYS:HG2	1:392:A:ASN:HD22	10	0.38
(1,1992)	1:354:A:LYS:HG3	1:392:A:ASN:HD21	10	0.38
(1,1992)	1:354:A:LYS:HG3	1:392:A:ASN:HD22	10	0.38
(1,1938)	1:350:A:ASN:HA	1:353:A:THR:HB	5	0.38
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD11	12	0.38
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD12	12	0.38
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD13	12	0.38
(1,1726)	1:331:A:PRO:HB2	1:338:A:ILE:HB	4	0.38
(1,1726)	1:331:A:PRO:HB3	1:338:A:ILE:HB	4	0.38
(1,1701)	1:329:A:ASP:HB2	1:344:A:VAL:HG21	10	0.38
(1,1701)	1:329:A:ASP:HB2	1:344:A:VAL:HG22	10	0.38
(1,1701)	1:329:A:ASP:HB2	1:344:A:VAL:HG23	10	0.38
(1,1701)	1:329:A:ASP:HB3	1:344:A:VAL:HG21	10	0.38
(1,1701)	1:329:A:ASP:HB3	1:344:A:VAL:HG22	10	0.38
(1,1701)	1:329:A:ASP:HB3	1:344:A:VAL:HG23	10	0.38
(1,1658)	1:322:A:ARG:HD2	1:323:A:GLY:H	1	0.38
(1,1658)	1:322:A:ARG:HD3	1:323:A:GLY:H	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1658)	1:322:A:ARG:HD2	1:323:A:GLY:H	18	0.38
(1,1658)	1:322:A:ARG:HD3	1:323:A:GLY:H	18	0.38
(1,1505)	1:315:A:PRO:HD2	1:350:A:ASN:HA	20	0.38
(1,1505)	1:315:A:PRO:HD3	1:350:A:ASN:HA	20	0.38
(1,1471)	1:314:A:MET:HA	1:353:A:THR:H	12	0.38
(1,1419)	1:312:A:GLN:HB2	1:345:A:THR:HG21	18	0.38
(1,1419)	1:312:A:GLN:HB2	1:345:A:THR:HG22	18	0.38
(1,1419)	1:312:A:GLN:HB2	1:345:A:THR:HG23	18	0.38
(1,1419)	1:312:A:GLN:HB3	1:345:A:THR:HG21	18	0.38
(1,1419)	1:312:A:GLN:HB3	1:345:A:THR:HG22	18	0.38
(1,1419)	1:312:A:GLN:HB3	1:345:A:THR:HG23	18	0.38
(1,1416)	1:312:A:GLN:HB2	1:349:A:ARG:HD2	14	0.38
(1,1416)	1:312:A:GLN:HB2	1:349:A:ARG:HD3	14	0.38
(1,1416)	1:312:A:GLN:HB3	1:349:A:ARG:HD2	14	0.38
(1,1416)	1:312:A:GLN:HB3	1:349:A:ARG:HD3	14	0.38
(1,1321)	1:302:A:GLN:HA	1:328:A:SER:HA	9	0.38
(1,1077)	1:295:A:HIS:HB2	1:296:A:GLY:H	8	0.38
(1,1077)	1:295:A:HIS:HB3	1:296:A:GLY:H	8	0.38
(1,1044)	1:291:A:ARG:HA	1:293:A:HIS:HA	13	0.38
(1,1023)	1:289:A:TRP:HZ2	1:381:A:VAL:H	2	0.38
(1,1008)	1:288:A:MET:HE1	1:320:A:PHE:HB2	17	0.38
(1,1008)	1:288:A:MET:HE1	1:320:A:PHE:HB3	17	0.38
(1,1008)	1:288:A:MET:HE2	1:320:A:PHE:HB2	17	0.38
(1,1008)	1:288:A:MET:HE2	1:320:A:PHE:HB3	17	0.38
(1,1008)	1:288:A:MET:HE3	1:320:A:PHE:HB2	17	0.38
(1,1008)	1:288:A:MET:HE3	1:320:A:PHE:HB3	17	0.38
(1,966)	1:285:A:PRO:HD2	1:288:A:MET:HE1	1	0.38
(1,966)	1:285:A:PRO:HD2	1:288:A:MET:HE2	1	0.38
(1,966)	1:285:A:PRO:HD2	1:288:A:MET:HE3	1	0.38
(1,966)	1:285:A:PRO:HD3	1:288:A:MET:HE1	1	0.38
(1,966)	1:285:A:PRO:HD3	1:288:A:MET:HE2	1	0.38
(1,966)	1:285:A:PRO:HD3	1:288:A:MET:HE3	1	0.38
(1,945)	1:284:A:ALA:HA	1:320:A:PHE:HB2	2	0.38
(1,945)	1:284:A:ALA:HA	1:320:A:PHE:HB3	2	0.38
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	9	0.38
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	9	0.38
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	15	0.38
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	15	0.38
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	17	0.38
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	17	0.38
(1,454)	1:257:A:PHE:H	1:258:A:ASN:HD21	3	0.38
(1,454)	1:257:A:PHE:H	1:258:A:ASN:HD22	3	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:255:A:HIS:HB2	1:294:A:LYS:HE2	3	0.38
(1,440)	1:255:A:HIS:HB2	1:294:A:LYS:HE3	3	0.38
(1,440)	1:255:A:HIS:HB3	1:294:A:LYS:HE2	3	0.38
(1,440)	1:255:A:HIS:HB3	1:294:A:LYS:HE3	3	0.38
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD2	18	0.38
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD3	18	0.38
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD2	18	0.38
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD3	18	0.38
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD2	18	0.38
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD3	18	0.38
(1,252)	1:246:A:TYR:HE1	1:263:A:TRP:HE1	11	0.38
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	3	0.38
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	18	0.38
(1,7)	1:231:A:GLN:HB2	1:236:A:ARG:HG2	12	0.38
(1,7)	1:231:A:GLN:HB2	1:236:A:ARG:HG3	12	0.38
(1,7)	1:231:A:GLN:HB3	1:236:A:ARG:HG2	12	0.38
(1,7)	1:231:A:GLN:HB3	1:236:A:ARG:HG3	12	0.38
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	4	0.37
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	4	0.37
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	4	0.37
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	4	0.37
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	4	0.37
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	4	0.37
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	4	0.37
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	4	0.37
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	4	0.37
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	18	0.37
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	18	0.37
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	18	0.37
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	18	0.37
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	18	0.37
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	18	0.37
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	18	0.37
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	18	0.37
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	18	0.37
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB2	13	0.37
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB3	13	0.37
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB2	13	0.37
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB3	13	0.37
(1,3700)	1:465:A:ASP:HA	1:468:A:MET:H	1	0.37
(1,3674)	1:462:A:ASP:HB2	1:464:A:ILE:H	18	0.37
(1,3674)	1:462:A:ASP:HB3	1:464:A:ILE:H	18	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3479)	1:446:A:HIS:HD2	1:484:A:SER:H	20	0.37
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD11	8	0.37
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD12	8	0.37
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD13	8	0.37
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB2	9	0.37
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB3	9	0.37
(1,3329)	1:435:A:ALA:H	1:461:A:SER:HA	4	0.37
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	3	0.37
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	3	0.37
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	3	0.37
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	3	0.37
(1,3235)	1:432:A:TYR:H	1:482:A:SER:HA	1	0.37
(1,3170)	1:430:A:ILE:H	1:481:A:GLN:H	17	0.37
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD11	8	0.37
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD12	8	0.37
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD13	8	0.37
(1,3159)	1:429:A:LYS:HG2	1:479:A:PRO:HG2	7	0.37
(1,3159)	1:429:A:LYS:HG2	1:479:A:PRO:HG3	7	0.37
(1,3159)	1:429:A:LYS:HG3	1:479:A:PRO:HG2	7	0.37
(1,3159)	1:429:A:LYS:HG3	1:479:A:PRO:HG3	7	0.37
(1,3144)	1:429:A:LYS:HD2	1:489:A:SER:HA	5	0.37
(1,3144)	1:429:A:LYS:HD3	1:489:A:SER:HA	5	0.37
(1,3136)	1:428:A:GLU:HG2	1:478:A:LYS:HA	3	0.37
(1,3136)	1:428:A:GLU:HG3	1:478:A:LYS:HA	3	0.37
(1,3126)	1:427:A:GLN:HG2	1:430:A:ILE:HA	10	0.37
(1,3126)	1:427:A:GLN:HG3	1:430:A:ILE:HA	10	0.37
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE21	2	0.37
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE22	2	0.37
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE21	5	0.37
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE22	5	0.37
(1,2989)	1:417:A:GLU:HA	1:420:A:VAL:HB	8	0.37
(1,2985)	1:417:A:GLU:HB2	1:421:A:SER:H	5	0.37
(1,2985)	1:417:A:GLU:HB3	1:421:A:SER:H	5	0.37
(1,2893)	1:408:A:ASP:HB2	1:442:A:LYS:HE2	7	0.37
(1,2893)	1:408:A:ASP:HB2	1:442:A:LYS:HE3	7	0.37
(1,2893)	1:408:A:ASP:HB3	1:442:A:LYS:HE2	7	0.37
(1,2893)	1:408:A:ASP:HB3	1:442:A:LYS:HE3	7	0.37
(1,2790)	1:403:A:ALA:HA	1:414:A:VAL:HB	10	0.37
(1,2631)	1:393:A:GLN:HA	1:396:A:ILE:H	18	0.37
(1,2484)	1:383:A:LYS:HB2	1:464:A:ILE:HD11	17	0.37
(1,2484)	1:383:A:LYS:HB2	1:464:A:ILE:HD12	17	0.37
(1,2484)	1:383:A:LYS:HB2	1:464:A:ILE:HD13	17	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2484)	1:383:A:LYS:HB3	1:464:A:ILE:HD11	17	0.37
(1,2484)	1:383:A:LYS:HB3	1:464:A:ILE:HD12	17	0.37
(1,2484)	1:383:A:LYS:HB3	1:464:A:ILE:HD13	17	0.37
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA2	5	0.37
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA3	5	0.37
(1,2227)	1:368:A:ALA:HA	1:371:A:TYR:H	12	0.37
(1,2042)	1:357:A:LEU:HD21	1:396:A:ILE:HA	10	0.37
(1,2042)	1:357:A:LEU:HD22	1:396:A:ILE:HA	10	0.37
(1,2042)	1:357:A:LEU:HD23	1:396:A:ILE:HA	10	0.37
(1,2013)	1:355:A:ARG:HA	1:358:A:GLN:H	12	0.37
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD21	5	0.37
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD22	5	0.37
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD21	5	0.37
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD22	5	0.37
(1,1790)	1:337:A:GLU:HG2	1:341:A:ASP:HB2	4	0.37
(1,1790)	1:337:A:GLU:HG2	1:341:A:ASP:HB3	4	0.37
(1,1790)	1:337:A:GLU:HG3	1:341:A:ASP:HB2	4	0.37
(1,1790)	1:337:A:GLU:HG3	1:341:A:ASP:HB3	4	0.37
(1,1790)	1:337:A:GLU:HG2	1:341:A:ASP:HB2	15	0.37
(1,1790)	1:337:A:GLU:HG2	1:341:A:ASP:HB3	15	0.37
(1,1790)	1:337:A:GLU:HG3	1:341:A:ASP:HB2	15	0.37
(1,1790)	1:337:A:GLU:HG3	1:341:A:ASP:HB3	15	0.37
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE1	8	0.37
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE2	8	0.37
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE3	8	0.37
(1,1552)	1:317:A:TYR:HB2	1:385:A:GLY:H	15	0.37
(1,1552)	1:317:A:TYR:HB3	1:385:A:GLY:H	15	0.37
(1,1542)	1:317:A:TYR:HE1	1:389:A:ASP:H	15	0.37
(1,1542)	1:317:A:TYR:HE2	1:389:A:ASP:H	15	0.37
(1,1488)	1:314:A:MET:HG2	1:319:A:ARG:HA	17	0.37
(1,1488)	1:314:A:MET:HG3	1:319:A:ARG:HA	17	0.37
(1,1445)	1:313:A:PHE:HA	1:349:A:ARG:H	18	0.37
(1,1442)	1:313:A:PHE:HA	1:352:A:LEU:HD11	6	0.37
(1,1442)	1:313:A:PHE:HA	1:352:A:LEU:HD12	6	0.37
(1,1442)	1:313:A:PHE:HA	1:352:A:LEU:HD13	6	0.37
(1,1037)	1:290:A:ASN:HB2	1:292:A:ASP:H	11	0.37
(1,1037)	1:290:A:ASN:HB3	1:292:A:ASP:H	11	0.37
(1,1024)	1:289:A:TRP:HH2	1:381:A:VAL:HA	11	0.37
(1,1020)	1:289:A:TRP:HH2	1:384:A:GLU:HG2	12	0.37
(1,1020)	1:289:A:TRP:HH2	1:384:A:GLU:HG3	12	0.37
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	3	0.37
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	1	0.37
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	1	0.37
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	2	0.37
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	17	0.37
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	17	0.37
(1,574)	1:264:A:SER:HB2	1:358:A:GLN:HB2	11	0.37
(1,574)	1:264:A:SER:HB2	1:358:A:GLN:HB3	11	0.37
(1,574)	1:264:A:SER:HB3	1:358:A:GLN:HB2	11	0.37
(1,574)	1:264:A:SER:HB3	1:358:A:GLN:HB3	11	0.37
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	15	0.37
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD2	18	0.37
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD3	18	0.37
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	19	0.37
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	19	0.37
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	19	0.37
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	19	0.37
(1,371)	1:251:A:LYS:HE2	1:259:A:ASP:HA	20	0.37
(1,371)	1:251:A:LYS:HE3	1:259:A:ASP:HA	20	0.37
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	8	0.37
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	7	0.37
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	7	0.37
(1,180)	1:241:A:ILE:HB	1:246:A:TYR:HD1	2	0.37
(1,180)	1:241:A:ILE:HB	1:246:A:TYR:HD2	2	0.37
(1,139)	1:237:A:ASN:HD21	1:239:A:SER:H	14	0.37
(1,139)	1:237:A:ASN:HD22	1:239:A:SER:H	14	0.37
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	14	0.37
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	14	0.37
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	14	0.37
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	14	0.37
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	14	0.37
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	14	0.37
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG21	11	0.37
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG22	11	0.37
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG23	11	0.37
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	5	0.36
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	5	0.36
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	5	0.36
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	5	0.36
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	5	0.36
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	5	0.36
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	5	0.36
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	5	0.36
(1,3972)	1:318:A:LEU:HD11	2:622:B:TYR:HE1	4	0.36
(1,3972)	1:318:A:LEU:HD12	2:622:B:TYR:HE1	4	0.36
(1,3972)	1:318:A:LEU:HD13	2:622:B:TYR:HE1	4	0.36
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	1	0.36
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	1	0.36
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	1	0.36
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	1	0.36
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	1	0.36
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	1	0.36
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	1	0.36
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	1	0.36
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	1	0.36
(1,3918)	1:488:A:GLU:HA	1:491:A:GLU:HA	14	0.36
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	2	0.36
(1,3887)	1:486:A:VAL:HG11	1:491:A:GLU:H	14	0.36
(1,3887)	1:486:A:VAL:HG12	1:491:A:GLU:H	14	0.36
(1,3887)	1:486:A:VAL:HG13	1:491:A:GLU:H	14	0.36
(1,3772)	1:472:A:LEU:HD21	1:474:A:GLU:HA	16	0.36
(1,3772)	1:472:A:LEU:HD22	1:474:A:GLU:HA	16	0.36
(1,3772)	1:472:A:LEU:HD23	1:474:A:GLU:HA	16	0.36
(1,3772)	1:472:A:LEU:HD21	1:474:A:GLU:HA	17	0.36
(1,3772)	1:472:A:LEU:HD22	1:474:A:GLU:HA	17	0.36
(1,3772)	1:472:A:LEU:HD23	1:474:A:GLU:HA	17	0.36
(1,3674)	1:462:A:ASP:HB2	1:464:A:ILE:H	16	0.36
(1,3674)	1:462:A:ASP:HB3	1:464:A:ILE:H	16	0.36
(1,3649)	1:460:A:LEU:HD21	1:472:A:LEU:HD11	6	0.36
(1,3649)	1:460:A:LEU:HD21	1:472:A:LEU:HD12	6	0.36
(1,3649)	1:460:A:LEU:HD21	1:472:A:LEU:HD13	6	0.36
(1,3649)	1:460:A:LEU:HD22	1:472:A:LEU:HD11	6	0.36
(1,3649)	1:460:A:LEU:HD22	1:472:A:LEU:HD12	6	0.36
(1,3649)	1:460:A:LEU:HD22	1:472:A:LEU:HD13	6	0.36
(1,3649)	1:460:A:LEU:HD23	1:472:A:LEU:HD11	6	0.36
(1,3649)	1:460:A:LEU:HD23	1:472:A:LEU:HD12	6	0.36
(1,3649)	1:460:A:LEU:HD23	1:472:A:LEU:HD13	6	0.36
(1,3605)	1:453:A:LYS:HG2	1:455:A:ILE:HD11	8	0.36
(1,3605)	1:453:A:LYS:HG2	1:455:A:ILE:HD12	8	0.36
(1,3605)	1:453:A:LYS:HG2	1:455:A:ILE:HD13	8	0.36
(1,3605)	1:453:A:LYS:HG3	1:455:A:ILE:HD11	8	0.36
(1,3605)	1:453:A:LYS:HG3	1:455:A:ILE:HD12	8	0.36
(1,3605)	1:453:A:LYS:HG3	1:455:A:ILE:HD13	8	0.36
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD11	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD12	8	0.36
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD13	8	0.36
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD11	8	0.36
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD12	8	0.36
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD13	8	0.36
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD11	8	0.36
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD12	8	0.36
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD13	8	0.36
(1,3478)	1:446:A:HIS:HD2	1:486:A:VAL:HG21	14	0.36
(1,3478)	1:446:A:HIS:HD2	1:486:A:VAL:HG22	14	0.36
(1,3478)	1:446:A:HIS:HD2	1:486:A:VAL:HG23	14	0.36
(1,3301)	1:434:A:THR:H	1:484:A:SER:H	11	0.36
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB2	4	0.36
(1,3247)	1:432:A:TYR:HB2	1:458:A:LEU:HB3	4	0.36
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB2	4	0.36
(1,3247)	1:432:A:TYR:HB3	1:458:A:LEU:HB3	4	0.36
(1,3214)	1:431:A:TYR:H	1:458:A:LEU:H	18	0.36
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB2	1	0.36
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB3	1	0.36
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB2	1	0.36
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB3	1	0.36
(1,3099)	1:424:A:LYS:HG2	1:427:A:GLN:HE21	8	0.36
(1,3099)	1:424:A:LYS:HG2	1:427:A:GLN:HE22	8	0.36
(1,3099)	1:424:A:LYS:HG3	1:427:A:GLN:HE21	8	0.36
(1,3099)	1:424:A:LYS:HG3	1:427:A:GLN:HE22	8	0.36
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE21	16	0.36
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE22	16	0.36
(1,3084)	1:423:A:MET:HE1	1:427:A:GLN:HG2	5	0.36
(1,3084)	1:423:A:MET:HE1	1:427:A:GLN:HG3	5	0.36
(1,3084)	1:423:A:MET:HE2	1:427:A:GLN:HG2	5	0.36
(1,3084)	1:423:A:MET:HE2	1:427:A:GLN:HG3	5	0.36
(1,3084)	1:423:A:MET:HE3	1:427:A:GLN:HG2	5	0.36
(1,3084)	1:423:A:MET:HE3	1:427:A:GLN:HG3	5	0.36
(1,3007)	1:419:A:TYR:HE2	1:478:A:LYS:HG2	1	0.36
(1,3007)	1:419:A:TYR:HE2	1:478:A:LYS:HG3	1	0.36
(1,3000)	1:418:A:ASP:HA	1:421:A:SER:HB2	20	0.36
(1,3000)	1:418:A:ASP:HA	1:421:A:SER:HB3	20	0.36
(1,2882)	1:407:A:THR:HG21	1:409:A:SER:H	16	0.36
(1,2882)	1:407:A:THR:HG22	1:409:A:SER:H	16	0.36
(1,2882)	1:407:A:THR:HG23	1:409:A:SER:H	16	0.36
(1,2827)	1:404:A:SER:H	1:413:A:THR:H	12	0.36
(1,2825)	1:404:A:SER:H	1:414:A:VAL:HG11	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2825)	1:404:A:SER:H	1:414:A:VAL:HG12	8	0.36
(1,2825)	1:404:A:SER:H	1:414:A:VAL:HG13	8	0.36
(1,2823)	1:404:A:SER:H	1:414:A:VAL:H	6	0.36
(1,2810)	1:404:A:SER:HA	1:459:A:LEU:HD11	8	0.36
(1,2810)	1:404:A:SER:HA	1:459:A:LEU:HD12	8	0.36
(1,2810)	1:404:A:SER:HA	1:459:A:LEU:HD13	8	0.36
(1,2694)	1:398:A:LYS:HA	1:475:A:PHE:HZ	6	0.36
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB2	2	0.36
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB3	2	0.36
(1,2508)	1:384:A:GLU:HA	1:464:A:ILE:HD11	16	0.36
(1,2508)	1:384:A:GLU:HA	1:464:A:ILE:HD12	16	0.36
(1,2508)	1:384:A:GLU:HA	1:464:A:ILE:HD13	16	0.36
(1,2487)	1:383:A:LYS:HE2	1:402:A:PHE:HA	10	0.36
(1,2487)	1:383:A:LYS:HE3	1:402:A:PHE:HA	10	0.36
(1,2487)	1:383:A:LYS:HE2	1:402:A:PHE:HA	19	0.36
(1,2487)	1:383:A:LYS:HE3	1:402:A:PHE:HA	19	0.36
(1,2444)	1:381:A:VAL:HA	1:464:A:ILE:HD11	13	0.36
(1,2444)	1:381:A:VAL:HA	1:464:A:ILE:HD12	13	0.36
(1,2444)	1:381:A:VAL:HA	1:464:A:ILE:HD13	13	0.36
(1,2353)	1:375:A:TRP:HZ3	1:400:A:LEU:HA	1	0.36
(1,2336)	1:375:A:TRP:HZ2	1:468:A:MET:HE1	13	0.36
(1,2336)	1:375:A:TRP:HZ2	1:468:A:MET:HE2	13	0.36
(1,2336)	1:375:A:TRP:HZ2	1:468:A:MET:HE3	13	0.36
(1,2290)	1:372:A:GLN:HG2	1:376:A:GLN:HE21	2	0.36
(1,2290)	1:372:A:GLN:HG2	1:376:A:GLN:HE22	2	0.36
(1,2290)	1:372:A:GLN:HG3	1:376:A:GLN:HE21	2	0.36
(1,2290)	1:372:A:GLN:HG3	1:376:A:GLN:HE22	2	0.36
(1,2181)	1:364:A:ALA:HA	1:371:A:TYR:HD1	4	0.36
(1,2181)	1:364:A:ALA:HA	1:371:A:TYR:HD2	4	0.36
(1,2045)	1:357:A:LEU:HD21	1:395:A:ALA:H	11	0.36
(1,2045)	1:357:A:LEU:HD22	1:395:A:ALA:H	11	0.36
(1,2045)	1:357:A:LEU:HD23	1:395:A:ALA:H	11	0.36
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	5	0.36
(1,1493)	1:314:A:MET:HB2	1:316:A:ASN:HA	10	0.36
(1,1493)	1:314:A:MET:HB3	1:316:A:ASN:HA	10	0.36
(1,1316)	1:302:A:GLN:HG2	1:332:A:LEU:HD11	4	0.36
(1,1316)	1:302:A:GLN:HG2	1:332:A:LEU:HD12	4	0.36
(1,1316)	1:302:A:GLN:HG2	1:332:A:LEU:HD13	4	0.36
(1,1316)	1:302:A:GLN:HG3	1:332:A:LEU:HD11	4	0.36
(1,1316)	1:302:A:GLN:HG3	1:332:A:LEU:HD12	4	0.36
(1,1316)	1:302:A:GLN:HG3	1:332:A:LEU:HD13	4	0.36
(1,1215)	1:299:A:LEU:H	1:307:A:MET:H	18	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1037)	1:290:A:ASN:HB2	1:292:A:ASP:H	18	0.36
(1,1037)	1:290:A:ASN:HB3	1:292:A:ASP:H	18	0.36
(1,1024)	1:289:A:TRP:HH2	1:381:A:VAL:HA	12	0.36
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	4	0.36
(1,934)	1:283:A:GLN:HG2	1:284:A:ALA:H	7	0.36
(1,934)	1:283:A:GLN:HG3	1:284:A:ALA:H	7	0.36
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	3	0.36
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	19	0.36
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	19	0.36
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	15	0.36
(1,371)	1:251:A:LYS:HE2	1:259:A:ASP:HA	16	0.36
(1,371)	1:251:A:LYS:HE3	1:259:A:ASP:HA	16	0.36
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	15	0.36
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	18	0.36
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	4	0.36
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	7	0.36
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	8	0.36
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	12	0.36
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	17	0.36
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	19	0.36
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	14	0.36
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	4	0.36
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	4	0.36
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	4	0.36
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	4	0.36
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	4	0.36
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	4	0.36
(1,8)	1:231:A:GLN:HG2	1:236:A:ARG:HG2	7	0.36
(1,8)	1:231:A:GLN:HG2	1:236:A:ARG:HG3	7	0.36
(1,8)	1:231:A:GLN:HG3	1:236:A:ARG:HG2	7	0.36
(1,8)	1:231:A:GLN:HG3	1:236:A:ARG:HG3	7	0.36
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	10	0.36
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE1	13	0.35
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE2	13	0.35
(1,3975)	1:400:A:LEU:HD11	2:629:B:MET:HE3	13	0.35
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE1	13	0.35
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE2	13	0.35
(1,3975)	1:400:A:LEU:HD12	2:629:B:MET:HE3	13	0.35
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE1	13	0.35
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE2	13	0.35
(1,3975)	1:400:A:LEU:HD13	2:629:B:MET:HE3	13	0.35
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3896)	1:486:A:VAL:HA	1:489:A:SER:HB2	8	0.35
(1,3896)	1:486:A:VAL:HA	1:489:A:SER:HB3	8	0.35
(1,3871)	1:483:A:VAL:HA	1:486:A:VAL:HA	11	0.35
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE2	2	0.35
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE3	2	0.35
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE2	2	0.35
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE3	2	0.35
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB2	8	0.35
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB3	8	0.35
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB2	8	0.35
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB3	8	0.35
(1,3771)	1:472:A:LEU:HD21	1:474:A:GLU:H	2	0.35
(1,3771)	1:472:A:LEU:HD22	1:474:A:GLU:H	2	0.35
(1,3771)	1:472:A:LEU:HD23	1:474:A:GLU:H	2	0.35
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB2	10	0.35
(1,3738)	1:469:A:MET:HE1	1:480:A:PHE:HB3	10	0.35
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB2	10	0.35
(1,3738)	1:469:A:MET:HE2	1:480:A:PHE:HB3	10	0.35
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB2	10	0.35
(1,3738)	1:469:A:MET:HE3	1:480:A:PHE:HB3	10	0.35
(1,3730)	1:468:A:MET:HA	1:471:A:TYR:HD1	4	0.35
(1,3730)	1:468:A:MET:HA	1:471:A:TYR:HD2	4	0.35
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	1	0.35
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	1	0.35
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	1	0.35
(1,3561)	1:450:A:LEU:HD11	1:456:A:GLU:H	17	0.35
(1,3561)	1:450:A:LEU:HD12	1:456:A:GLU:H	17	0.35
(1,3561)	1:450:A:LEU:HD13	1:456:A:GLU:H	17	0.35
(1,3555)	1:450:A:LEU:HD11	1:457:A:VAL:HA	14	0.35
(1,3555)	1:450:A:LEU:HD12	1:457:A:VAL:HA	14	0.35
(1,3555)	1:450:A:LEU:HD13	1:457:A:VAL:HA	14	0.35
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD11	10	0.35
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD12	10	0.35
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD13	10	0.35
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD11	10	0.35
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD12	10	0.35
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD13	10	0.35
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD11	10	0.35
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD12	10	0.35
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD13	10	0.35
(1,3479)	1:446:A:HIS:HD2	1:484:A:SER:H	6	0.35
(1,3356)	1:436:A:ASP:HB2	1:440:A:ALA:HB1	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3356)	1:436:A:ASP:HB2	1:440:A:ALA:HB2	8	0.35
(1,3356)	1:436:A:ASP:HB2	1:440:A:ALA:HB3	8	0.35
(1,3356)	1:436:A:ASP:HB3	1:440:A:ALA:HB1	8	0.35
(1,3356)	1:436:A:ASP:HB3	1:440:A:ALA:HB2	8	0.35
(1,3356)	1:436:A:ASP:HB3	1:440:A:ALA:HB3	8	0.35
(1,3235)	1:432:A:TYR:H	1:482:A:SER:HA	20	0.35
(1,3187)	1:430:A:ILE:HD11	1:474:A:GLU:HA	17	0.35
(1,3187)	1:430:A:ILE:HD12	1:474:A:GLU:HA	17	0.35
(1,3187)	1:430:A:ILE:HD13	1:474:A:GLU:HA	17	0.35
(1,3185)	1:430:A:ILE:HD11	1:475:A:PHE:H	18	0.35
(1,3185)	1:430:A:ILE:HD12	1:475:A:PHE:H	18	0.35
(1,3185)	1:430:A:ILE:HD13	1:475:A:PHE:H	18	0.35
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB2	8	0.35
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB3	8	0.35
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB2	8	0.35
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB3	8	0.35
(1,3144)	1:429:A:LYS:HD2	1:489:A:SER:HA	10	0.35
(1,3144)	1:429:A:LYS:HD3	1:489:A:SER:HA	10	0.35
(1,3128)	1:427:A:GLN:HG2	1:429:A:LYS:H	16	0.35
(1,3128)	1:427:A:GLN:HG3	1:429:A:LYS:H	16	0.35
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE21	8	0.35
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE22	8	0.35
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE21	15	0.35
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE22	15	0.35
(1,3078)	1:423:A:MET:HE1	1:428:A:GLU:H	14	0.35
(1,3078)	1:423:A:MET:HE2	1:428:A:GLU:H	14	0.35
(1,3078)	1:423:A:MET:HE3	1:428:A:GLU:H	14	0.35
(1,3072)	1:423:A:MET:HE1	1:431:A:TYR:HD1	2	0.35
(1,3072)	1:423:A:MET:HE1	1:431:A:TYR:HD2	2	0.35
(1,3072)	1:423:A:MET:HE2	1:431:A:TYR:HD1	2	0.35
(1,3072)	1:423:A:MET:HE2	1:431:A:TYR:HD2	2	0.35
(1,3072)	1:423:A:MET:HE3	1:431:A:TYR:HD1	2	0.35
(1,3072)	1:423:A:MET:HE3	1:431:A:TYR:HD2	2	0.35
(1,2988)	1:417:A:GLU:HA	1:420:A:VAL:H	8	0.35
(1,2914)	1:410:A:SER:HA	1:438:A:TYR:HD1	14	0.35
(1,2824)	1:404:A:SER:H	1:414:A:VAL:HB	8	0.35
(1,2811)	1:404:A:SER:HB2	1:458:A:LEU:H	3	0.35
(1,2811)	1:404:A:SER:HB3	1:458:A:LEU:H	3	0.35
(1,2621)	1:393:A:GLN:HE21	1:473:A:THR:H	1	0.35
(1,2621)	1:393:A:GLN:HE22	1:473:A:THR:H	1	0.35
(1,2620)	1:393:A:GLN:HE21	1:474:A:GLU:HB2	7	0.35
(1,2620)	1:393:A:GLN:HE21	1:474:A:GLU:HB3	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2620)	1:393:A:GLN:HE22	1:474:A:GLU:HB2	7	0.35
(1,2620)	1:393:A:GLN:HE22	1:474:A:GLU:HB3	7	0.35
(1,2591)	1:390:A:PHE:HD1	1:471:A:TYR:HD1	5	0.35
(1,2591)	1:390:A:PHE:HD1	1:471:A:TYR:HD2	5	0.35
(1,2591)	1:390:A:PHE:HD2	1:471:A:TYR:HD1	5	0.35
(1,2591)	1:390:A:PHE:HD2	1:471:A:TYR:HD2	5	0.35
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB2	13	0.35
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB3	13	0.35
(1,2432)	1:380:A:LEU:HA	1:384:A:GLU:H	6	0.35
(1,2429)	1:380:A:LEU:HA	1:462:A:ASP:HB2	7	0.35
(1,2429)	1:380:A:LEU:HA	1:462:A:ASP:HB3	7	0.35
(1,2425)	1:380:A:LEU:HB2	1:464:A:ILE:H	20	0.35
(1,2425)	1:380:A:LEU:HB3	1:464:A:ILE:H	20	0.35
(1,2344)	1:375:A:TRP:HZ2	1:402:A:PHE:HA	11	0.35
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA2	12	0.35
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA3	12	0.35
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA2	18	0.35
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA3	18	0.35
(1,2318)	1:374:A:PHE:HZ	1:382:A:LEU:HB2	8	0.35
(1,2318)	1:374:A:PHE:HZ	1:382:A:LEU:HB3	8	0.35
(1,2200)	1:365:A:LYS:HA	1:368:A:ALA:HA	20	0.35
(1,2107)	1:360:A:LEU:HA	1:364:A:ALA:H	4	0.35
(1,2014)	1:355:A:ARG:HA	1:358:A:GLN:HB2	5	0.35
(1,2014)	1:355:A:ARG:HA	1:358:A:GLN:HB3	5	0.35
(1,2002)	1:354:A:LYS:HG2	1:357:A:LEU:HD11	14	0.35
(1,2002)	1:354:A:LYS:HG2	1:357:A:LEU:HD12	14	0.35
(1,2002)	1:354:A:LYS:HG2	1:357:A:LEU:HD13	14	0.35
(1,2002)	1:354:A:LYS:HG3	1:357:A:LEU:HD11	14	0.35
(1,2002)	1:354:A:LYS:HG3	1:357:A:LEU:HD12	14	0.35
(1,2002)	1:354:A:LYS:HG3	1:357:A:LEU:HD13	14	0.35
(1,1997)	1:354:A:LYS:HB2	1:358:A:GLN:HE21	14	0.35
(1,1997)	1:354:A:LYS:HB2	1:358:A:GLN:HE22	14	0.35
(1,1997)	1:354:A:LYS:HB3	1:358:A:GLN:HE21	14	0.35
(1,1997)	1:354:A:LYS:HB3	1:358:A:GLN:HE22	14	0.35
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD21	16	0.35
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD22	16	0.35
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD21	16	0.35
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD22	16	0.35
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD21	7	0.35
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD22	7	0.35
(1,1790)	1:337:A:GLU:HG2	1:341:A:ASP:HB2	17	0.35
(1,1790)	1:337:A:GLU:HG2	1:341:A:ASP:HB3	17	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1790)	1:337:A:GLU:HG3	1:341:A:ASP:HB2	17	0.35
(1,1790)	1:337:A:GLU:HG3	1:341:A:ASP:HB3	17	0.35
(1,1762)	1:335:A:SER:H	1:339:A:LEU:H	1	0.35
(1,1658)	1:322:A:ARG:HD2	1:323:A:GLY:H	20	0.35
(1,1658)	1:322:A:ARG:HD3	1:323:A:GLY:H	20	0.35
(1,1621)	1:320:A:PHE:HE1	1:378:A:PHE:HB2	7	0.35
(1,1621)	1:320:A:PHE:HE1	1:378:A:PHE:HB3	7	0.35
(1,1621)	1:320:A:PHE:HE2	1:378:A:PHE:HB2	7	0.35
(1,1621)	1:320:A:PHE:HE2	1:378:A:PHE:HB3	7	0.35
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG21	16	0.35
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG22	16	0.35
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG23	16	0.35
(1,1159)	1:298:A:LYS:H	1:322:A:ARG:HD2	4	0.35
(1,1159)	1:298:A:LYS:H	1:322:A:ARG:HD3	4	0.35
(1,1149)	1:298:A:LYS:HB2	1:325:A:ILE:H	5	0.35
(1,1149)	1:298:A:LYS:HB3	1:325:A:ILE:H	5	0.35
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD2	18	0.35
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD3	18	0.35
(1,1037)	1:290:A:ASN:HB2	1:292:A:ASP:H	10	0.35
(1,1037)	1:290:A:ASN:HB3	1:292:A:ASP:H	10	0.35
(1,1037)	1:290:A:ASN:HB2	1:292:A:ASP:H	17	0.35
(1,1037)	1:290:A:ASN:HB3	1:292:A:ASP:H	17	0.35
(1,1037)	1:290:A:ASN:HB2	1:292:A:ASP:H	19	0.35
(1,1037)	1:290:A:ASN:HB3	1:292:A:ASP:H	19	0.35
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	19	0.35
(1,848)	1:279:A:TYR:H	1:322:A:ARG:H	1	0.35
(1,848)	1:279:A:TYR:H	1:322:A:ARG:H	2	0.35
(1,848)	1:279:A:TYR:H	1:322:A:ARG:H	16	0.35
(1,620)	1:266:A:ASN:HB2	1:274:A:TYR:HE1	12	0.35
(1,620)	1:266:A:ASN:HB2	1:274:A:TYR:HE2	12	0.35
(1,620)	1:266:A:ASN:HB3	1:274:A:TYR:HE1	12	0.35
(1,620)	1:266:A:ASN:HB3	1:274:A:TYR:HE2	12	0.35
(1,549)	1:263:A:TRP:H	1:359:A:MET:HG2	5	0.35
(1,549)	1:263:A:TRP:H	1:359:A:MET:HG3	5	0.35
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	10	0.35
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	12	0.35
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	15	0.35
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	15	0.35
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE21	9	0.35
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE22	9	0.35
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE21	9	0.35
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE22	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE21	11	0.35
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE22	11	0.35
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE21	11	0.35
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE22	11	0.35
(1,352)	1:250:A:TYR:HE1	1:256:A:ASP:H	16	0.35
(1,352)	1:250:A:TYR:HE2	1:256:A:ASP:H	16	0.35
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	14	0.35
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	15	0.35
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	5	0.35
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	17	0.35
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	17	0.35
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	17	0.35
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	17	0.35
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	17	0.35
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	17	0.35
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	17	0.35
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	7	0.35
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG11	8	0.34
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG12	8	0.34
(2,16)	1:467:A:TRP:NE1	2:630:B:VAL:HG13	8	0.34
(1,3943)	1:490:A:LEU:HA	1:492:A:LYS:H	8	0.34
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD11	4	0.34
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD12	4	0.34
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD13	4	0.34
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD11	4	0.34
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD12	4	0.34
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD13	4	0.34
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD11	4	0.34
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD12	4	0.34
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD13	4	0.34
(1,3938)	1:490:A:LEU:HA	1:493:A:LEU:H	10	0.34
(1,3785)	1:474:A:GLU:HA	1:480:A:PHE:H	13	0.34
(1,3767)	1:472:A:LEU:HD23	1:480:A:PHE:HE2	9	0.34
(1,3730)	1:468:A:MET:HA	1:471:A:TYR:HD1	17	0.34
(1,3730)	1:468:A:MET:HA	1:471:A:TYR:HD2	17	0.34
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD11	1	0.34
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD12	1	0.34
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD13	1	0.34
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD11	1	0.34
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD12	1	0.34
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD13	1	0.34
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD11	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD12	1	0.34
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD13	1	0.34
(1,3245)	1:432:A:TYR:HB2	1:458:A:LEU:H	3	0.34
(1,3245)	1:432:A:TYR:HB3	1:458:A:LEU:H	3	0.34
(1,3207)	1:431:A:TYR:HA	1:482:A:SER:HA	1	0.34
(1,3207)	1:431:A:TYR:HA	1:482:A:SER:HA	20	0.34
(1,3185)	1:430:A:ILE:HD11	1:475:A:PHE:H	19	0.34
(1,3185)	1:430:A:ILE:HD12	1:475:A:PHE:H	19	0.34
(1,3185)	1:430:A:ILE:HD13	1:475:A:PHE:H	19	0.34
(1,3135)	1:428:A:GLU:HA	1:478:A:LYS:HA	2	0.34
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE21	18	0.34
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE22	18	0.34
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD11	5	0.34
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD12	5	0.34
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD13	5	0.34
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD11	5	0.34
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD12	5	0.34
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD13	5	0.34
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD11	16	0.34
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD12	16	0.34
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD13	16	0.34
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD11	16	0.34
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD12	16	0.34
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD13	16	0.34
(1,2982)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	12	0.34
(1,2982)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	12	0.34
(1,2862)	1:405:A:THR:HG21	1:408:A:ASP:HA	7	0.34
(1,2862)	1:405:A:THR:HG22	1:408:A:ASP:HA	7	0.34
(1,2862)	1:405:A:THR:HG23	1:408:A:ASP:HA	7	0.34
(1,2861)	1:405:A:THR:HA	1:408:A:ASP:HA	8	0.34
(1,2848)	1:405:A:THR:H	1:457:A:VAL:HB	9	0.34
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG11	18	0.34
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG12	18	0.34
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG13	18	0.34
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	14	0.34
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	14	0.34
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	14	0.34
(1,2695)	1:398:A:LYS:HD2	1:475:A:PHE:HZ	11	0.34
(1,2695)	1:398:A:LYS:HD3	1:475:A:PHE:HZ	11	0.34
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB2	3	0.34
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB3	3	0.34
(1,2536)	1:386:A:PRO:HB2	1:472:A:LEU:HB2	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2536)	1:386:A:PRO:HB2	1:472:A:LEU:HB3	1	0.34
(1,2536)	1:386:A:PRO:HB3	1:472:A:LEU:HB2	1	0.34
(1,2536)	1:386:A:PRO:HB3	1:472:A:LEU:HB3	1	0.34
(1,2348)	1:375:A:TRP:HZ3	1:401:A:ARG:H	8	0.34
(1,2042)	1:357:A:LEU:HD21	1:396:A:ILE:HA	5	0.34
(1,2042)	1:357:A:LEU:HD22	1:396:A:ILE:HA	5	0.34
(1,2042)	1:357:A:LEU:HD23	1:396:A:ILE:HA	5	0.34
(1,2042)	1:357:A:LEU:HD21	1:396:A:ILE:HA	15	0.34
(1,2042)	1:357:A:LEU:HD22	1:396:A:ILE:HA	15	0.34
(1,2042)	1:357:A:LEU:HD23	1:396:A:ILE:HA	15	0.34
(1,1959)	1:352:A:LEU:HD21	1:356:A:VAL:H	12	0.34
(1,1959)	1:352:A:LEU:HD22	1:356:A:VAL:H	12	0.34
(1,1959)	1:352:A:LEU:HD23	1:356:A:VAL:H	12	0.34
(1,1937)	1:350:A:ASN:HA	1:353:A:THR:H	10	0.34
(1,1726)	1:331:A:PRO:HB2	1:338:A:ILE:HB	17	0.34
(1,1726)	1:331:A:PRO:HB3	1:338:A:ILE:HB	17	0.34
(1,1415)	1:312:A:GLN:HA	1:349:A:ARG:HD2	20	0.34
(1,1415)	1:312:A:GLN:HA	1:349:A:ARG:HD3	20	0.34
(1,1367)	1:307:A:MET:HE1	1:339:A:LEU:H	17	0.34
(1,1367)	1:307:A:MET:HE2	1:339:A:LEU:H	17	0.34
(1,1367)	1:307:A:MET:HE3	1:339:A:LEU:H	17	0.34
(1,1321)	1:302:A:GLN:HA	1:328:A:SER:HA	19	0.34
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD11	15	0.34
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD12	15	0.34
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD13	15	0.34
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HA	20	0.34
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	18	0.34
(1,883)	1:280:A:ILE:HD11	1:318:A:LEU:HD21	14	0.34
(1,883)	1:280:A:ILE:HD11	1:318:A:LEU:HD22	14	0.34
(1,883)	1:280:A:ILE:HD11	1:318:A:LEU:HD23	14	0.34
(1,883)	1:280:A:ILE:HD12	1:318:A:LEU:HD21	14	0.34
(1,883)	1:280:A:ILE:HD12	1:318:A:LEU:HD22	14	0.34
(1,883)	1:280:A:ILE:HD12	1:318:A:LEU:HD23	14	0.34
(1,883)	1:280:A:ILE:HD13	1:318:A:LEU:HD21	14	0.34
(1,883)	1:280:A:ILE:HD13	1:318:A:LEU:HD22	14	0.34
(1,883)	1:280:A:ILE:HD13	1:318:A:LEU:HD23	14	0.34
(1,879)	1:280:A:ILE:HA	1:321:A:VAL:HA	2	0.34
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	8	0.34
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	8	0.34
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	16	0.34
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	16	0.34
(1,574)	1:264:A:SER:HB2	1:358:A:GLN:HB2	18	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,574)	1:264:A:SER:HB2	1:358:A:GLN:HB3	18	0.34
(1,574)	1:264:A:SER:HB3	1:358:A:GLN:HB2	18	0.34
(1,574)	1:264:A:SER:HB3	1:358:A:GLN:HB3	18	0.34
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	16	0.34
(1,564)	1:263:A:TRP:HE1	1:265:A:HIS:H	3	0.34
(1,439)	1:255:A:HIS:HE1	1:308:A:ASP:HB2	6	0.34
(1,439)	1:255:A:HIS:HE1	1:308:A:ASP:HB3	6	0.34
(1,408)	1:253:A:ILE:HB	1:298:A:LYS:H	3	0.34
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	15	0.34
(1,112)	1:235:A:THR:HA	1:265:A:HIS:HE1	16	0.34
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD2	6	0.34
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD3	6	0.34
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD2	18	0.34
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD3	18	0.34
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	12	0.34
(1,3938)	1:490:A:LEU:HA	1:493:A:LEU:H	13	0.33
(1,3938)	1:490:A:LEU:HA	1:493:A:LEU:H	16	0.33
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	7	0.33
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	10	0.33
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB2	19	0.33
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB3	19	0.33
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB2	19	0.33
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB3	19	0.33
(1,3848)	1:481:A:GLN:HG2	1:486:A:VAL:HA	16	0.33
(1,3848)	1:481:A:GLN:HG3	1:486:A:VAL:HA	16	0.33
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	15	0.33
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	15	0.33
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	15	0.33
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD11	11	0.33
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD12	11	0.33
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD13	11	0.33
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD11	11	0.33
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD12	11	0.33
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD13	11	0.33
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD11	11	0.33
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD12	11	0.33
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD13	11	0.33
(1,3463)	1:444:A:SER:H	1:447:A:LEU:HD11	5	0.33
(1,3463)	1:444:A:SER:H	1:447:A:LEU:HD12	5	0.33
(1,3463)	1:444:A:SER:H	1:447:A:LEU:HD13	5	0.33
(1,3389)	1:438:A:TYR:HE1	1:442:A:LYS:HD2	7	0.33
(1,3389)	1:438:A:TYR:HE1	1:442:A:LYS:HD3	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3389)	1:438:A:TYR:HE2	1:442:A:LYS:HD2	7	0.33
(1,3389)	1:438:A:TYR:HE2	1:442:A:LYS:HD3	7	0.33
(1,3329)	1:435:A:ALA:H	1:461:A:SER:HA	7	0.33
(1,3315)	1:434:A:THR:HA	1:461:A:SER:HA	4	0.33
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD21	10	0.33
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD22	10	0.33
(1,3282)	1:433:A:ILE:HB	1:447:A:LEU:HD23	10	0.33
(1,3235)	1:432:A:TYR:H	1:482:A:SER:HA	3	0.33
(1,3188)	1:430:A:ILE:HB	1:469:A:MET:HE1	10	0.33
(1,3188)	1:430:A:ILE:HB	1:469:A:MET:HE2	10	0.33
(1,3188)	1:430:A:ILE:HB	1:469:A:MET:HE3	10	0.33
(1,3170)	1:430:A:ILE:H	1:481:A:GLN:H	4	0.33
(1,3144)	1:429:A:LYS:HD2	1:489:A:SER:HA	12	0.33
(1,3144)	1:429:A:LYS:HD3	1:489:A:SER:HA	12	0.33
(1,3136)	1:428:A:GLU:HG2	1:478:A:LYS:HA	13	0.33
(1,3136)	1:428:A:GLU:HG3	1:478:A:LYS:HA	13	0.33
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	13	0.33
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	13	0.33
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	13	0.33
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	13	0.33
(1,3070)	1:423:A:MET:HA	1:456:A:GLU:H	2	0.33
(1,2982)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	3	0.33
(1,2982)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	3	0.33
(1,2937)	1:414:A:VAL:HG21	1:419:A:TYR:HA	18	0.33
(1,2937)	1:414:A:VAL:HG22	1:419:A:TYR:HA	18	0.33
(1,2937)	1:414:A:VAL:HG23	1:419:A:TYR:HA	18	0.33
(1,2888)	1:408:A:ASP:HA	1:459:A:LEU:HD11	6	0.33
(1,2888)	1:408:A:ASP:HA	1:459:A:LEU:HD12	6	0.33
(1,2888)	1:408:A:ASP:HA	1:459:A:LEU:HD13	6	0.33
(1,2887)	1:407:A:THR:HG21	1:408:A:ASP:H	19	0.33
(1,2887)	1:407:A:THR:HG22	1:408:A:ASP:H	19	0.33
(1,2887)	1:407:A:THR:HG23	1:408:A:ASP:H	19	0.33
(1,2880)	1:407:A:THR:H	1:409:A:SER:H	7	0.33
(1,2755)	1:402:A:PHE:HD2	1:460:A:LEU:HD12	19	0.33
(1,2745)	1:402:A:PHE:HE1	1:480:A:PHE:HE1	16	0.33
(1,2745)	1:402:A:PHE:HE1	1:480:A:PHE:HE2	16	0.33
(1,2745)	1:402:A:PHE:HE2	1:480:A:PHE:HE1	16	0.33
(1,2745)	1:402:A:PHE:HE2	1:480:A:PHE:HE2	16	0.33
(1,2694)	1:398:A:LYS:HA	1:475:A:PHE:HZ	13	0.33
(1,2562)	1:387:A:ALA:HB1	1:471:A:TYR:HD1	12	0.33
(1,2562)	1:387:A:ALA:HB1	1:471:A:TYR:HD2	12	0.33
(1,2562)	1:387:A:ALA:HB2	1:471:A:TYR:HD1	12	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2562)	1:387:A:ALA:HB2	1:471:A:TYR:HD2	12	0.33
(1,2562)	1:387:A:ALA:HB3	1:471:A:TYR:HD1	12	0.33
(1,2562)	1:387:A:ALA:HB3	1:471:A:TYR:HD2	12	0.33
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB2	12	0.33
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB3	12	0.33
(1,2290)	1:372:A:GLN:HG2	1:376:A:GLN:HE21	9	0.33
(1,2290)	1:372:A:GLN:HG2	1:376:A:GLN:HE22	9	0.33
(1,2290)	1:372:A:GLN:HG3	1:376:A:GLN:HE21	9	0.33
(1,2290)	1:372:A:GLN:HG3	1:376:A:GLN:HE22	9	0.33
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	6	0.33
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	6	0.33
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	6	0.33
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	6	0.33
(1,2185)	1:364:A:ALA:HA	1:368:A:ALA:HA	6	0.33
(1,2042)	1:357:A:LEU:HD21	1:396:A:ILE:HA	20	0.33
(1,2042)	1:357:A:LEU:HD22	1:396:A:ILE:HA	20	0.33
(1,2042)	1:357:A:LEU:HD23	1:396:A:ILE:HA	20	0.33
(1,2041)	1:357:A:LEU:HD21	1:396:A:ILE:H	19	0.33
(1,2041)	1:357:A:LEU:HD22	1:396:A:ILE:H	19	0.33
(1,2041)	1:357:A:LEU:HD23	1:396:A:ILE:H	19	0.33
(1,1933)	1:350:A:ASN:HA	1:354:A:LYS:H	10	0.33
(1,1676)	1:325:A:ILE:HD11	1:327:A:SER:HB2	1	0.33
(1,1676)	1:325:A:ILE:HD11	1:327:A:SER:HB3	1	0.33
(1,1676)	1:325:A:ILE:HD12	1:327:A:SER:HB2	1	0.33
(1,1676)	1:325:A:ILE:HD12	1:327:A:SER:HB3	1	0.33
(1,1676)	1:325:A:ILE:HD13	1:327:A:SER:HB2	1	0.33
(1,1676)	1:325:A:ILE:HD13	1:327:A:SER:HB3	1	0.33
(1,1674)	1:325:A:ILE:HD11	1:327:A:SER:H	6	0.33
(1,1674)	1:325:A:ILE:HD12	1:327:A:SER:H	6	0.33
(1,1674)	1:325:A:ILE:HD13	1:327:A:SER:H	6	0.33
(1,1671)	1:325:A:ILE:HB	1:348:A:LEU:HD11	19	0.33
(1,1671)	1:325:A:ILE:HB	1:348:A:LEU:HD12	19	0.33
(1,1671)	1:325:A:ILE:HB	1:348:A:LEU:HD13	19	0.33
(1,1626)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	7	0.33
(1,1391)	1:309:A:ASP:HB2	1:311:A:GLU:HB2	3	0.33
(1,1391)	1:309:A:ASP:HB2	1:311:A:GLU:HB3	3	0.33
(1,1391)	1:309:A:ASP:HB3	1:311:A:GLU:HB2	3	0.33
(1,1391)	1:309:A:ASP:HB3	1:311:A:GLU:HB3	3	0.33
(1,1140)	1:297:A:LEU:HA	1:309:A:ASP:HA	13	0.33
(1,1140)	1:297:A:LEU:HA	1:309:A:ASP:HA	16	0.33
(1,1044)	1:291:A:ARG:HA	1:293:A:HIS:HA	9	0.33
(1,970)	1:285:A:PRO:HG2	1:287:A:ASP:H	14	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:285:A:PRO:HG3	1:287:A:ASP:H	14	0.33
(1,707)	1:273:A:GLU:H	1:327:A:SER:HA	1	0.33
(1,454)	1:257:A:PHE:H	1:258:A:ASN:HD21	1	0.33
(1,454)	1:257:A:PHE:H	1:258:A:ASN:HD22	1	0.33
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	18	0.33
(1,145)	1:238:A:LYS:HD2	1:267:A:ARG:H	15	0.33
(1,145)	1:238:A:LYS:HD3	1:267:A:ARG:H	15	0.33
(1,103)	1:235:A:THR:H	1:303:A:ARG:HD2	6	0.33
(1,103)	1:235:A:THR:H	1:303:A:ARG:HD3	6	0.33
(1,92)	1:234:A:TRP:HZ3	1:249:A:PHE:HZ	20	0.33
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	4	0.32
(1,3972)	1:318:A:LEU:HD11	2:622:B:TYR:HE1	5	0.32
(1,3972)	1:318:A:LEU:HD12	2:622:B:TYR:HE1	5	0.32
(1,3972)	1:318:A:LEU:HD13	2:622:B:TYR:HE1	5	0.32
(1,3943)	1:490:A:LEU:HA	1:492:A:LYS:H	17	0.32
(1,3938)	1:490:A:LEU:HA	1:493:A:LEU:H	4	0.32
(1,3935)	1:490:A:LEU:HA	1:494:A:ALA:H	13	0.32
(1,3891)	1:486:A:VAL:HG11	1:490:A:LEU:H	9	0.32
(1,3891)	1:486:A:VAL:HG12	1:490:A:LEU:H	9	0.32
(1,3891)	1:486:A:VAL:HG13	1:490:A:LEU:H	9	0.32
(1,3817)	1:475:A:PHE:HE2	1:476:A:ASP:HB2	8	0.32
(1,3772)	1:472:A:LEU:HD21	1:474:A:GLU:HA	12	0.32
(1,3772)	1:472:A:LEU:HD22	1:474:A:GLU:HA	12	0.32
(1,3772)	1:472:A:LEU:HD23	1:474:A:GLU:HA	12	0.32
(1,3567)	1:450:A:LEU:HA	1:454:A:GLY:H	1	0.32
(1,3560)	1:450:A:LEU:HB2	1:456:A:GLU:H	18	0.32
(1,3560)	1:450:A:LEU:HB3	1:456:A:GLU:H	18	0.32
(1,3536)	1:449:A:LEU:HA	1:453:A:LYS:H	9	0.32
(1,3535)	1:449:A:LEU:HD21	1:483:A:VAL:HB	16	0.32
(1,3535)	1:449:A:LEU:HD22	1:483:A:VAL:HB	16	0.32
(1,3535)	1:449:A:LEU:HD23	1:483:A:VAL:HB	16	0.32
(1,3523)	1:448:A:GLU:HA	1:451:A:ARG:HB2	14	0.32
(1,3523)	1:448:A:GLU:HA	1:451:A:ARG:HB3	14	0.32
(1,3476)	1:445:A:PRO:HG2	1:446:A:HIS:H	6	0.32
(1,3476)	1:445:A:PRO:HG3	1:446:A:HIS:H	6	0.32
(1,3389)	1:438:A:TYR:HE1	1:442:A:LYS:HD2	2	0.32
(1,3389)	1:438:A:TYR:HE1	1:442:A:LYS:HD3	2	0.32
(1,3389)	1:438:A:TYR:HE2	1:442:A:LYS:HD2	2	0.32
(1,3389)	1:438:A:TYR:HE2	1:442:A:LYS:HD3	2	0.32
(1,3311)	1:434:A:THR:HB	1:466:A:GLU:HA	16	0.32
(1,3062)	1:422:A:ARG:HD2	1:456:A:GLU:HG2	5	0.32
(1,3062)	1:422:A:ARG:HD2	1:456:A:GLU:HG3	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3062)	1:422:A:ARG:HD3	1:456:A:GLU:HG2	5	0.32
(1,3062)	1:422:A:ARG:HD3	1:456:A:GLU:HG3	5	0.32
(1,3039)	1:420:A:VAL:HB	1:475:A:PHE:HZ	17	0.32
(1,2982)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	17	0.32
(1,2982)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	17	0.32
(1,2941)	1:414:A:VAL:HG11	1:416:A:LEU:H	11	0.32
(1,2941)	1:414:A:VAL:HG12	1:416:A:LEU:H	11	0.32
(1,2941)	1:414:A:VAL:HG13	1:416:A:LEU:H	11	0.32
(1,2855)	1:405:A:THR:HB	1:451:A:ARG:HA	4	0.32
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	12	0.32
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	12	0.32
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	12	0.32
(1,2565)	1:387:A:ALA:HB1	1:471:A:TYR:HD1	1	0.32
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB2	18	0.32
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB3	18	0.32
(1,2545)	1:386:A:PRO:HG2	1:397:A:ALA:HA	20	0.32
(1,2545)	1:386:A:PRO:HG3	1:397:A:ALA:HA	20	0.32
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD11	19	0.32
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD12	19	0.32
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD13	19	0.32
(1,2483)	1:383:A:LYS:HD2	1:465:A:ASP:HA	10	0.32
(1,2483)	1:383:A:LYS:HD3	1:465:A:ASP:HA	10	0.32
(1,2344)	1:375:A:TRP:HZ2	1:402:A:PHE:HA	8	0.32
(1,2200)	1:365:A:LYS:HA	1:368:A:ALA:HA	10	0.32
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	1	0.32
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	1	0.32
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	1	0.32
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	1	0.32
(1,2166)	1:363:A:LEU:HA	1:367:A:ASP:HB2	4	0.32
(1,2166)	1:363:A:LEU:HA	1:367:A:ASP:HB3	4	0.32
(1,2132)	1:361:A:GLU:HA	1:371:A:TYR:HE1	7	0.32
(1,2045)	1:357:A:LEU:HD21	1:395:A:ALA:H	16	0.32
(1,2045)	1:357:A:LEU:HD22	1:395:A:ALA:H	16	0.32
(1,2045)	1:357:A:LEU:HD23	1:395:A:ALA:H	16	0.32
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE21	14	0.32
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE22	14	0.32
(1,1992)	1:354:A:LYS:HG2	1:392:A:ASN:HD21	9	0.32
(1,1992)	1:354:A:LYS:HG2	1:392:A:ASN:HD22	9	0.32
(1,1992)	1:354:A:LYS:HG3	1:392:A:ASN:HD21	9	0.32
(1,1992)	1:354:A:LYS:HG3	1:392:A:ASN:HD22	9	0.32
(1,1990)	1:354:A:LYS:HD2	1:392:A:ASN:HD21	18	0.32
(1,1990)	1:354:A:LYS:HD2	1:392:A:ASN:HD22	18	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1990)	1:354:A:LYS:HD3	1:392:A:ASN:HD21	18	0.32
(1,1990)	1:354:A:LYS:HD3	1:392:A:ASN:HD22	18	0.32
(1,1989)	1:354:A:LYS:HA	1:392:A:ASN:HD21	6	0.32
(1,1989)	1:354:A:LYS:HA	1:392:A:ASN:HD22	6	0.32
(1,1909)	1:348:A:LEU:HA	1:352:A:LEU:H	12	0.32
(1,1889)	1:346:A:ARG:HA	1:349:A:ARG:HG2	8	0.32
(1,1529)	1:316:A:ASN:HA	1:319:A:ARG:HA	2	0.32
(1,1471)	1:314:A:MET:HA	1:353:A:THR:H	1	0.32
(1,1318)	1:302:A:GLN:H	1:329:A:ASP:H	11	0.32
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE1	18	0.32
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE2	18	0.32
(1,1037)	1:290:A:ASN:HB2	1:292:A:ASP:H	8	0.32
(1,1037)	1:290:A:ASN:HB3	1:292:A:ASP:H	8	0.32
(1,1024)	1:289:A:TRP:HH2	1:381:A:VAL:HA	2	0.32
(1,1023)	1:289:A:TRP:HZ2	1:381:A:VAL:H	4	0.32
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	10	0.32
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	15	0.32
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE1	13	0.32
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE2	13	0.32
(1,967)	1:285:A:PRO:HG2	1:288:A:MET:HE3	13	0.32
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE1	13	0.32
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE2	13	0.32
(1,967)	1:285:A:PRO:HG3	1:288:A:MET:HE3	13	0.32
(1,799)	1:278:A:LEU:H	1:359:A:MET:HE1	18	0.32
(1,799)	1:278:A:LEU:H	1:359:A:MET:HE2	18	0.32
(1,799)	1:278:A:LEU:H	1:359:A:MET:HE3	18	0.32
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	11	0.32
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	11	0.32
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	20	0.32
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	20	0.32
(1,693)	1:272:A:GLN:HB2	1:274:A:TYR:H	5	0.32
(1,693)	1:272:A:GLN:HB3	1:274:A:TYR:H	5	0.32
(1,693)	1:272:A:GLN:HB2	1:274:A:TYR:H	13	0.32
(1,693)	1:272:A:GLN:HB3	1:274:A:TYR:H	13	0.32
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD21	8	0.32
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD22	8	0.32
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD21	12	0.32
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD22	12	0.32
(1,574)	1:264:A:SER:HB2	1:358:A:GLN:HB2	8	0.32
(1,574)	1:264:A:SER:HB2	1:358:A:GLN:HB3	8	0.32
(1,574)	1:264:A:SER:HB3	1:358:A:GLN:HB2	8	0.32
(1,574)	1:264:A:SER:HB3	1:358:A:GLN:HB3	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	18	0.32
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	18	0.32
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	17	0.32
(1,426)	1:254:A:ALA:HA	1:322:A:ARG:HD2	1	0.32
(1,426)	1:254:A:ALA:HA	1:322:A:ARG:HD3	1	0.32
(1,382)	1:251:A:LYS:HA	1:255:A:HIS:HA	16	0.32
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	18	0.32
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	18	0.32
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	18	0.32
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	18	0.32
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	20	0.32
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	12	0.32
(1,252)	1:246:A:TYR:HD1	1:263:A:TRP:HE1	12	0.32
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	12	0.32
(1,37)	1:233:A:LEU:HD11	1:249:A:PHE:H	2	0.32
(1,37)	1:233:A:LEU:HD12	1:249:A:PHE:H	2	0.32
(1,37)	1:233:A:LEU:HD13	1:249:A:PHE:H	2	0.32
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	11	0.32
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	16	0.32
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	17	0.32
(2,9)	1:338:A:ILE:HD11	1:342:A:SER:H	2	0.31
(2,9)	1:338:A:ILE:HD12	1:342:A:SER:H	2	0.31
(2,9)	1:338:A:ILE:HD13	1:342:A:SER:H	2	0.31
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD11	8	0.31
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD12	8	0.31
(1,3941)	1:490:A:LEU:HD21	1:493:A:LEU:HD13	8	0.31
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD11	8	0.31
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD12	8	0.31
(1,3941)	1:490:A:LEU:HD22	1:493:A:LEU:HD13	8	0.31
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD11	8	0.31
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD12	8	0.31
(1,3941)	1:490:A:LEU:HD23	1:493:A:LEU:HD13	8	0.31
(1,3938)	1:490:A:LEU:HA	1:493:A:LEU:H	15	0.31
(1,3919)	1:488:A:GLU:HA	1:491:A:GLU:HB2	14	0.31
(1,3919)	1:488:A:GLU:HA	1:491:A:GLU:HB3	14	0.31
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	18	0.31
(1,3891)	1:486:A:VAL:HG11	1:490:A:LEU:H	20	0.31
(1,3891)	1:486:A:VAL:HG12	1:490:A:LEU:H	20	0.31
(1,3891)	1:486:A:VAL:HG13	1:490:A:LEU:H	20	0.31
(1,3841)	1:481:A:GLN:HG2	1:489:A:SER:HA	12	0.31
(1,3841)	1:481:A:GLN:HG3	1:489:A:SER:HA	12	0.31
(1,3821)	1:476:A:ASP:HB2	1:478:A:LYS:HD2	15	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3821)	1:476:A:ASP:HB2	1:478:A:LYS:HD3	15	0.31
(1,3821)	1:476:A:ASP:HB3	1:478:A:LYS:HD2	15	0.31
(1,3821)	1:476:A:ASP:HB3	1:478:A:LYS:HD3	15	0.31
(1,3788)	1:474:A:GLU:HA	1:479:A:PRO:HA	13	0.31
(1,3674)	1:462:A:ASP:HB2	1:464:A:ILE:H	10	0.31
(1,3674)	1:462:A:ASP:HB3	1:464:A:ILE:H	10	0.31
(1,3492)	1:447:A:LEU:HA	1:483:A:VAL:HB	12	0.31
(1,3476)	1:445:A:PRO:HG2	1:446:A:HIS:H	16	0.31
(1,3476)	1:445:A:PRO:HG3	1:446:A:HIS:H	16	0.31
(1,3461)	1:444:A:SER:HA	1:447:A:LEU:H	5	0.31
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD11	3	0.31
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD12	3	0.31
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD13	3	0.31
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD11	6	0.31
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD12	6	0.31
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD13	6	0.31
(1,3351)	1:436:A:ASP:HA	1:463:A:ARG:HA	5	0.31
(1,3235)	1:432:A:TYR:H	1:482:A:SER:HA	15	0.31
(1,3235)	1:432:A:TYR:H	1:482:A:SER:HA	17	0.31
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD11	1	0.31
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD12	1	0.31
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD13	1	0.31
(1,3137)	1:428:A:GLU:HA	1:478:A:LYS:HG2	8	0.31
(1,3137)	1:428:A:GLU:HA	1:478:A:LYS:HG3	8	0.31
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD11	3	0.31
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD12	3	0.31
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD13	3	0.31
(1,3063)	1:422:A:ARG:HB2	1:427:A:GLN:HE21	7	0.31
(1,3063)	1:422:A:ARG:HB2	1:427:A:GLN:HE22	7	0.31
(1,3063)	1:422:A:ARG:HB3	1:427:A:GLN:HE21	7	0.31
(1,3063)	1:422:A:ARG:HB3	1:427:A:GLN:HE22	7	0.31
(1,3000)	1:418:A:ASP:HA	1:421:A:SER:HB2	11	0.31
(1,3000)	1:418:A:ASP:HA	1:421:A:SER:HB3	11	0.31
(1,2985)	1:417:A:GLU:HB2	1:421:A:SER:H	19	0.31
(1,2985)	1:417:A:GLU:HB3	1:421:A:SER:H	19	0.31
(1,2915)	1:410:A:SER:HB3	1:438:A:TYR:HD2	6	0.31
(1,2828)	1:404:A:SER:H	1:412:A:GLN:HA	14	0.31
(1,2827)	1:404:A:SER:H	1:413:A:THR:H	18	0.31
(1,2797)	1:403:A:ALA:HA	1:412:A:GLN:HA	11	0.31
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG11	7	0.31
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG12	7	0.31
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG13	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG11	3	0.31
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG12	3	0.31
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG13	3	0.31
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG11	3	0.31
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG12	3	0.31
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG13	3	0.31
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG11	2	0.31
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG12	2	0.31
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG13	2	0.31
(1,2593)	1:390:A:PHE:HA	1:393:A:GLN:H	12	0.31
(1,2575)	1:388:A:GLU:HA	1:390:A:PHE:H	5	0.31
(1,2538)	1:386:A:PRO:HA	1:471:A:TYR:HB2	17	0.31
(1,2538)	1:386:A:PRO:HA	1:471:A:TYR:HB3	17	0.31
(1,2365)	1:375:A:TRP:HA	1:379:A:GLY:H	18	0.31
(1,2359)	1:375:A:TRP:HH2	1:383:A:LYS:HG2	13	0.31
(1,2359)	1:375:A:TRP:HH2	1:383:A:LYS:HG3	13	0.31
(1,2358)	1:375:A:TRP:HZ2	1:383:A:LYS:HE2	10	0.31
(1,2358)	1:375:A:TRP:HZ2	1:383:A:LYS:HE3	10	0.31
(1,2318)	1:374:A:PHE:HZ	1:382:A:LEU:HB2	7	0.31
(1,2318)	1:374:A:PHE:HZ	1:382:A:LEU:HB3	7	0.31
(1,2045)	1:357:A:LEU:HD21	1:395:A:ALA:H	10	0.31
(1,2045)	1:357:A:LEU:HD22	1:395:A:ALA:H	10	0.31
(1,2045)	1:357:A:LEU:HD23	1:395:A:ALA:H	10	0.31
(1,2042)	1:357:A:LEU:HD21	1:396:A:ILE:HA	14	0.31
(1,2042)	1:357:A:LEU:HD22	1:396:A:ILE:HA	14	0.31
(1,2042)	1:357:A:LEU:HD23	1:396:A:ILE:HA	14	0.31
(1,2042)	1:357:A:LEU:HD21	1:396:A:ILE:HA	18	0.31
(1,2042)	1:357:A:LEU:HD22	1:396:A:ILE:HA	18	0.31
(1,2042)	1:357:A:LEU:HD23	1:396:A:ILE:HA	18	0.31
(1,1996)	1:354:A:LYS:HA	1:358:A:GLN:HE21	15	0.31
(1,1996)	1:354:A:LYS:HA	1:358:A:GLN:HE22	15	0.31
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD21	12	0.31
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD22	12	0.31
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD21	12	0.31
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD22	12	0.31
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD11	1	0.31
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD12	1	0.31
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD13	1	0.31
(1,1964)	1:352:A:LEU:HA	1:355:A:ARG:HD2	9	0.31
(1,1964)	1:352:A:LEU:HA	1:355:A:ARG:HD3	9	0.31
(1,1937)	1:350:A:ASN:HA	1:353:A:THR:H	19	0.31
(1,1472)	1:314:A:MET:HA	1:353:A:THR:HA	12	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1324)	1:302:A:GLN:H	1:327:A:SER:H	19	0.31
(1,1321)	1:302:A:GLN:HA	1:328:A:SER:HA	20	0.31
(1,1318)	1:302:A:GLN:H	1:329:A:ASP:H	19	0.31
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE1	5	0.31
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE2	5	0.31
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE1	19	0.31
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE2	19	0.31
(1,1219)	1:299:A:LEU:H	1:306:A:ILE:H	3	0.31
(1,1219)	1:299:A:LEU:H	1:306:A:ILE:H	11	0.31
(1,1132)	1:297:A:LEU:H	1:310:A:ALA:H	15	0.31
(1,1072)	1:295:A:HIS:HE1	1:311:A:GLU:HA	7	0.31
(1,1029)	1:289:A:TRP:HZ2	1:380:A:LEU:HB2	13	0.31
(1,1029)	1:289:A:TRP:HZ2	1:380:A:LEU:HB3	13	0.31
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	16	0.31
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD21	9	0.31
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD22	9	0.31
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	1	0.31
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	3	0.31
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	3	0.31
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	14	0.31
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	14	0.31
(1,764)	1:276:A:SER:HB2	1:326:A:ASP:H	20	0.31
(1,764)	1:276:A:SER:HB3	1:326:A:ASP:H	20	0.31
(1,719)	1:274:A:TYR:HD2	1:348:A:LEU:HD23	13	0.31
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	10	0.31
(1,702)	1:273:A:GLU:H	1:329:A:ASP:HB2	1	0.31
(1,702)	1:273:A:GLU:H	1:329:A:ASP:HB3	1	0.31
(1,648)	1:268:A:VAL:HB	1:274:A:TYR:H	20	0.31
(1,550)	1:263:A:TRP:HA	1:359:A:MET:HG2	13	0.31
(1,550)	1:263:A:TRP:HA	1:359:A:MET:HG3	13	0.31
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD2	3	0.31
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD3	3	0.31
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD2	3	0.31
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD3	3	0.31
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD2	3	0.31
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD3	3	0.31
(1,353)	1:250:A:TYR:HE1	1:256:A:ASP:HB2	3	0.31
(1,353)	1:250:A:TYR:HE1	1:256:A:ASP:HB3	3	0.31
(1,353)	1:250:A:TYR:HE2	1:256:A:ASP:HB2	3	0.31
(1,353)	1:250:A:TYR:HE2	1:256:A:ASP:HB3	3	0.31
(1,293)	1:248:A:GLU:HA	1:251:A:LYS:H	17	0.31
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB2	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB3	9	0.31
(1,123)	1:236:A:ARG:HB2	1:240:A:GLU:H	13	0.31
(1,123)	1:236:A:ARG:HB3	1:240:A:GLU:H	13	0.31
(1,23)	1:232:A:ALA:HB1	1:235:A:THR:HB	15	0.31
(1,23)	1:232:A:ALA:HB2	1:235:A:THR:HB	15	0.31
(1,23)	1:232:A:ALA:HB3	1:235:A:THR:HB	15	0.31
(1,3936)	1:490:A:LEU:HB2	1:494:A:ALA:H	14	0.3
(1,3936)	1:490:A:LEU:HB3	1:494:A:ALA:H	14	0.3
(1,3915)	1:488:A:GLU:HA	1:492:A:LYS:H	14	0.3
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	7	0.3
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	18	0.3
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE2	19	0.3
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE3	19	0.3
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE2	19	0.3
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE3	19	0.3
(1,3846)	1:481:A:GLN:HE21	1:486:A:VAL:H	17	0.3
(1,3846)	1:481:A:GLN:HE22	1:486:A:VAL:H	17	0.3
(1,3492)	1:447:A:LEU:HA	1:483:A:VAL:HB	20	0.3
(1,3365)	1:437:A:SER:H	1:441:A:ALA:H	8	0.3
(1,3360)	1:437:A:SER:HA	1:462:A:ASP:HA	6	0.3
(1,3329)	1:435:A:ALA:H	1:461:A:SER:HA	17	0.3
(1,3254)	1:433:A:ILE:HA	1:484:A:SER:H	14	0.3
(1,3214)	1:431:A:TYR:H	1:458:A:LEU:H	7	0.3
(1,3207)	1:431:A:TYR:HA	1:482:A:SER:HA	10	0.3
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD11	9	0.3
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD12	9	0.3
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD13	9	0.3
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD11	13	0.3
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD12	13	0.3
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD13	13	0.3
(1,3155)	1:429:A:LYS:HB2	1:480:A:PHE:HA	17	0.3
(1,3155)	1:429:A:LYS:HB3	1:480:A:PHE:HA	17	0.3
(1,3144)	1:429:A:LYS:HD2	1:489:A:SER:HA	20	0.3
(1,3144)	1:429:A:LYS:HD3	1:489:A:SER:HA	20	0.3
(1,3136)	1:428:A:GLU:HG2	1:478:A:LYS:HA	8	0.3
(1,3136)	1:428:A:GLU:HG3	1:478:A:LYS:HA	8	0.3
(1,3133)	1:428:A:GLU:HG2	1:479:A:PRO:HD2	13	0.3
(1,3133)	1:428:A:GLU:HG2	1:479:A:PRO:HD3	13	0.3
(1,3133)	1:428:A:GLU:HG3	1:479:A:PRO:HD2	13	0.3
(1,3133)	1:428:A:GLU:HG3	1:479:A:PRO:HD3	13	0.3
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD11	6	0.3
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD12	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3092)	1:424:A:LYS:HG2	1:455:A:ILE:HD13	6	0.3
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD11	6	0.3
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD12	6	0.3
(1,3092)	1:424:A:LYS:HG3	1:455:A:ILE:HD13	6	0.3
(1,3091)	1:424:A:LYS:HG2	1:455:A:ILE:HA	1	0.3
(1,3091)	1:424:A:LYS:HG3	1:455:A:ILE:HA	1	0.3
(1,2982)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	16	0.3
(1,2982)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	16	0.3
(1,2945)	1:415:A:SER:H	1:419:A:TYR:H	18	0.3
(1,2859)	1:405:A:THR:HG21	1:442:A:LYS:HA	5	0.3
(1,2859)	1:405:A:THR:HG22	1:442:A:LYS:HA	5	0.3
(1,2859)	1:405:A:THR:HG23	1:442:A:LYS:HA	5	0.3
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG11	7	0.3
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG12	7	0.3
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG13	7	0.3
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	16	0.3
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	16	0.3
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	16	0.3
(1,2575)	1:388:A:GLU:HA	1:390:A:PHE:H	3	0.3
(1,2575)	1:388:A:GLU:HA	1:390:A:PHE:H	7	0.3
(1,2353)	1:375:A:TRP:HZ3	1:400:A:LEU:HA	9	0.3
(1,2351)	1:375:A:TRP:HE3	1:400:A:LEU:HA	1	0.3
(1,2336)	1:375:A:TRP:HZ2	1:468:A:MET:HE1	17	0.3
(1,2336)	1:375:A:TRP:HZ2	1:468:A:MET:HE2	17	0.3
(1,2336)	1:375:A:TRP:HZ2	1:468:A:MET:HE3	17	0.3
(1,2318)	1:374:A:PHE:HZ	1:382:A:LEU:HB2	17	0.3
(1,2318)	1:374:A:PHE:HZ	1:382:A:LEU:HB3	17	0.3
(1,2245)	1:369:A:GLU:HG2	1:370:A:LYS:H	20	0.3
(1,2245)	1:369:A:GLU:HG3	1:370:A:LYS:H	20	0.3
(1,2216)	1:367:A:ASP:HB2	1:370:A:LYS:HD2	12	0.3
(1,2216)	1:367:A:ASP:HB2	1:370:A:LYS:HD3	12	0.3
(1,2216)	1:367:A:ASP:HB3	1:370:A:LYS:HD2	12	0.3
(1,2216)	1:367:A:ASP:HB3	1:370:A:LYS:HD3	12	0.3
(1,2181)	1:364:A:ALA:HA	1:371:A:TYR:HD1	7	0.3
(1,2181)	1:364:A:ALA:HA	1:371:A:TYR:HD2	7	0.3
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG2	17	0.3
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG3	17	0.3
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG2	17	0.3
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG3	17	0.3
(1,2108)	1:360:A:LEU:HD21	1:364:A:ALA:H	4	0.3
(1,2108)	1:360:A:LEU:HD22	1:364:A:ALA:H	4	0.3
(1,2108)	1:360:A:LEU:HD23	1:364:A:ALA:H	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2045)	1:357:A:LEU:HD21	1:395:A:ALA:H	3	0.3
(1,2045)	1:357:A:LEU:HD22	1:395:A:ALA:H	3	0.3
(1,2045)	1:357:A:LEU:HD23	1:395:A:ALA:H	3	0.3
(1,2042)	1:357:A:LEU:HD21	1:396:A:ILE:HA	2	0.3
(1,2042)	1:357:A:LEU:HD22	1:396:A:ILE:HA	2	0.3
(1,2042)	1:357:A:LEU:HD23	1:396:A:ILE:HA	2	0.3
(1,1973)	1:353:A:THR:HG21	1:392:A:ASN:HB2	2	0.3
(1,1973)	1:353:A:THR:HG21	1:392:A:ASN:HB3	2	0.3
(1,1973)	1:353:A:THR:HG22	1:392:A:ASN:HB2	2	0.3
(1,1973)	1:353:A:THR:HG22	1:392:A:ASN:HB3	2	0.3
(1,1973)	1:353:A:THR:HG23	1:392:A:ASN:HB2	2	0.3
(1,1973)	1:353:A:THR:HG23	1:392:A:ASN:HB3	2	0.3
(1,1938)	1:350:A:ASN:HA	1:353:A:THR:HB	10	0.3
(1,1909)	1:348:A:LEU:HA	1:352:A:LEU:H	8	0.3
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	11	0.3
(1,1626)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	13	0.3
(1,1478)	1:314:A:MET:HE1	1:349:A:ARG:HA	2	0.3
(1,1478)	1:314:A:MET:HE2	1:349:A:ARG:HA	2	0.3
(1,1478)	1:314:A:MET:HE3	1:349:A:ARG:HA	2	0.3
(1,1416)	1:312:A:GLN:HB2	1:349:A:ARG:HD2	12	0.3
(1,1416)	1:312:A:GLN:HB2	1:349:A:ARG:HD3	12	0.3
(1,1416)	1:312:A:GLN:HB3	1:349:A:ARG:HD2	12	0.3
(1,1416)	1:312:A:GLN:HB3	1:349:A:ARG:HD3	12	0.3
(1,1354)	1:305:A:PHE:HE2	1:307:A:MET:HA	9	0.3
(1,1324)	1:302:A:GLN:H	1:327:A:SER:H	3	0.3
(1,1322)	1:302:A:GLN:HG2	1:328:A:SER:HA	16	0.3
(1,1322)	1:302:A:GLN:HG3	1:328:A:SER:HA	16	0.3
(1,1321)	1:302:A:GLN:HA	1:328:A:SER:HA	15	0.3
(1,1139)	1:297:A:LEU:H	1:309:A:ASP:HA	16	0.3
(1,1130)	1:297:A:LEU:H	1:311:A:GLU:HA	7	0.3
(1,1072)	1:295:A:HIS:HE1	1:311:A:GLU:HA	10	0.3
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	3	0.3
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	3	0.3
(1,1066)	1:295:A:HIS:HB2	1:320:A:PHE:HA	8	0.3
(1,1066)	1:295:A:HIS:HB3	1:320:A:PHE:HA	8	0.3
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD2	11	0.3
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD3	11	0.3
(1,1024)	1:289:A:TRP:HH2	1:381:A:VAL:HA	10	0.3
(1,1013)	1:288:A:MET:HA	1:294:A:LYS:H	2	0.3
(1,949)	1:284:A:ALA:HA	1:288:A:MET:HE1	9	0.3
(1,949)	1:284:A:ALA:HA	1:288:A:MET:HE2	9	0.3
(1,949)	1:284:A:ALA:HA	1:288:A:MET:HE3	9	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	6	0.3
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	6	0.3
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	6	0.3
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	10	0.3
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	10	0.3
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	19	0.3
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	19	0.3
(1,723)	1:274:A:TYR:H	1:328:A:SER:H	8	0.3
(1,675)	1:270:A:GLY:H	1:272:A:GLN:H	16	0.3
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	20	0.3
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	20	0.3
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB2	6	0.3
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB3	6	0.3
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB2	6	0.3
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB3	6	0.3
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB2	6	0.3
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB3	6	0.3
(1,376)	1:251:A:LYS:HG2	1:257:A:PHE:HA	14	0.3
(1,376)	1:251:A:LYS:HG3	1:257:A:PHE:HA	14	0.3
(1,374)	1:251:A:LYS:HA	1:257:A:PHE:HA	15	0.3
(1,293)	1:248:A:GLU:HA	1:251:A:LYS:H	2	0.3
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	1	0.3
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	13	0.3
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	18	0.3
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	15	0.3
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	15	0.3
(1,144)	1:237:A:ASN:HD21	1:238:A:LYS:H	14	0.3
(1,144)	1:237:A:ASN:HD22	1:238:A:LYS:H	14	0.3
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG21	2	0.3
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG22	2	0.3
(1,11)	1:231:A:GLN:HG2	1:235:A:THR:HG23	2	0.3
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG21	2	0.3
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG22	2	0.3
(1,11)	1:231:A:GLN:HG3	1:235:A:THR:HG23	2	0.3
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	4	0.3
(2,14)	1:442:A:LYS:H	1:461:A:SER:HB2	3	0.29
(2,14)	1:442:A:LYS:H	1:461:A:SER:HB3	3	0.29
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	1	0.29
(1,3938)	1:490:A:LEU:HA	1:493:A:LEU:H	14	0.29
(1,3936)	1:490:A:LEU:HB2	1:494:A:ALA:H	10	0.29
(1,3936)	1:490:A:LEU:HB3	1:494:A:ALA:H	10	0.29
(1,3935)	1:490:A:LEU:HA	1:494:A:ALA:H	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3886)	1:486:A:VAL:HG11	1:494:A:ALA:HB1	14	0.29
(1,3886)	1:486:A:VAL:HG11	1:494:A:ALA:HB2	14	0.29
(1,3886)	1:486:A:VAL:HG11	1:494:A:ALA:HB3	14	0.29
(1,3886)	1:486:A:VAL:HG12	1:494:A:ALA:HB1	14	0.29
(1,3886)	1:486:A:VAL:HG12	1:494:A:ALA:HB2	14	0.29
(1,3886)	1:486:A:VAL:HG12	1:494:A:ALA:HB3	14	0.29
(1,3886)	1:486:A:VAL:HG13	1:494:A:ALA:HB1	14	0.29
(1,3886)	1:486:A:VAL:HG13	1:494:A:ALA:HB2	14	0.29
(1,3886)	1:486:A:VAL:HG13	1:494:A:ALA:HB3	14	0.29
(1,3740)	1:469:A:MET:HE1	1:473:A:THR:H	3	0.29
(1,3740)	1:469:A:MET:HE2	1:473:A:THR:H	3	0.29
(1,3740)	1:469:A:MET:HE3	1:473:A:THR:H	3	0.29
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	4	0.29
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	4	0.29
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	4	0.29
(1,3523)	1:448:A:GLU:HA	1:451:A:ARG:HB2	16	0.29
(1,3523)	1:448:A:GLU:HA	1:451:A:ARG:HB3	16	0.29
(1,3522)	1:448:A:GLU:HA	1:451:A:ARG:H	16	0.29
(1,3476)	1:445:A:PRO:HG2	1:446:A:HIS:H	14	0.29
(1,3476)	1:445:A:PRO:HG3	1:446:A:HIS:H	14	0.29
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD11	1	0.29
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD12	1	0.29
(1,3447)	1:442:A:LYS:HA	1:447:A:LEU:HD13	1	0.29
(1,3235)	1:432:A:TYR:H	1:482:A:SER:HA	2	0.29
(1,3226)	1:431:A:TYR:HD1	1:450:A:LEU:HD12	17	0.29
(1,3222)	1:431:A:TYR:HD1	1:456:A:GLU:H	6	0.29
(1,3222)	1:431:A:TYR:HD2	1:456:A:GLU:H	6	0.29
(1,3165)	1:429:A:LYS:HB2	1:431:A:TYR:HE1	14	0.29
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG2	12	0.29
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG3	12	0.29
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG2	12	0.29
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG3	12	0.29
(1,3144)	1:429:A:LYS:HD2	1:489:A:SER:HA	11	0.29
(1,3144)	1:429:A:LYS:HD3	1:489:A:SER:HA	11	0.29
(1,3090)	1:424:A:LYS:HE2	1:455:A:ILE:HA	1	0.29
(1,3090)	1:424:A:LYS:HE3	1:455:A:ILE:HA	1	0.29
(1,2986)	1:417:A:GLU:HA	1:421:A:SER:HB2	4	0.29
(1,2986)	1:417:A:GLU:HA	1:421:A:SER:HB3	4	0.29
(1,2968)	1:416:A:LEU:HA	1:420:A:VAL:H	10	0.29
(1,2838)	1:405:A:THR:H	1:459:A:LEU:H	2	0.29
(1,2828)	1:404:A:SER:H	1:412:A:GLN:HA	1	0.29
(1,2818)	1:404:A:SER:HA	1:456:A:GLU:HG2	16	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2818)	1:404:A:SER:HA	1:456:A:GLU:HG3	16	0.29
(1,2767)	1:402:A:PHE:H	1:413:A:THR:H	14	0.29
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG11	8	0.29
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG12	8	0.29
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG13	8	0.29
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG11	8	0.29
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG12	8	0.29
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG13	8	0.29
(1,2620)	1:393:A:GLN:HE21	1:474:A:GLU:HB2	5	0.29
(1,2620)	1:393:A:GLN:HE21	1:474:A:GLU:HB3	5	0.29
(1,2620)	1:393:A:GLN:HE22	1:474:A:GLU:HB2	5	0.29
(1,2620)	1:393:A:GLN:HE22	1:474:A:GLU:HB3	5	0.29
(1,2575)	1:388:A:GLU:HA	1:390:A:PHE:H	6	0.29
(1,2562)	1:387:A:ALA:HB1	1:471:A:TYR:HD1	17	0.29
(1,2562)	1:387:A:ALA:HB1	1:471:A:TYR:HD2	17	0.29
(1,2562)	1:387:A:ALA:HB2	1:471:A:TYR:HD1	17	0.29
(1,2562)	1:387:A:ALA:HB2	1:471:A:TYR:HD2	17	0.29
(1,2562)	1:387:A:ALA:HB3	1:471:A:TYR:HD1	17	0.29
(1,2562)	1:387:A:ALA:HB3	1:471:A:TYR:HD2	17	0.29
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB2	17	0.29
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB3	17	0.29
(1,2432)	1:380:A:LEU:HA	1:384:A:GLU:H	3	0.29
(1,2398)	1:378:A:PHE:HA	1:382:A:LEU:H	6	0.29
(1,2398)	1:378:A:PHE:HA	1:382:A:LEU:H	13	0.29
(1,2398)	1:378:A:PHE:HA	1:382:A:LEU:H	17	0.29
(1,2359)	1:375:A:TRP:HH2	1:383:A:LYS:HG2	5	0.29
(1,2359)	1:375:A:TRP:HH2	1:383:A:LYS:HG3	5	0.29
(1,2317)	1:374:A:PHE:HZ	1:382:A:LEU:H	4	0.29
(1,2045)	1:357:A:LEU:HD21	1:395:A:ALA:H	6	0.29
(1,2045)	1:357:A:LEU:HD22	1:395:A:ALA:H	6	0.29
(1,2045)	1:357:A:LEU:HD23	1:395:A:ALA:H	6	0.29
(1,2042)	1:357:A:LEU:HD21	1:396:A:ILE:HA	13	0.29
(1,2042)	1:357:A:LEU:HD22	1:396:A:ILE:HA	13	0.29
(1,2042)	1:357:A:LEU:HD23	1:396:A:ILE:HA	13	0.29
(1,2041)	1:357:A:LEU:HD21	1:396:A:ILE:H	2	0.29
(1,2041)	1:357:A:LEU:HD22	1:396:A:ILE:H	2	0.29
(1,2041)	1:357:A:LEU:HD23	1:396:A:ILE:H	2	0.29
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD11	1	0.29
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD12	1	0.29
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD13	1	0.29
(1,1897)	1:347:A:ASN:HA	1:351:A:ALA:H	3	0.29
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	12	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD11	13	0.29
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD12	13	0.29
(1,1754)	1:334:A:VAL:HA	1:338:A:ILE:HD13	13	0.29
(1,1508)	1:315:A:PRO:HA	1:349:A:ARG:HG2	15	0.29
(1,1508)	1:315:A:PRO:HA	1:349:A:ARG:HG3	15	0.29
(1,1493)	1:314:A:MET:HB2	1:316:A:ASN:HA	8	0.29
(1,1493)	1:314:A:MET:HB3	1:316:A:ASN:HA	8	0.29
(1,1446)	1:313:A:PHE:HA	1:349:A:ARG:HA	18	0.29
(1,1415)	1:312:A:GLN:HA	1:349:A:ARG:HD2	12	0.29
(1,1415)	1:312:A:GLN:HA	1:349:A:ARG:HD3	12	0.29
(1,1367)	1:307:A:MET:HE1	1:339:A:LEU:H	11	0.29
(1,1367)	1:307:A:MET:HE2	1:339:A:LEU:H	11	0.29
(1,1367)	1:307:A:MET:HE3	1:339:A:LEU:H	11	0.29
(1,1367)	1:307:A:MET:HE1	1:339:A:LEU:H	12	0.29
(1,1367)	1:307:A:MET:HE2	1:339:A:LEU:H	12	0.29
(1,1367)	1:307:A:MET:HE3	1:339:A:LEU:H	12	0.29
(1,1298)	1:301:A:VAL:H	1:306:A:ILE:HB	13	0.29
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD11	7	0.29
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD12	7	0.29
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD13	7	0.29
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD11	14	0.29
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD12	14	0.29
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD13	14	0.29
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HA	6	0.29
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HA	16	0.29
(1,1008)	1:288:A:MET:HE1	1:320:A:PHE:HB2	9	0.29
(1,1008)	1:288:A:MET:HE1	1:320:A:PHE:HB3	9	0.29
(1,1008)	1:288:A:MET:HE2	1:320:A:PHE:HB2	9	0.29
(1,1008)	1:288:A:MET:HE2	1:320:A:PHE:HB3	9	0.29
(1,1008)	1:288:A:MET:HE3	1:320:A:PHE:HB2	9	0.29
(1,1008)	1:288:A:MET:HE3	1:320:A:PHE:HB3	9	0.29
(1,936)	1:284:A:ALA:HA	1:378:A:PHE:HZ	16	0.29
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	5	0.29
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	5	0.29
(1,720)	1:274:A:TYR:HB2	1:330:A:LEU:HD11	5	0.29
(1,720)	1:274:A:TYR:HB2	1:330:A:LEU:HD12	5	0.29
(1,720)	1:274:A:TYR:HB2	1:330:A:LEU:HD13	5	0.29
(1,720)	1:274:A:TYR:HB3	1:330:A:LEU:HD11	5	0.29
(1,720)	1:274:A:TYR:HB3	1:330:A:LEU:HD12	5	0.29
(1,720)	1:274:A:TYR:HB3	1:330:A:LEU:HD13	5	0.29
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	13	0.29
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	11	0.29
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	3	0.29
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	6	0.29
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	6	0.29
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD1	7	0.29
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD2	7	0.29
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	5	0.29
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	5	0.29
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD2	20	0.29
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD3	20	0.29
(1,293)	1:248:A:GLU:HA	1:251:A:LYS:H	5	0.29
(1,219)	1:244:A:GLU:HA	1:248:A:GLU:H	9	0.29
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	12	0.29
(1,158)	1:238:A:LYS:HA	1:241:A:ILE:HB	12	0.29
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD2	7	0.29
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD3	7	0.29
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	9	0.29
(1,3936)	1:490:A:LEU:HB2	1:494:A:ALA:H	20	0.28
(1,3936)	1:490:A:LEU:HB3	1:494:A:ALA:H	20	0.28
(1,3927)	1:489:A:SER:HB2	1:493:A:LEU:HD11	15	0.28
(1,3927)	1:489:A:SER:HB2	1:493:A:LEU:HD12	15	0.28
(1,3927)	1:489:A:SER:HB2	1:493:A:LEU:HD13	15	0.28
(1,3927)	1:489:A:SER:HB3	1:493:A:LEU:HD11	15	0.28
(1,3927)	1:489:A:SER:HB3	1:493:A:LEU:HD12	15	0.28
(1,3927)	1:489:A:SER:HB3	1:493:A:LEU:HD13	15	0.28
(1,3857)	1:481:A:GLN:HE21	1:482:A:SER:H	2	0.28
(1,3857)	1:481:A:GLN:HE22	1:482:A:SER:H	2	0.28
(1,3848)	1:481:A:GLN:HG2	1:486:A:VAL:HA	15	0.28
(1,3848)	1:481:A:GLN:HG3	1:486:A:VAL:HA	15	0.28
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	17	0.28
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	17	0.28
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	17	0.28
(1,3674)	1:462:A:ASP:HB2	1:464:A:ILE:H	11	0.28
(1,3674)	1:462:A:ASP:HB3	1:464:A:ILE:H	11	0.28
(1,3567)	1:450:A:LEU:HA	1:454:A:GLY:H	20	0.28
(1,3360)	1:437:A:SER:HA	1:462:A:ASP:HA	1	0.28
(1,3353)	1:436:A:ASP:HA	1:461:A:SER:HA	4	0.28
(1,3235)	1:432:A:TYR:H	1:482:A:SER:HA	14	0.28
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD11	10	0.28
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD12	10	0.28
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD13	10	0.28
(1,3165)	1:429:A:LYS:HB2	1:431:A:TYR:HE2	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3144)	1:429:A:LYS:HD2	1:489:A:SER:HA	15	0.28
(1,3144)	1:429:A:LYS:HD3	1:489:A:SER:HA	15	0.28
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG2	17	0.28
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG3	17	0.28
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG2	17	0.28
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG3	17	0.28
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD11	10	0.28
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD12	10	0.28
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD13	10	0.28
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD11	18	0.28
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD12	18	0.28
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD13	18	0.28
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE21	14	0.28
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE22	14	0.28
(1,3081)	1:423:A:MET:HE1	1:427:A:GLN:HB2	15	0.28
(1,3081)	1:423:A:MET:HE1	1:427:A:GLN:HB3	15	0.28
(1,3081)	1:423:A:MET:HE2	1:427:A:GLN:HB2	15	0.28
(1,3081)	1:423:A:MET:HE2	1:427:A:GLN:HB3	15	0.28
(1,3081)	1:423:A:MET:HE3	1:427:A:GLN:HB2	15	0.28
(1,3081)	1:423:A:MET:HE3	1:427:A:GLN:HB3	15	0.28
(1,2989)	1:417:A:GLU:HA	1:420:A:VAL:HB	5	0.28
(1,2989)	1:417:A:GLU:HA	1:420:A:VAL:HB	11	0.28
(1,2986)	1:417:A:GLU:HA	1:421:A:SER:HB2	17	0.28
(1,2986)	1:417:A:GLU:HA	1:421:A:SER:HB3	17	0.28
(1,2984)	1:417:A:GLU:HA	1:421:A:SER:H	2	0.28
(1,2982)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	11	0.28
(1,2982)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	11	0.28
(1,2940)	1:414:A:VAL:HG21	1:418:A:ASP:HB2	8	0.28
(1,2940)	1:414:A:VAL:HG21	1:418:A:ASP:HB3	8	0.28
(1,2940)	1:414:A:VAL:HG22	1:418:A:ASP:HB2	8	0.28
(1,2940)	1:414:A:VAL:HG22	1:418:A:ASP:HB3	8	0.28
(1,2940)	1:414:A:VAL:HG23	1:418:A:ASP:HB2	8	0.28
(1,2940)	1:414:A:VAL:HG23	1:418:A:ASP:HB3	8	0.28
(1,2937)	1:414:A:VAL:HG21	1:419:A:TYR:HA	6	0.28
(1,2937)	1:414:A:VAL:HG22	1:419:A:TYR:HA	6	0.28
(1,2937)	1:414:A:VAL:HG23	1:419:A:TYR:HA	6	0.28
(1,2848)	1:405:A:THR:H	1:457:A:VAL:HB	5	0.28
(1,2838)	1:405:A:THR:H	1:459:A:LEU:H	15	0.28
(1,2814)	1:404:A:SER:HA	1:457:A:VAL:H	13	0.28
(1,2793)	1:403:A:ALA:H	1:413:A:THR:H	14	0.28
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG11	4	0.28
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG12	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG13	4	0.28
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG11	17	0.28
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG12	17	0.28
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG13	17	0.28
(1,2764)	1:402:A:PHE:H	1:414:A:VAL:HB	20	0.28
(1,2755)	1:402:A:PHE:HD2	1:460:A:LEU:HD13	4	0.28
(1,2755)	1:402:A:PHE:HD1	1:460:A:LEU:HD13	16	0.28
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	7	0.28
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	7	0.28
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	7	0.28
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	20	0.28
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	20	0.28
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	20	0.28
(1,2736)	1:401:A:ARG:HD2	1:414:A:VAL:H	9	0.28
(1,2736)	1:401:A:ARG:HD3	1:414:A:VAL:H	9	0.28
(1,2640)	1:394:A:GLU:HA	1:475:A:PHE:HA	6	0.28
(1,2575)	1:388:A:GLU:HA	1:390:A:PHE:H	19	0.28
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB2	9	0.28
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB3	9	0.28
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB2	15	0.28
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB3	15	0.28
(1,2436)	1:380:A:LEU:HA	1:383:A:LYS:HD2	2	0.28
(1,2436)	1:380:A:LEU:HA	1:383:A:LYS:HD3	2	0.28
(1,2425)	1:380:A:LEU:HB2	1:464:A:ILE:H	3	0.28
(1,2425)	1:380:A:LEU:HB3	1:464:A:ILE:H	3	0.28
(1,2368)	1:375:A:TRP:HZ2	1:379:A:GLY:HA2	2	0.28
(1,2368)	1:375:A:TRP:HZ2	1:379:A:GLY:HA3	2	0.28
(1,2337)	1:375:A:TRP:HD1	1:413:A:THR:HA	7	0.28
(1,2323)	1:374:A:PHE:HZ	1:378:A:PHE:HB2	14	0.28
(1,2323)	1:374:A:PHE:HZ	1:378:A:PHE:HB3	14	0.28
(1,2231)	1:368:A:ALA:HA	1:370:A:LYS:H	12	0.28
(1,2123)	1:361:A:GLU:HA	1:399:A:LEU:HA	16	0.28
(1,2042)	1:357:A:LEU:HD21	1:396:A:ILE:HA	17	0.28
(1,2042)	1:357:A:LEU:HD22	1:396:A:ILE:HA	17	0.28
(1,2042)	1:357:A:LEU:HD23	1:396:A:ILE:HA	17	0.28
(1,1992)	1:354:A:LYS:HG2	1:392:A:ASN:HD21	1	0.28
(1,1992)	1:354:A:LYS:HG2	1:392:A:ASN:HD22	1	0.28
(1,1992)	1:354:A:LYS:HG3	1:392:A:ASN:HD21	1	0.28
(1,1992)	1:354:A:LYS:HG3	1:392:A:ASN:HD22	1	0.28
(1,1938)	1:350:A:ASN:HA	1:353:A:THR:HB	12	0.28
(1,1937)	1:350:A:ASN:HA	1:353:A:THR:H	15	0.28
(1,1767)	1:335:A:SER:H	1:338:A:ILE:HB	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1726)	1:331:A:PRO:HB2	1:338:A:ILE:HB	18	0.28
(1,1726)	1:331:A:PRO:HB3	1:338:A:ILE:HB	18	0.28
(1,1487)	1:314:A:MET:HB2	1:319:A:ARG:HA	14	0.28
(1,1487)	1:314:A:MET:HB3	1:319:A:ARG:HA	14	0.28
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG21	8	0.28
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG22	8	0.28
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG23	8	0.28
(1,1349)	1:305:A:PHE:HZ	1:308:A:ASP:HA	1	0.28
(1,1255)	1:300:A:TYR:HA	1:306:A:ILE:HB	6	0.28
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD11	1	0.28
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD12	1	0.28
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD13	1	0.28
(1,1154)	1:298:A:LYS:HB2	1:324:A:LEU:HB2	5	0.28
(1,1154)	1:298:A:LYS:HB2	1:324:A:LEU:HB3	5	0.28
(1,1154)	1:298:A:LYS:HB3	1:324:A:LEU:HB2	5	0.28
(1,1154)	1:298:A:LYS:HB3	1:324:A:LEU:HB3	5	0.28
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HA	1	0.28
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD2	5	0.28
(1,1058)	1:294:A:LYS:H	1:319:A:ARG:HD3	5	0.28
(1,1053)	1:293:A:HIS:HB2	1:295:A:HIS:H	11	0.28
(1,1053)	1:293:A:HIS:HB3	1:295:A:HIS:H	11	0.28
(1,1003)	1:288:A:MET:HG2	1:381:A:VAL:HG21	1	0.28
(1,1003)	1:288:A:MET:HG2	1:381:A:VAL:HG22	1	0.28
(1,1003)	1:288:A:MET:HG2	1:381:A:VAL:HG23	1	0.28
(1,1003)	1:288:A:MET:HG3	1:381:A:VAL:HG21	1	0.28
(1,1003)	1:288:A:MET:HG3	1:381:A:VAL:HG22	1	0.28
(1,1003)	1:288:A:MET:HG3	1:381:A:VAL:HG23	1	0.28
(1,958)	1:285:A:PRO:HG2	1:320:A:PHE:HA	17	0.28
(1,958)	1:285:A:PRO:HG3	1:320:A:PHE:HA	17	0.28
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	14	0.28
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	20	0.28
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	20	0.28
(1,719)	1:274:A:TYR:HD2	1:348:A:LEU:HD22	15	0.28
(1,684)	1:272:A:GLN:HE21	1:351:A:ALA:H	19	0.28
(1,684)	1:272:A:GLN:HE22	1:351:A:ALA:H	19	0.28
(1,653)	1:268:A:VAL:HB	1:273:A:GLU:HA	6	0.28
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	4	0.28
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	4	0.28
(1,600)	1:265:A:HIS:HA	1:276:A:SER:H	1	0.28
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD21	2	0.28
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD22	2	0.28
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	4	0.28
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	14	0.28
(1,447)	1:256:A:ASP:HA	1:258:A:ASN:HD21	14	0.28
(1,447)	1:256:A:ASP:HA	1:258:A:ASN:HD22	14	0.28
(1,376)	1:251:A:LYS:HG2	1:257:A:PHE:HA	10	0.28
(1,376)	1:251:A:LYS:HG3	1:257:A:PHE:HA	10	0.28
(1,376)	1:251:A:LYS:HG2	1:257:A:PHE:HA	12	0.28
(1,376)	1:251:A:LYS:HG3	1:257:A:PHE:HA	12	0.28
(1,353)	1:250:A:TYR:HE1	1:256:A:ASP:HB2	18	0.28
(1,353)	1:250:A:TYR:HE1	1:256:A:ASP:HB3	18	0.28
(1,353)	1:250:A:TYR:HE2	1:256:A:ASP:HB2	18	0.28
(1,353)	1:250:A:TYR:HE2	1:256:A:ASP:HB3	18	0.28
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	10	0.28
(1,109)	1:235:A:THR:HA	1:267:A:ARG:HD2	8	0.28
(1,109)	1:235:A:THR:HA	1:267:A:ARG:HD3	8	0.28
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	14	0.27
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	18	0.27
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	2	0.27
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE2	10	0.27
(1,3851)	1:481:A:GLN:HE21	1:485:A:LYS:HE3	10	0.27
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE2	10	0.27
(1,3851)	1:481:A:GLN:HE22	1:485:A:LYS:HE3	10	0.27
(1,3848)	1:481:A:GLN:HG2	1:486:A:VAL:HA	11	0.27
(1,3848)	1:481:A:GLN:HG3	1:486:A:VAL:HA	11	0.27
(1,3846)	1:481:A:GLN:HE21	1:486:A:VAL:H	3	0.27
(1,3846)	1:481:A:GLN:HE22	1:486:A:VAL:H	3	0.27
(1,3772)	1:472:A:LEU:HD21	1:474:A:GLU:HA	1	0.27
(1,3772)	1:472:A:LEU:HD22	1:474:A:GLU:HA	1	0.27
(1,3772)	1:472:A:LEU:HD23	1:474:A:GLU:HA	1	0.27
(1,3726)	1:468:A:MET:HG2	1:472:A:LEU:HB2	13	0.27
(1,3726)	1:468:A:MET:HG2	1:472:A:LEU:HB3	13	0.27
(1,3726)	1:468:A:MET:HG3	1:472:A:LEU:HB2	13	0.27
(1,3726)	1:468:A:MET:HG3	1:472:A:LEU:HB3	13	0.27
(1,3538)	1:449:A:LEU:HD11	1:453:A:LYS:HB2	4	0.27
(1,3538)	1:449:A:LEU:HD11	1:453:A:LYS:HB3	4	0.27
(1,3538)	1:449:A:LEU:HD12	1:453:A:LYS:HB2	4	0.27
(1,3538)	1:449:A:LEU:HD12	1:453:A:LYS:HB3	4	0.27
(1,3538)	1:449:A:LEU:HD13	1:453:A:LYS:HB2	4	0.27
(1,3538)	1:449:A:LEU:HD13	1:453:A:LYS:HB3	4	0.27
(1,3483)	1:446:A:HIS:HB2	1:483:A:VAL:HB	13	0.27
(1,3483)	1:446:A:HIS:HB3	1:483:A:VAL:HB	13	0.27
(1,3354)	1:436:A:ASP:H	1:441:A:ALA:H	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3208)	1:431:A:TYR:HB2	1:482:A:SER:HA	20	0.27
(1,3208)	1:431:A:TYR:HB3	1:482:A:SER:HA	20	0.27
(1,3162)	1:429:A:LYS:HA	1:478:A:LYS:HG2	19	0.27
(1,3162)	1:429:A:LYS:HA	1:478:A:LYS:HG3	19	0.27
(1,3076)	1:423:A:MET:HE1	1:429:A:LYS:H	19	0.27
(1,3076)	1:423:A:MET:HE2	1:429:A:LYS:H	19	0.27
(1,3076)	1:423:A:MET:HE3	1:429:A:LYS:H	19	0.27
(1,2984)	1:417:A:GLU:HA	1:421:A:SER:H	16	0.27
(1,2824)	1:404:A:SER:H	1:414:A:VAL:HB	1	0.27
(1,2797)	1:403:A:ALA:HA	1:412:A:GLN:HA	14	0.27
(1,2764)	1:402:A:PHE:H	1:414:A:VAL:HB	15	0.27
(1,2719)	1:400:A:LEU:H	1:416:A:LEU:H	18	0.27
(1,2699)	1:398:A:LYS:HE2	1:417:A:GLU:HG2	18	0.27
(1,2699)	1:398:A:LYS:HE2	1:417:A:GLU:HG3	18	0.27
(1,2699)	1:398:A:LYS:HE3	1:417:A:GLU:HG2	18	0.27
(1,2699)	1:398:A:LYS:HE3	1:417:A:GLU:HG3	18	0.27
(1,2508)	1:384:A:GLU:HA	1:464:A:ILE:HD11	11	0.27
(1,2508)	1:384:A:GLU:HA	1:464:A:ILE:HD12	11	0.27
(1,2508)	1:384:A:GLU:HA	1:464:A:ILE:HD13	11	0.27
(1,2341)	1:375:A:TRP:HE1	1:412:A:GLN:HE21	5	0.27
(1,2341)	1:375:A:TRP:HE1	1:412:A:GLN:HE22	5	0.27
(1,2337)	1:375:A:TRP:HD1	1:413:A:THR:HA	1	0.27
(1,2288)	1:372:A:GLN:HE21	1:376:A:GLN:H	10	0.27
(1,2288)	1:372:A:GLN:HE22	1:376:A:GLN:H	10	0.27
(1,2227)	1:368:A:ALA:HA	1:371:A:TYR:H	4	0.27
(1,2203)	1:365:A:LYS:HA	1:367:A:ASP:H	7	0.27
(1,2166)	1:363:A:LEU:HA	1:367:A:ASP:HB2	9	0.27
(1,2166)	1:363:A:LEU:HA	1:367:A:ASP:HB3	9	0.27
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG2	3	0.27
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG3	3	0.27
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG2	3	0.27
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG3	3	0.27
(1,2041)	1:357:A:LEU:HD21	1:396:A:ILE:H	18	0.27
(1,2041)	1:357:A:LEU:HD22	1:396:A:ILE:H	18	0.27
(1,2041)	1:357:A:LEU:HD23	1:396:A:ILE:H	18	0.27
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE21	1	0.27
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE22	1	0.27
(1,1994)	1:354:A:LYS:HA	1:358:A:GLN:H	2	0.27
(1,1989)	1:354:A:LYS:HA	1:392:A:ASN:HD21	15	0.27
(1,1989)	1:354:A:LYS:HA	1:392:A:ASN:HD22	15	0.27
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE1	5	0.27
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE2	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE3	5	0.27
(1,1490)	1:314:A:MET:HB2	1:318:A:LEU:H	3	0.27
(1,1490)	1:314:A:MET:HB3	1:318:A:LEU:H	3	0.27
(1,1471)	1:314:A:MET:HA	1:353:A:THR:H	6	0.27
(1,1318)	1:302:A:GLN:H	1:329:A:ASP:H	20	0.27
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE1	2	0.27
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE2	2	0.27
(1,1139)	1:297:A:LEU:H	1:309:A:ASP:HA	11	0.27
(1,1037)	1:290:A:ASN:HB2	1:292:A:ASP:H	16	0.27
(1,1037)	1:290:A:ASN:HB3	1:292:A:ASP:H	16	0.27
(1,1022)	1:289:A:TRP:HH2	1:381:A:VAL:H	14	0.27
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	8	0.27
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	11	0.27
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD21	15	0.27
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD22	15	0.27
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	5	0.27
(1,970)	1:285:A:PRO:HG2	1:287:A:ASP:H	7	0.27
(1,970)	1:285:A:PRO:HG3	1:287:A:ASP:H	7	0.27
(1,764)	1:276:A:SER:HB2	1:326:A:ASP:H	17	0.27
(1,764)	1:276:A:SER:HB3	1:326:A:ASP:H	17	0.27
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB2	6	0.27
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB3	6	0.27
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	7	0.27
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD1	8	0.27
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD2	8	0.27
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	9	0.27
(1,457)	1:258:A:ASN:HD21	1:283:A:GLN:HB2	19	0.27
(1,457)	1:258:A:ASN:HD21	1:283:A:GLN:HB3	19	0.27
(1,457)	1:258:A:ASN:HD22	1:283:A:GLN:HB2	19	0.27
(1,457)	1:258:A:ASN:HD22	1:283:A:GLN:HB3	19	0.27
(1,423)	1:254:A:ALA:HA	1:323:A:GLY:H	3	0.27
(1,376)	1:251:A:LYS:HG2	1:257:A:PHE:HA	8	0.27
(1,376)	1:251:A:LYS:HG3	1:257:A:PHE:HA	8	0.27
(1,371)	1:251:A:LYS:HE2	1:259:A:ASP:HA	1	0.27
(1,371)	1:251:A:LYS:HE3	1:259:A:ASP:HA	1	0.27
(1,296)	1:248:A:GLU:HA	1:251:A:LYS:HE2	13	0.27
(1,296)	1:248:A:GLU:HA	1:251:A:LYS:HE3	13	0.27
(1,293)	1:248:A:GLU:HA	1:251:A:LYS:H	1	0.27
(1,293)	1:248:A:GLU:HA	1:251:A:LYS:H	13	0.27
(1,208)	1:243:A:ASP:HB2	1:247:A:LYS:HD2	4	0.27
(1,208)	1:243:A:ASP:HB2	1:247:A:LYS:HD3	4	0.27
(1,208)	1:243:A:ASP:HB3	1:247:A:LYS:HD2	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,208)	1:243:A:ASP:HB3	1:247:A:LYS:HD3	4	0.27
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	3	0.27
(1,174)	1:240:A:GLU:HA	1:242:A:THR:H	11	0.27
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	3	0.27
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD11	7	0.27
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD12	7	0.27
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD13	7	0.27
(1,8)	1:231:A:GLN:HG2	1:236:A:ARG:HG2	20	0.27
(1,8)	1:231:A:GLN:HG2	1:236:A:ARG:HG3	20	0.27
(1,8)	1:231:A:GLN:HG3	1:236:A:ARG:HG2	20	0.27
(1,8)	1:231:A:GLN:HG3	1:236:A:ARG:HG3	20	0.27
(1,5)	1:231:A:GLN:HG2	1:236:A:ARG:H	11	0.27
(1,5)	1:231:A:GLN:HG3	1:236:A:ARG:H	11	0.27
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB1	9	0.26
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB2	9	0.26
(1,3982)	1:450:A:LEU:HD21	2:640:B:ALA:HB3	9	0.26
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB1	9	0.26
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB2	9	0.26
(1,3982)	1:450:A:LEU:HD22	2:640:B:ALA:HB3	9	0.26
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB1	9	0.26
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB2	9	0.26
(1,3982)	1:450:A:LEU:HD23	2:640:B:ALA:HB3	9	0.26
(1,3936)	1:490:A:LEU:HB2	1:494:A:ALA:H	15	0.26
(1,3936)	1:490:A:LEU:HB3	1:494:A:ALA:H	15	0.26
(1,3891)	1:486:A:VAL:HG11	1:490:A:LEU:H	8	0.26
(1,3891)	1:486:A:VAL:HG12	1:490:A:LEU:H	8	0.26
(1,3891)	1:486:A:VAL:HG13	1:490:A:LEU:H	8	0.26
(1,3882)	1:485:A:LYS:HB2	1:487:A:ASP:HB3	18	0.26
(1,3857)	1:481:A:GLN:HE21	1:482:A:SER:H	15	0.26
(1,3857)	1:481:A:GLN:HE22	1:482:A:SER:H	15	0.26
(1,3772)	1:472:A:LEU:HD21	1:474:A:GLU:HA	11	0.26
(1,3772)	1:472:A:LEU:HD22	1:474:A:GLU:HA	11	0.26
(1,3772)	1:472:A:LEU:HD23	1:474:A:GLU:HA	11	0.26
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	14	0.26
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	14	0.26
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	14	0.26
(1,3674)	1:462:A:ASP:HB2	1:464:A:ILE:H	20	0.26
(1,3674)	1:462:A:ASP:HB3	1:464:A:ILE:H	20	0.26
(1,3617)	1:456:A:GLU:HG2	1:458:A:LEU:H	14	0.26
(1,3617)	1:456:A:GLU:HG3	1:458:A:LEU:H	14	0.26
(1,3538)	1:449:A:LEU:HD11	1:453:A:LYS:HB2	1	0.26
(1,3538)	1:449:A:LEU:HD11	1:453:A:LYS:HB3	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3538)	1:449:A:LEU:HD12	1:453:A:LYS:HB2	1	0.26
(1,3538)	1:449:A:LEU:HD12	1:453:A:LYS:HB3	1	0.26
(1,3538)	1:449:A:LEU:HD13	1:453:A:LYS:HB2	1	0.26
(1,3538)	1:449:A:LEU:HD13	1:453:A:LYS:HB3	1	0.26
(1,3534)	1:449:A:LEU:HD21	1:490:A:LEU:HD11	10	0.26
(1,3534)	1:449:A:LEU:HD21	1:490:A:LEU:HD12	10	0.26
(1,3534)	1:449:A:LEU:HD21	1:490:A:LEU:HD13	10	0.26
(1,3534)	1:449:A:LEU:HD22	1:490:A:LEU:HD11	10	0.26
(1,3534)	1:449:A:LEU:HD22	1:490:A:LEU:HD12	10	0.26
(1,3534)	1:449:A:LEU:HD22	1:490:A:LEU:HD13	10	0.26
(1,3534)	1:449:A:LEU:HD23	1:490:A:LEU:HD11	10	0.26
(1,3534)	1:449:A:LEU:HD23	1:490:A:LEU:HD12	10	0.26
(1,3534)	1:449:A:LEU:HD23	1:490:A:LEU:HD13	10	0.26
(1,3534)	1:449:A:LEU:HD21	1:490:A:LEU:HD21	10	0.26
(1,3534)	1:449:A:LEU:HD21	1:490:A:LEU:HD22	10	0.26
(1,3534)	1:449:A:LEU:HD21	1:490:A:LEU:HD23	10	0.26
(1,3534)	1:449:A:LEU:HD22	1:490:A:LEU:HD21	10	0.26
(1,3534)	1:449:A:LEU:HD22	1:490:A:LEU:HD22	10	0.26
(1,3534)	1:449:A:LEU:HD22	1:490:A:LEU:HD23	10	0.26
(1,3534)	1:449:A:LEU:HD23	1:490:A:LEU:HD21	10	0.26
(1,3534)	1:449:A:LEU:HD23	1:490:A:LEU:HD22	10	0.26
(1,3534)	1:449:A:LEU:HD23	1:490:A:LEU:HD23	10	0.26
(1,3488)	1:446:A:HIS:HA	1:448:A:GLU:H	12	0.26
(1,3471)	1:445:A:PRO:HA	1:448:A:GLU:HG2	8	0.26
(1,3471)	1:445:A:PRO:HA	1:448:A:GLU:HG3	8	0.26
(1,3311)	1:434:A:THR:HB	1:466:A:GLU:HA	7	0.26
(1,3225)	1:431:A:TYR:HB2	1:450:A:LEU:HD11	14	0.26
(1,3225)	1:431:A:TYR:HB2	1:450:A:LEU:HD12	14	0.26
(1,3225)	1:431:A:TYR:HB2	1:450:A:LEU:HD13	14	0.26
(1,3225)	1:431:A:TYR:HB3	1:450:A:LEU:HD11	14	0.26
(1,3225)	1:431:A:TYR:HB3	1:450:A:LEU:HD12	14	0.26
(1,3225)	1:431:A:TYR:HB3	1:450:A:LEU:HD13	14	0.26
(1,3207)	1:431:A:TYR:HA	1:482:A:SER:HA	3	0.26
(1,3206)	1:431:A:TYR:HA	1:482:A:SER:H	18	0.26
(1,3199)	1:431:A:TYR:HE1	1:489:A:SER:HA	3	0.26
(1,3199)	1:431:A:TYR:HE2	1:489:A:SER:HA	3	0.26
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB2	9	0.26
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB3	9	0.26
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB2	9	0.26
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB3	9	0.26
(1,3133)	1:428:A:GLU:HG2	1:479:A:PRO:HD2	3	0.26
(1,3133)	1:428:A:GLU:HG2	1:479:A:PRO:HD3	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3133)	1:428:A:GLU:HG3	1:479:A:PRO:HD2	3	0.26
(1,3133)	1:428:A:GLU:HG3	1:479:A:PRO:HD3	3	0.26
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	5	0.26
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	5	0.26
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	5	0.26
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	5	0.26
(1,3083)	1:423:A:MET:HB2	1:427:A:GLN:HE21	18	0.26
(1,3083)	1:423:A:MET:HB2	1:427:A:GLN:HE22	18	0.26
(1,3083)	1:423:A:MET:HB3	1:427:A:GLN:HE21	18	0.26
(1,3083)	1:423:A:MET:HB3	1:427:A:GLN:HE22	18	0.26
(1,2989)	1:417:A:GLU:HA	1:420:A:VAL:HB	6	0.26
(1,2986)	1:417:A:GLU:HA	1:421:A:SER:HB2	14	0.26
(1,2986)	1:417:A:GLU:HA	1:421:A:SER:HB3	14	0.26
(1,2883)	1:407:A:THR:HG21	1:409:A:SER:HB2	6	0.26
(1,2883)	1:407:A:THR:HG21	1:409:A:SER:HB3	6	0.26
(1,2883)	1:407:A:THR:HG22	1:409:A:SER:HB2	6	0.26
(1,2883)	1:407:A:THR:HG22	1:409:A:SER:HB3	6	0.26
(1,2883)	1:407:A:THR:HG23	1:409:A:SER:HB2	6	0.26
(1,2883)	1:407:A:THR:HG23	1:409:A:SER:HB3	6	0.26
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG11	4	0.26
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG12	4	0.26
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG13	4	0.26
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	17	0.26
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	17	0.26
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	17	0.26
(1,2736)	1:401:A:ARG:HD2	1:414:A:VAL:H	8	0.26
(1,2736)	1:401:A:ARG:HD3	1:414:A:VAL:H	8	0.26
(1,2711)	1:399:A:LEU:H	1:416:A:LEU:HD11	7	0.26
(1,2711)	1:399:A:LEU:H	1:416:A:LEU:HD12	7	0.26
(1,2711)	1:399:A:LEU:H	1:416:A:LEU:HD13	7	0.26
(1,2632)	1:393:A:GLN:HA	1:396:A:ILE:HB	6	0.26
(1,2632)	1:393:A:GLN:HA	1:396:A:ILE:HB	12	0.26
(1,2575)	1:388:A:GLU:HA	1:390:A:PHE:H	18	0.26
(1,2524)	1:385:A:GLY:HA2	1:389:A:ASP:H	19	0.26
(1,2524)	1:385:A:GLY:HA3	1:389:A:ASP:H	19	0.26
(1,2491)	1:383:A:LYS:HE2	1:401:A:ARG:H	10	0.26
(1,2491)	1:383:A:LYS:HE3	1:401:A:ARG:H	10	0.26
(1,2380)	1:376:A:GLN:HE21	1:412:A:GLN:H	12	0.26
(1,2380)	1:376:A:GLN:HE22	1:412:A:GLN:H	12	0.26
(1,2014)	1:355:A:ARG:HA	1:358:A:GLN:HB2	13	0.26
(1,2014)	1:355:A:ARG:HA	1:358:A:GLN:HB3	13	0.26
(1,1964)	1:352:A:LEU:HA	1:355:A:ARG:HD2	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1964)	1:352:A:LEU:HA	1:355:A:ARG:HD3	17	0.26
(1,1937)	1:350:A:ASN:HA	1:353:A:THR:H	8	0.26
(1,1910)	1:348:A:LEU:HD11	1:352:A:LEU:H	9	0.26
(1,1910)	1:348:A:LEU:HD12	1:352:A:LEU:H	9	0.26
(1,1910)	1:348:A:LEU:HD13	1:352:A:LEU:H	9	0.26
(1,1764)	1:335:A:SER:H	1:339:A:LEU:HD21	14	0.26
(1,1764)	1:335:A:SER:H	1:339:A:LEU:HD22	14	0.26
(1,1764)	1:335:A:SER:H	1:339:A:LEU:HD23	14	0.26
(1,1540)	1:317:A:TYR:HE1	1:392:A:ASN:HB2	10	0.26
(1,1540)	1:317:A:TYR:HE1	1:392:A:ASN:HB3	10	0.26
(1,1540)	1:317:A:TYR:HE2	1:392:A:ASN:HB2	10	0.26
(1,1540)	1:317:A:TYR:HE2	1:392:A:ASN:HB3	10	0.26
(1,1511)	1:315:A:PRO:HG2	1:319:A:ARG:H	17	0.26
(1,1511)	1:315:A:PRO:HG3	1:319:A:ARG:H	17	0.26
(1,1505)	1:315:A:PRO:HD2	1:350:A:ASN:HA	8	0.26
(1,1505)	1:315:A:PRO:HD3	1:350:A:ASN:HA	8	0.26
(1,1487)	1:314:A:MET:HB2	1:319:A:ARG:HA	17	0.26
(1,1487)	1:314:A:MET:HB3	1:319:A:ARG:HA	17	0.26
(1,1415)	1:312:A:GLN:HA	1:349:A:ARG:HD2	14	0.26
(1,1415)	1:312:A:GLN:HA	1:349:A:ARG:HD3	14	0.26
(1,1367)	1:307:A:MET:HE1	1:339:A:LEU:H	13	0.26
(1,1367)	1:307:A:MET:HE2	1:339:A:LEU:H	13	0.26
(1,1367)	1:307:A:MET:HE3	1:339:A:LEU:H	13	0.26
(1,1334)	1:303:A:ARG:H	1:327:A:SER:H	20	0.26
(1,1317)	1:302:A:GLN:HE21	1:332:A:LEU:HD21	14	0.26
(1,1317)	1:302:A:GLN:HE21	1:332:A:LEU:HD22	14	0.26
(1,1317)	1:302:A:GLN:HE21	1:332:A:LEU:HD23	14	0.26
(1,1317)	1:302:A:GLN:HE22	1:332:A:LEU:HD21	14	0.26
(1,1317)	1:302:A:GLN:HE22	1:332:A:LEU:HD22	14	0.26
(1,1317)	1:302:A:GLN:HE22	1:332:A:LEU:HD23	14	0.26
(1,1152)	1:298:A:LYS:HB2	1:324:A:LEU:HA	5	0.26
(1,1152)	1:298:A:LYS:HB3	1:324:A:LEU:HA	5	0.26
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	7	0.26
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	7	0.26
(1,1069)	1:295:A:HIS:HE1	1:316:A:ASN:HA	5	0.26
(1,1044)	1:291:A:ARG:HA	1:293:A:HIS:HA	8	0.26
(1,1010)	1:288:A:MET:HA	1:319:A:ARG:HD2	7	0.26
(1,1010)	1:288:A:MET:HA	1:319:A:ARG:HD3	7	0.26
(1,879)	1:280:A:ILE:HA	1:321:A:VAL:HA	9	0.26
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	12	0.26
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	12	0.26
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	17	0.26
(1,701)	1:273:A:GLU:H	1:329:A:ASP:HA	1	0.26
(1,680)	1:271:A:LYS:HA	1:273:A:GLU:H	6	0.26
(1,423)	1:254:A:ALA:HA	1:323:A:GLY:H	18	0.26
(1,382)	1:251:A:LYS:HA	1:255:A:HIS:HA	3	0.26
(1,218)	1:243:A:ASP:HB2	1:244:A:GLU:H	4	0.26
(1,218)	1:243:A:ASP:HB3	1:244:A:GLU:H	4	0.26
(1,130)	1:237:A:ASN:HA	1:265:A:HIS:HE1	7	0.26
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD2	12	0.26
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD3	12	0.26
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	20	0.26
(1,65)	1:234:A:TRP:HH2	1:305:A:PHE:HB2	15	0.26
(1,65)	1:234:A:TRP:HH2	1:305:A:PHE:HB3	15	0.26
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG21	14	0.25
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG22	14	0.25
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG23	14	0.25
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG21	14	0.25
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG22	14	0.25
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG23	14	0.25
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG21	14	0.25
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG22	14	0.25
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG23	14	0.25
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG11	7	0.25
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG12	7	0.25
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG13	7	0.25
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG11	7	0.25
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG12	7	0.25
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG13	7	0.25
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG11	7	0.25
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG12	7	0.25
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG13	7	0.25
(1,3922)	1:488:A:GLU:HA	1:490:A:LEU:H	19	0.25
(1,3891)	1:486:A:VAL:HG11	1:490:A:LEU:H	5	0.25
(1,3891)	1:486:A:VAL:HG12	1:490:A:LEU:H	5	0.25
(1,3891)	1:486:A:VAL:HG13	1:490:A:LEU:H	5	0.25
(1,3891)	1:486:A:VAL:HG11	1:490:A:LEU:H	13	0.25
(1,3891)	1:486:A:VAL:HG12	1:490:A:LEU:H	13	0.25
(1,3891)	1:486:A:VAL:HG13	1:490:A:LEU:H	13	0.25
(1,3848)	1:481:A:GLN:HG2	1:486:A:VAL:HA	2	0.25
(1,3848)	1:481:A:GLN:HG3	1:486:A:VAL:HA	2	0.25
(1,3807)	1:475:A:PHE:H	1:479:A:PRO:HA	7	0.25
(1,3788)	1:474:A:GLU:HA	1:479:A:PRO:HA	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3777)	1:473:A:THR:HB	1:480:A:PHE:H	10	0.25
(1,3601)	1:453:A:LYS:HG2	1:493:A:LEU:HD21	14	0.25
(1,3601)	1:453:A:LYS:HG2	1:493:A:LEU:HD22	14	0.25
(1,3601)	1:453:A:LYS:HG2	1:493:A:LEU:HD23	14	0.25
(1,3601)	1:453:A:LYS:HG3	1:493:A:LEU:HD21	14	0.25
(1,3601)	1:453:A:LYS:HG3	1:493:A:LEU:HD22	14	0.25
(1,3601)	1:453:A:LYS:HG3	1:493:A:LEU:HD23	14	0.25
(1,3538)	1:449:A:LEU:HD11	1:453:A:LYS:HB2	13	0.25
(1,3538)	1:449:A:LEU:HD11	1:453:A:LYS:HB3	13	0.25
(1,3538)	1:449:A:LEU:HD12	1:453:A:LYS:HB2	13	0.25
(1,3538)	1:449:A:LEU:HD12	1:453:A:LYS:HB3	13	0.25
(1,3538)	1:449:A:LEU:HD13	1:453:A:LYS:HB2	13	0.25
(1,3538)	1:449:A:LEU:HD13	1:453:A:LYS:HB3	13	0.25
(1,3476)	1:445:A:PRO:HG2	1:446:A:HIS:H	2	0.25
(1,3476)	1:445:A:PRO:HG3	1:446:A:HIS:H	2	0.25
(1,3353)	1:436:A:ASP:HA	1:461:A:SER:HA	3	0.25
(1,3248)	1:432:A:TYR:HA	1:457:A:VAL:HA	10	0.25
(1,3248)	1:432:A:TYR:HA	1:457:A:VAL:HA	12	0.25
(1,3207)	1:431:A:TYR:HA	1:482:A:SER:HA	14	0.25
(1,3174)	1:430:A:ILE:H	1:480:A:PHE:HA	14	0.25
(1,3174)	1:430:A:ILE:H	1:480:A:PHE:HA	20	0.25
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD11	20	0.25
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD12	20	0.25
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD13	20	0.25
(1,3153)	1:429:A:LYS:HA	1:480:A:PHE:H	8	0.25
(1,3150)	1:429:A:LYS:HD2	1:481:A:GLN:HB2	12	0.25
(1,3150)	1:429:A:LYS:HD2	1:481:A:GLN:HB3	12	0.25
(1,3150)	1:429:A:LYS:HD3	1:481:A:GLN:HB2	12	0.25
(1,3150)	1:429:A:LYS:HD3	1:481:A:GLN:HB3	12	0.25
(1,3128)	1:427:A:GLN:HG2	1:429:A:LYS:H	6	0.25
(1,3128)	1:427:A:GLN:HG3	1:429:A:LYS:H	6	0.25
(1,3121)	1:427:A:GLN:HE21	1:455:A:ILE:HA	14	0.25
(1,3121)	1:427:A:GLN:HE22	1:455:A:ILE:HA	14	0.25
(1,3096)	1:424:A:LYS:H	1:427:A:GLN:HB2	11	0.25
(1,3096)	1:424:A:LYS:H	1:427:A:GLN:HB3	11	0.25
(1,3076)	1:423:A:MET:HE1	1:429:A:LYS:H	18	0.25
(1,3076)	1:423:A:MET:HE2	1:429:A:LYS:H	18	0.25
(1,3076)	1:423:A:MET:HE3	1:429:A:LYS:H	18	0.25
(1,2940)	1:414:A:VAL:HG21	1:418:A:ASP:HB2	3	0.25
(1,2940)	1:414:A:VAL:HG21	1:418:A:ASP:HB3	3	0.25
(1,2940)	1:414:A:VAL:HG22	1:418:A:ASP:HB2	3	0.25
(1,2940)	1:414:A:VAL:HG22	1:418:A:ASP:HB3	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2940)	1:414:A:VAL:HG23	1:418:A:ASP:HB2	3	0.25
(1,2940)	1:414:A:VAL:HG23	1:418:A:ASP:HB3	3	0.25
(1,2927)	1:412:A:GLN:HA	1:414:A:VAL:HB	20	0.25
(1,2914)	1:410:A:SER:HA	1:438:A:TYR:HD1	16	0.25
(1,2912)	1:410:A:SER:HB2	1:438:A:TYR:HD1	17	0.25
(1,2912)	1:410:A:SER:HB2	1:438:A:TYR:HD2	17	0.25
(1,2912)	1:410:A:SER:HB3	1:438:A:TYR:HD1	17	0.25
(1,2912)	1:410:A:SER:HB3	1:438:A:TYR:HD2	17	0.25
(1,2898)	1:409:A:SER:H	1:442:A:LYS:HE2	16	0.25
(1,2898)	1:409:A:SER:H	1:442:A:LYS:HE3	16	0.25
(1,2873)	1:406:A:HIS:HA	1:422:A:ARG:HD2	9	0.25
(1,2873)	1:406:A:HIS:HA	1:422:A:ARG:HD3	9	0.25
(1,2824)	1:404:A:SER:H	1:414:A:VAL:HB	6	0.25
(1,2808)	1:404:A:SER:HB2	1:459:A:LEU:H	2	0.25
(1,2808)	1:404:A:SER:HB3	1:459:A:LEU:H	2	0.25
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG11	4	0.25
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG12	4	0.25
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG13	4	0.25
(1,2631)	1:393:A:GLN:HA	1:396:A:ILE:H	20	0.25
(1,2574)	1:388:A:GLU:H	1:390:A:PHE:H	15	0.25
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD1	12	0.25
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD2	12	0.25
(1,2535)	1:386:A:PRO:HB2	1:472:A:LEU:HA	17	0.25
(1,2535)	1:386:A:PRO:HB3	1:472:A:LEU:HA	17	0.25
(1,2381)	1:376:A:GLN:HA	1:412:A:GLN:HE21	19	0.25
(1,2381)	1:376:A:GLN:HA	1:412:A:GLN:HE22	19	0.25
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA2	17	0.25
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA3	17	0.25
(1,2317)	1:374:A:PHE:HZ	1:382:A:LEU:H	17	0.25
(1,2203)	1:365:A:LYS:HA	1:367:A:ASP:H	13	0.25
(1,2108)	1:360:A:LEU:HD21	1:364:A:ALA:H	5	0.25
(1,2108)	1:360:A:LEU:HD22	1:364:A:ALA:H	5	0.25
(1,2108)	1:360:A:LEU:HD23	1:364:A:ALA:H	5	0.25
(1,2042)	1:357:A:LEU:HD21	1:396:A:ILE:HA	4	0.25
(1,2042)	1:357:A:LEU:HD22	1:396:A:ILE:HA	4	0.25
(1,2042)	1:357:A:LEU:HD23	1:396:A:ILE:HA	4	0.25
(1,2014)	1:355:A:ARG:HA	1:358:A:GLN:HB2	12	0.25
(1,2014)	1:355:A:ARG:HA	1:358:A:GLN:HB3	12	0.25
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD11	4	0.25
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD12	4	0.25
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD13	4	0.25
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB1	18	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB2	18	0.25
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB3	18	0.25
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB1	18	0.25
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB2	18	0.25
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB3	18	0.25
(1,1937)	1:350:A:ASN:HA	1:353:A:THR:H	5	0.25
(1,1937)	1:350:A:ASN:HA	1:353:A:THR:H	7	0.25
(1,1935)	1:350:A:ASN:HA	1:354:A:LYS:HG2	17	0.25
(1,1935)	1:350:A:ASN:HA	1:354:A:LYS:HG3	17	0.25
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD21	5	0.25
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD22	5	0.25
(1,1716)	1:330:A:LEU:HB2	1:334:A:VAL:HB	5	0.25
(1,1716)	1:330:A:LEU:HB3	1:334:A:VAL:HB	5	0.25
(1,1452)	1:313:A:PHE:HZ	1:345:A:THR:HA	11	0.25
(1,1416)	1:312:A:GLN:HB2	1:349:A:ARG:HD2	3	0.25
(1,1416)	1:312:A:GLN:HB2	1:349:A:ARG:HD3	3	0.25
(1,1416)	1:312:A:GLN:HB3	1:349:A:ARG:HD2	3	0.25
(1,1416)	1:312:A:GLN:HB3	1:349:A:ARG:HD3	3	0.25
(1,1349)	1:305:A:PHE:HZ	1:308:A:ASP:HA	16	0.25
(1,1318)	1:302:A:GLN:H	1:329:A:ASP:H	9	0.25
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE1	15	0.25
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE2	15	0.25
(1,1218)	1:299:A:LEU:HD21	1:307:A:MET:HE1	18	0.25
(1,1218)	1:299:A:LEU:HD21	1:307:A:MET:HE2	18	0.25
(1,1218)	1:299:A:LEU:HD21	1:307:A:MET:HE3	18	0.25
(1,1218)	1:299:A:LEU:HD22	1:307:A:MET:HE1	18	0.25
(1,1218)	1:299:A:LEU:HD22	1:307:A:MET:HE2	18	0.25
(1,1218)	1:299:A:LEU:HD22	1:307:A:MET:HE3	18	0.25
(1,1218)	1:299:A:LEU:HD23	1:307:A:MET:HE1	18	0.25
(1,1218)	1:299:A:LEU:HD23	1:307:A:MET:HE2	18	0.25
(1,1218)	1:299:A:LEU:HD23	1:307:A:MET:HE3	18	0.25
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD11	11	0.25
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD12	11	0.25
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD13	11	0.25
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD11	11	0.25
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD12	11	0.25
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD13	11	0.25
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD11	11	0.25
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD12	11	0.25
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD13	11	0.25
(1,1159)	1:298:A:LYS:H	1:322:A:ARG:HD2	10	0.25
(1,1159)	1:298:A:LYS:H	1:322:A:ARG:HD3	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1118)	1:297:A:LEU:HA	1:322:A:ARG:HD2	19	0.25
(1,1118)	1:297:A:LEU:HA	1:322:A:ARG:HD3	19	0.25
(1,1090)	1:296:A:GLY:H	1:311:A:GLU:HA	20	0.25
(1,1072)	1:295:A:HIS:HE1	1:311:A:GLU:HA	19	0.25
(1,1067)	1:295:A:HIS:HB2	1:319:A:ARG:HA	6	0.25
(1,1067)	1:295:A:HIS:HB3	1:319:A:ARG:HA	6	0.25
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	20	0.25
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD21	5	0.25
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD22	5	0.25
(1,574)	1:264:A:SER:HB2	1:358:A:GLN:HB2	4	0.25
(1,574)	1:264:A:SER:HB2	1:358:A:GLN:HB3	4	0.25
(1,574)	1:264:A:SER:HB3	1:358:A:GLN:HB2	4	0.25
(1,574)	1:264:A:SER:HB3	1:358:A:GLN:HB3	4	0.25
(1,570)	1:264:A:SER:HB2	1:359:A:MET:HA	4	0.25
(1,570)	1:264:A:SER:HB3	1:359:A:MET:HA	4	0.25
(1,564)	1:263:A:TRP:HE1	1:265:A:HIS:H	16	0.25
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	1	0.25
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	13	0.25
(1,547)	1:263:A:TRP:HZ3	1:370:A:LYS:HZ3	17	0.25
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	8	0.25
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	8	0.25
(1,513)	1:261:A:LEU:H	1:281:A:PRO:HA	8	0.25
(1,410)	1:253:A:ILE:HB	1:298:A:LYS:HD2	10	0.25
(1,410)	1:253:A:ILE:HB	1:298:A:LYS:HD3	10	0.25
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB2	13	0.25
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB3	13	0.25
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB2	13	0.25
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB3	13	0.25
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB2	13	0.25
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB3	13	0.25
(1,346)	1:250:A:TYR:HB2	1:263:A:TRP:HE3	19	0.25
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	2	0.25
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	15	0.25
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG21	15	0.25
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG22	15	0.25
(1,9)	1:231:A:GLN:HA	1:235:A:THR:HG23	15	0.25
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD11	7	0.24
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD12	7	0.24
(1,3981)	1:455:A:ILE:HD11	2:639:B:LEU:HD13	7	0.24
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD11	7	0.24
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD12	7	0.24
(1,3981)	1:455:A:ILE:HD12	2:639:B:LEU:HD13	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD11	7	0.24
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD12	7	0.24
(1,3981)	1:455:A:ILE:HD13	2:639:B:LEU:HD13	7	0.24
(1,3938)	1:490:A:LEU:HA	1:493:A:LEU:H	3	0.24
(1,3938)	1:490:A:LEU:HA	1:493:A:LEU:H	19	0.24
(1,3908)	1:487:A:ASP:H	1:489:A:SER:H	8	0.24
(1,3894)	1:486:A:VAL:HA	1:489:A:SER:H	8	0.24
(1,3807)	1:475:A:PHE:H	1:479:A:PRO:HA	2	0.24
(1,3634)	1:458:A:LEU:HD11	1:480:A:PHE:HE1	19	0.24
(1,3634)	1:458:A:LEU:HD11	1:480:A:PHE:HE2	19	0.24
(1,3634)	1:458:A:LEU:HD12	1:480:A:PHE:HE1	19	0.24
(1,3634)	1:458:A:LEU:HD12	1:480:A:PHE:HE2	19	0.24
(1,3634)	1:458:A:LEU:HD13	1:480:A:PHE:HE1	19	0.24
(1,3634)	1:458:A:LEU:HD13	1:480:A:PHE:HE2	19	0.24
(1,3538)	1:449:A:LEU:HD11	1:453:A:LYS:HB2	9	0.24
(1,3538)	1:449:A:LEU:HD11	1:453:A:LYS:HB3	9	0.24
(1,3538)	1:449:A:LEU:HD12	1:453:A:LYS:HB2	9	0.24
(1,3538)	1:449:A:LEU:HD12	1:453:A:LYS:HB3	9	0.24
(1,3538)	1:449:A:LEU:HD13	1:453:A:LYS:HB2	9	0.24
(1,3538)	1:449:A:LEU:HD13	1:453:A:LYS:HB3	9	0.24
(1,3479)	1:446:A:HIS:HD2	1:484:A:SER:H	9	0.24
(1,3406)	1:439:A:ALA:HA	1:442:A:LYS:HD2	2	0.24
(1,3406)	1:439:A:ALA:HA	1:442:A:LYS:HD3	2	0.24
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB2	16	0.24
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB3	16	0.24
(1,3301)	1:434:A:THR:H	1:484:A:SER:H	10	0.24
(1,3235)	1:432:A:TYR:H	1:482:A:SER:HA	10	0.24
(1,3231)	1:432:A:TYR:H	1:483:A:VAL:H	18	0.24
(1,3222)	1:431:A:TYR:HD1	1:456:A:GLU:H	20	0.24
(1,3222)	1:431:A:TYR:HD2	1:456:A:GLU:H	20	0.24
(1,3207)	1:431:A:TYR:HA	1:482:A:SER:HA	2	0.24
(1,3178)	1:430:A:ILE:HD11	1:479:A:PRO:HA	13	0.24
(1,3178)	1:430:A:ILE:HD12	1:479:A:PRO:HA	13	0.24
(1,3178)	1:430:A:ILE:HD13	1:479:A:PRO:HA	13	0.24
(1,3170)	1:430:A:ILE:H	1:481:A:GLN:H	20	0.24
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD11	7	0.24
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD12	7	0.24
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD13	7	0.24
(1,3165)	1:429:A:LYS:HB2	1:431:A:TYR:HE1	16	0.24
(1,3153)	1:429:A:LYS:HA	1:480:A:PHE:H	14	0.24
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG2	19	0.24
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG3	19	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG2	19	0.24
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG3	19	0.24
(1,3135)	1:428:A:GLU:HA	1:478:A:LYS:HA	19	0.24
(1,3133)	1:428:A:GLU:HG2	1:479:A:PRO:HD2	16	0.24
(1,3133)	1:428:A:GLU:HG2	1:479:A:PRO:HD3	16	0.24
(1,3133)	1:428:A:GLU:HG3	1:479:A:PRO:HD2	16	0.24
(1,3133)	1:428:A:GLU:HG3	1:479:A:PRO:HD3	16	0.24
(1,3121)	1:427:A:GLN:HE21	1:455:A:ILE:HA	7	0.24
(1,3121)	1:427:A:GLN:HE22	1:455:A:ILE:HA	7	0.24
(1,3112)	1:426:A:GLY:HA2	1:428:A:GLU:HA	15	0.24
(1,3112)	1:426:A:GLY:HA3	1:428:A:GLU:HA	15	0.24
(1,3095)	1:424:A:LYS:H	1:427:A:GLN:H	6	0.24
(1,3076)	1:423:A:MET:HE1	1:429:A:LYS:H	14	0.24
(1,3076)	1:423:A:MET:HE2	1:429:A:LYS:H	14	0.24
(1,3076)	1:423:A:MET:HE3	1:429:A:LYS:H	14	0.24
(1,2873)	1:406:A:HIS:HA	1:422:A:ARG:HD2	20	0.24
(1,2873)	1:406:A:HIS:HA	1:422:A:ARG:HD3	20	0.24
(1,2871)	1:406:A:HIS:HA	1:456:A:GLU:HG2	4	0.24
(1,2871)	1:406:A:HIS:HA	1:456:A:GLU:HG3	4	0.24
(1,2813)	1:404:A:SER:HB2	1:458:A:LEU:HA	2	0.24
(1,2813)	1:404:A:SER:HB3	1:458:A:LEU:HA	2	0.24
(1,2781)	1:403:A:ALA:H	1:459:A:LEU:H	13	0.24
(1,2575)	1:388:A:GLU:HA	1:390:A:PHE:H	9	0.24
(1,2566)	1:387:A:ALA:H	1:468:A:MET:HA	17	0.24
(1,2436)	1:380:A:LEU:HA	1:383:A:LYS:HD2	14	0.24
(1,2436)	1:380:A:LEU:HA	1:383:A:LYS:HD3	14	0.24
(1,2260)	1:371:A:TYR:HE1	1:399:A:LEU:HA	12	0.24
(1,2260)	1:371:A:TYR:HE2	1:399:A:LEU:HA	12	0.24
(1,2203)	1:365:A:LYS:HA	1:367:A:ASP:H	20	0.24
(1,2133)	1:361:A:GLU:HA	1:365:A:LYS:H	11	0.24
(1,2133)	1:361:A:GLU:HA	1:365:A:LYS:H	17	0.24
(1,2042)	1:357:A:LEU:HD21	1:396:A:ILE:HA	3	0.24
(1,2042)	1:357:A:LEU:HD22	1:396:A:ILE:HA	3	0.24
(1,2042)	1:357:A:LEU:HD23	1:396:A:ILE:HA	3	0.24
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD21	15	0.24
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD22	15	0.24
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD21	15	0.24
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD22	15	0.24
(1,1951)	1:351:A:ALA:HA	1:354:A:LYS:HD2	9	0.24
(1,1951)	1:351:A:ALA:HA	1:354:A:LYS:HD3	9	0.24
(1,1776)	1:336:A:ARG:HA	1:340:A:GLN:H	1	0.24
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE1	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE2	3	0.24
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE3	3	0.24
(1,1479)	1:314:A:MET:H	1:349:A:ARG:HD2	6	0.24
(1,1479)	1:314:A:MET:H	1:349:A:ARG:HD3	6	0.24
(1,1159)	1:298:A:LYS:H	1:322:A:ARG:HD2	19	0.24
(1,1159)	1:298:A:LYS:H	1:322:A:ARG:HD3	19	0.24
(1,1159)	1:298:A:LYS:H	1:322:A:ARG:HD2	20	0.24
(1,1159)	1:298:A:LYS:H	1:322:A:ARG:HD3	20	0.24
(1,1154)	1:298:A:LYS:HB2	1:324:A:LEU:HB2	15	0.24
(1,1154)	1:298:A:LYS:HB2	1:324:A:LEU:HB3	15	0.24
(1,1154)	1:298:A:LYS:HB3	1:324:A:LEU:HB2	15	0.24
(1,1154)	1:298:A:LYS:HB3	1:324:A:LEU:HB3	15	0.24
(1,1035)	1:290:A:ASN:H	1:292:A:ASP:H	2	0.24
(1,1023)	1:289:A:TRP:HZ2	1:381:A:VAL:H	7	0.24
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	9	0.24
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	1	0.24
(1,914)	1:282:A:SER:H	1:378:A:PHE:HZ	6	0.24
(1,752)	1:275:A:THR:HG21	1:324:A:LEU:HD21	12	0.24
(1,752)	1:275:A:THR:HG21	1:324:A:LEU:HD22	12	0.24
(1,752)	1:275:A:THR:HG21	1:324:A:LEU:HD23	12	0.24
(1,752)	1:275:A:THR:HG22	1:324:A:LEU:HD21	12	0.24
(1,752)	1:275:A:THR:HG22	1:324:A:LEU:HD22	12	0.24
(1,752)	1:275:A:THR:HG22	1:324:A:LEU:HD23	12	0.24
(1,752)	1:275:A:THR:HG23	1:324:A:LEU:HD21	12	0.24
(1,752)	1:275:A:THR:HG23	1:324:A:LEU:HD22	12	0.24
(1,752)	1:275:A:THR:HG23	1:324:A:LEU:HD23	12	0.24
(1,715)	1:274:A:TYR:HE1	1:348:A:LEU:HA	18	0.24
(1,715)	1:274:A:TYR:HE2	1:348:A:LEU:HA	18	0.24
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	5	0.24
(1,648)	1:268:A:VAL:HB	1:274:A:TYR:H	6	0.24
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD21	10	0.24
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD22	10	0.24
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	5	0.24
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	5	0.24
(1,539)	1:262:A:THR:HG21	1:280:A:ILE:HB	14	0.24
(1,539)	1:262:A:THR:HG22	1:280:A:ILE:HB	14	0.24
(1,539)	1:262:A:THR:HG23	1:280:A:ILE:HB	14	0.24
(1,382)	1:251:A:LYS:HA	1:255:A:HIS:HA	10	0.24
(1,382)	1:251:A:LYS:HA	1:255:A:HIS:HA	18	0.24
(1,376)	1:251:A:LYS:HG2	1:257:A:PHE:HA	18	0.24
(1,376)	1:251:A:LYS:HG3	1:257:A:PHE:HA	18	0.24
(1,370)	1:251:A:LYS:HE2	1:259:A:ASP:H	16	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:251:A:LYS:HE3	1:259:A:ASP:H	16	0.24
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	5	0.24
(1,252)	1:246:A:TYR:HD1	1:263:A:TRP:HE1	15	0.24
(1,130)	1:237:A:ASN:HA	1:265:A:HIS:HE1	14	0.24
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD2	15	0.24
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD3	15	0.24
(1,95)	1:234:A:TRP:HA	1:246:A:TYR:HE2	16	0.24
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	13	0.24
(1,84)	1:234:A:TRP:HD1	1:275:A:THR:HB	5	0.24
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	12	0.24
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD11	17	0.24
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD12	17	0.24
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD13	17	0.24
(2,14)	1:442:A:LYS:H	1:461:A:SER:HB2	10	0.23
(2,14)	1:442:A:LYS:H	1:461:A:SER:HB3	10	0.23
(1,3891)	1:486:A:VAL:HG11	1:490:A:LEU:H	1	0.23
(1,3891)	1:486:A:VAL:HG12	1:490:A:LEU:H	1	0.23
(1,3891)	1:486:A:VAL:HG13	1:490:A:LEU:H	1	0.23
(1,3891)	1:486:A:VAL:HG11	1:490:A:LEU:H	18	0.23
(1,3891)	1:486:A:VAL:HG12	1:490:A:LEU:H	18	0.23
(1,3891)	1:486:A:VAL:HG13	1:490:A:LEU:H	18	0.23
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB2	5	0.23
(1,3850)	1:481:A:GLN:HE21	1:485:A:LYS:HB3	5	0.23
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB2	5	0.23
(1,3850)	1:481:A:GLN:HE22	1:485:A:LYS:HB3	5	0.23
(1,3817)	1:475:A:PHE:HD2	1:476:A:ASP:HB3	18	0.23
(1,3807)	1:475:A:PHE:H	1:479:A:PRO:HA	13	0.23
(1,3776)	1:473:A:THR:HA	1:480:A:PHE:H	13	0.23
(1,3688)	1:464:A:ILE:HD11	1:467:A:TRP:HE3	4	0.23
(1,3688)	1:464:A:ILE:HD12	1:467:A:TRP:HE3	4	0.23
(1,3688)	1:464:A:ILE:HD13	1:467:A:TRP:HE3	4	0.23
(1,3537)	1:449:A:LEU:HD11	1:453:A:LYS:H	13	0.23
(1,3537)	1:449:A:LEU:HD12	1:453:A:LYS:H	13	0.23
(1,3537)	1:449:A:LEU:HD13	1:453:A:LYS:H	13	0.23
(1,3533)	1:449:A:LEU:HD21	1:490:A:LEU:HB2	10	0.23
(1,3533)	1:449:A:LEU:HD21	1:490:A:LEU:HB3	10	0.23
(1,3533)	1:449:A:LEU:HD22	1:490:A:LEU:HB2	10	0.23
(1,3533)	1:449:A:LEU:HD22	1:490:A:LEU:HB3	10	0.23
(1,3533)	1:449:A:LEU:HD23	1:490:A:LEU:HB2	10	0.23
(1,3533)	1:449:A:LEU:HD23	1:490:A:LEU:HB3	10	0.23
(1,3482)	1:446:A:HIS:HA	1:483:A:VAL:HB	17	0.23
(1,3364)	1:437:A:SER:HA	1:461:A:SER:HB2	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3364)	1:437:A:SER:HA	1:461:A:SER:HB3	11	0.23
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB2	7	0.23
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB3	7	0.23
(1,3317)	1:434:A:THR:HA	1:460:A:LEU:H	1	0.23
(1,3272)	1:433:A:ILE:HB	1:459:A:LEU:HD21	16	0.23
(1,3272)	1:433:A:ILE:HB	1:459:A:LEU:HD22	16	0.23
(1,3272)	1:433:A:ILE:HB	1:459:A:LEU:HD23	16	0.23
(1,3238)	1:432:A:TYR:HB2	1:460:A:LEU:H	12	0.23
(1,3238)	1:432:A:TYR:HB3	1:460:A:LEU:H	12	0.23
(1,3174)	1:430:A:ILE:H	1:480:A:PHE:HA	8	0.23
(1,3155)	1:429:A:LYS:HB2	1:480:A:PHE:HA	1	0.23
(1,3155)	1:429:A:LYS:HB3	1:480:A:PHE:HA	1	0.23
(1,3150)	1:429:A:LYS:HD2	1:481:A:GLN:HB2	7	0.23
(1,3150)	1:429:A:LYS:HD2	1:481:A:GLN:HB3	7	0.23
(1,3150)	1:429:A:LYS:HD3	1:481:A:GLN:HB2	7	0.23
(1,3150)	1:429:A:LYS:HD3	1:481:A:GLN:HB3	7	0.23
(1,3137)	1:428:A:GLU:HA	1:478:A:LYS:HG2	19	0.23
(1,3137)	1:428:A:GLU:HA	1:478:A:LYS:HG3	19	0.23
(1,3061)	1:422:A:ARG:HD2	1:456:A:GLU:HB2	5	0.23
(1,3061)	1:422:A:ARG:HD2	1:456:A:GLU:HB3	5	0.23
(1,3061)	1:422:A:ARG:HD3	1:456:A:GLU:HB2	5	0.23
(1,3061)	1:422:A:ARG:HD3	1:456:A:GLU:HB3	5	0.23
(1,2980)	1:417:A:GLU:H	1:475:A:PHE:HZ	9	0.23
(1,2980)	1:417:A:GLU:H	1:475:A:PHE:HZ	13	0.23
(1,2913)	1:410:A:SER:HA	1:438:A:TYR:HE1	14	0.23
(1,2913)	1:410:A:SER:HA	1:438:A:TYR:HE2	14	0.23
(1,2887)	1:407:A:THR:HG21	1:408:A:ASP:H	8	0.23
(1,2887)	1:407:A:THR:HG22	1:408:A:ASP:H	8	0.23
(1,2887)	1:407:A:THR:HG23	1:408:A:ASP:H	8	0.23
(1,2848)	1:405:A:THR:H	1:457:A:VAL:HB	14	0.23
(1,2807)	1:404:A:SER:HA	1:459:A:LEU:H	2	0.23
(1,2794)	1:403:A:ALA:HA	1:413:A:THR:H	12	0.23
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG11	1	0.23
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG12	1	0.23
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG13	1	0.23
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG11	13	0.23
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG12	13	0.23
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG13	13	0.23
(1,2642)	1:394:A:GLU:HA	1:398:A:LYS:H	7	0.23
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB2	16	0.23
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB3	16	0.23
(1,2524)	1:385:A:GLY:HA2	1:389:A:ASP:H	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2524)	1:385:A:GLY:HA3	1:389:A:ASP:H	7	0.23
(1,2524)	1:385:A:GLY:HA2	1:389:A:ASP:H	20	0.23
(1,2524)	1:385:A:GLY:HA3	1:389:A:ASP:H	20	0.23
(1,2448)	1:381:A:VAL:HA	1:384:A:GLU:H	9	0.23
(1,2357)	1:375:A:TRP:HH2	1:383:A:LYS:HE2	15	0.23
(1,2357)	1:375:A:TRP:HH2	1:383:A:LYS:HE3	15	0.23
(1,2170)	1:363:A:LEU:HA	1:366:A:ASP:HB2	3	0.23
(1,2170)	1:363:A:LEU:HA	1:366:A:ASP:HB3	3	0.23
(1,2014)	1:355:A:ARG:HA	1:358:A:GLN:HB2	3	0.23
(1,2014)	1:355:A:ARG:HA	1:358:A:GLN:HB3	3	0.23
(1,1996)	1:354:A:LYS:HA	1:358:A:GLN:HE21	7	0.23
(1,1996)	1:354:A:LYS:HA	1:358:A:GLN:HE22	7	0.23
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD21	14	0.23
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD22	14	0.23
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD21	14	0.23
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD22	14	0.23
(1,1945)	1:351:A:ALA:HA	1:355:A:ARG:H	1	0.23
(1,1886)	1:346:A:ARG:HG2	1:350:A:ASN:HD21	19	0.23
(1,1886)	1:346:A:ARG:HG2	1:350:A:ASN:HD22	19	0.23
(1,1886)	1:346:A:ARG:HG3	1:350:A:ASN:HD21	19	0.23
(1,1886)	1:346:A:ARG:HG3	1:350:A:ASN:HD22	19	0.23
(1,1884)	1:346:A:ARG:HA	1:350:A:ASN:H	16	0.23
(1,1810)	1:339:A:LEU:HA	1:345:A:THR:H	8	0.23
(1,1768)	1:335:A:SER:H	1:338:A:ILE:HD11	12	0.23
(1,1768)	1:335:A:SER:H	1:338:A:ILE:HD12	12	0.23
(1,1768)	1:335:A:SER:H	1:338:A:ILE:HD13	12	0.23
(1,1701)	1:329:A:ASP:HB2	1:344:A:VAL:HG21	5	0.23
(1,1701)	1:329:A:ASP:HB2	1:344:A:VAL:HG22	5	0.23
(1,1701)	1:329:A:ASP:HB2	1:344:A:VAL:HG23	5	0.23
(1,1701)	1:329:A:ASP:HB3	1:344:A:VAL:HG21	5	0.23
(1,1701)	1:329:A:ASP:HB3	1:344:A:VAL:HG22	5	0.23
(1,1701)	1:329:A:ASP:HB3	1:344:A:VAL:HG23	5	0.23
(1,1658)	1:322:A:ARG:HD2	1:323:A:GLY:H	10	0.23
(1,1658)	1:322:A:ARG:HD3	1:323:A:GLY:H	10	0.23
(1,1621)	1:320:A:PHE:HE1	1:378:A:PHE:HB2	13	0.23
(1,1621)	1:320:A:PHE:HE1	1:378:A:PHE:HB3	13	0.23
(1,1621)	1:320:A:PHE:HE2	1:378:A:PHE:HB2	13	0.23
(1,1621)	1:320:A:PHE:HE2	1:378:A:PHE:HB3	13	0.23
(1,1445)	1:313:A:PHE:HA	1:349:A:ARG:H	4	0.23
(1,1432)	1:312:A:GLN:HE21	1:336:A:ARG:HG2	3	0.23
(1,1432)	1:312:A:GLN:HE21	1:336:A:ARG:HG3	3	0.23
(1,1432)	1:312:A:GLN:HE22	1:336:A:ARG:HG2	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1432)	1:312:A:GLN:HE22	1:336:A:ARG:HG3	3	0.23
(1,1334)	1:303:A:ARG:H	1:327:A:SER:H	7	0.23
(1,1139)	1:297:A:LEU:H	1:309:A:ASP:HA	15	0.23
(1,1072)	1:295:A:HIS:HE1	1:311:A:GLU:HA	12	0.23
(1,1044)	1:291:A:ARG:HA	1:293:A:HIS:HA	6	0.23
(1,1035)	1:290:A:ASN:H	1:292:A:ASP:H	3	0.23
(1,1024)	1:289:A:TRP:HH2	1:381:A:VAL:HA	3	0.23
(1,1022)	1:289:A:TRP:HH2	1:381:A:VAL:H	11	0.23
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	7	0.23
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	13	0.23
(1,962)	1:285:A:PRO:HB2	1:294:A:LYS:HG2	15	0.23
(1,962)	1:285:A:PRO:HB2	1:294:A:LYS:HG3	15	0.23
(1,962)	1:285:A:PRO:HB3	1:294:A:LYS:HG2	15	0.23
(1,962)	1:285:A:PRO:HB3	1:294:A:LYS:HG3	15	0.23
(1,957)	1:285:A:PRO:HD2	1:320:A:PHE:HA	2	0.23
(1,957)	1:285:A:PRO:HD3	1:320:A:PHE:HA	2	0.23
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	17	0.23
(1,914)	1:282:A:SER:H	1:378:A:PHE:HZ	4	0.23
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	20	0.23
(1,703)	1:273:A:GLU:H	1:328:A:SER:H	1	0.23
(1,680)	1:271:A:LYS:HA	1:273:A:GLU:H	18	0.23
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB2	12	0.23
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB3	12	0.23
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	3	0.23
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE21	13	0.23
(1,458)	1:258:A:ASN:HD21	1:283:A:GLN:HE22	13	0.23
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE21	13	0.23
(1,458)	1:258:A:ASN:HD22	1:283:A:GLN:HE22	13	0.23
(1,408)	1:253:A:ILE:HB	1:298:A:LYS:H	18	0.23
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB2	2	0.23
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB3	2	0.23
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB2	2	0.23
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB3	2	0.23
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB2	2	0.23
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB3	2	0.23
(1,346)	1:250:A:TYR:HB2	1:263:A:TRP:HE3	6	0.23
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	3	0.23
(1,293)	1:248:A:GLU:HA	1:251:A:LYS:H	14	0.23
(1,282)	1:247:A:LYS:HA	1:250:A:TYR:H	4	0.23
(1,220)	1:244:A:GLU:HB2	1:248:A:GLU:H	12	0.23
(1,220)	1:244:A:GLU:HB3	1:248:A:GLU:H	12	0.23
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3970)	1:357:A:LEU:HD11	2:620:B:LEU:HD21	12	0.22
(1,3970)	1:357:A:LEU:HD11	2:620:B:LEU:HD22	12	0.22
(1,3970)	1:357:A:LEU:HD11	2:620:B:LEU:HD23	12	0.22
(1,3970)	1:357:A:LEU:HD12	2:620:B:LEU:HD21	12	0.22
(1,3970)	1:357:A:LEU:HD12	2:620:B:LEU:HD22	12	0.22
(1,3970)	1:357:A:LEU:HD12	2:620:B:LEU:HD23	12	0.22
(1,3970)	1:357:A:LEU:HD13	2:620:B:LEU:HD21	12	0.22
(1,3970)	1:357:A:LEU:HD13	2:620:B:LEU:HD22	12	0.22
(1,3970)	1:357:A:LEU:HD13	2:620:B:LEU:HD23	12	0.22
(1,3726)	1:468:A:MET:HG2	1:472:A:LEU:HB2	2	0.22
(1,3726)	1:468:A:MET:HG2	1:472:A:LEU:HB3	2	0.22
(1,3726)	1:468:A:MET:HG3	1:472:A:LEU:HB2	2	0.22
(1,3726)	1:468:A:MET:HG3	1:472:A:LEU:HB3	2	0.22
(1,3709)	1:466:A:GLU:HA	1:470:A:ASN:H	4	0.22
(1,3605)	1:453:A:LYS:HG2	1:455:A:ILE:HD11	1	0.22
(1,3605)	1:453:A:LYS:HG2	1:455:A:ILE:HD12	1	0.22
(1,3605)	1:453:A:LYS:HG2	1:455:A:ILE:HD13	1	0.22
(1,3605)	1:453:A:LYS:HG3	1:455:A:ILE:HD11	1	0.22
(1,3605)	1:453:A:LYS:HG3	1:455:A:ILE:HD12	1	0.22
(1,3605)	1:453:A:LYS:HG3	1:455:A:ILE:HD13	1	0.22
(1,3570)	1:450:A:LEU:HA	1:453:A:LYS:H	17	0.22
(1,3536)	1:449:A:LEU:HA	1:453:A:LYS:H	4	0.22
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB2	17	0.22
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB3	17	0.22
(1,3351)	1:436:A:ASP:HA	1:463:A:ARG:HA	15	0.22
(1,3329)	1:435:A:ALA:H	1:461:A:SER:HA	16	0.22
(1,3259)	1:433:A:ILE:HB	1:483:A:VAL:H	7	0.22
(1,3255)	1:433:A:ILE:HB	1:484:A:SER:H	11	0.22
(1,3235)	1:432:A:TYR:H	1:482:A:SER:HA	7	0.22
(1,3214)	1:431:A:TYR:H	1:458:A:LEU:H	6	0.22
(1,3214)	1:431:A:TYR:H	1:458:A:LEU:H	16	0.22
(1,3143)	1:429:A:LYS:HD2	1:489:A:SER:H	20	0.22
(1,3143)	1:429:A:LYS:HD3	1:489:A:SER:H	20	0.22
(1,3135)	1:428:A:GLU:HA	1:478:A:LYS:HA	14	0.22
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG2	20	0.22
(1,3119)	1:427:A:GLN:HG2	1:478:A:LYS:HG3	20	0.22
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG2	20	0.22
(1,3119)	1:427:A:GLN:HG3	1:478:A:LYS:HG3	20	0.22
(1,3013)	1:419:A:TYR:HA	1:456:A:GLU:HB2	2	0.22
(1,3013)	1:419:A:TYR:HA	1:456:A:GLU:HB3	2	0.22
(1,2982)	1:417:A:GLU:HG2	1:475:A:PHE:HZ	1	0.22
(1,2982)	1:417:A:GLU:HG3	1:475:A:PHE:HZ	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2937)	1:414:A:VAL:HG21	1:419:A:TYR:HA	14	0.22
(1,2937)	1:414:A:VAL:HG22	1:419:A:TYR:HA	14	0.22
(1,2937)	1:414:A:VAL:HG23	1:419:A:TYR:HA	14	0.22
(1,2913)	1:410:A:SER:HA	1:438:A:TYR:HE1	12	0.22
(1,2913)	1:410:A:SER:HA	1:438:A:TYR:HE2	12	0.22
(1,2911)	1:410:A:SER:HA	1:438:A:TYR:HD1	5	0.22
(1,2911)	1:410:A:SER:HA	1:438:A:TYR:HD2	5	0.22
(1,2875)	1:406:A:HIS:HB2	1:414:A:VAL:HB	9	0.22
(1,2875)	1:406:A:HIS:HB3	1:414:A:VAL:HB	9	0.22
(1,2861)	1:405:A:THR:HA	1:408:A:ASP:HA	3	0.22
(1,2861)	1:405:A:THR:HA	1:408:A:ASP:HA	11	0.22
(1,2794)	1:403:A:ALA:HA	1:413:A:THR:H	18	0.22
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG11	9	0.22
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG12	9	0.22
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG13	9	0.22
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	1	0.22
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	1	0.22
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	1	0.22
(1,2704)	1:398:A:LYS:HA	1:416:A:LEU:HD11	15	0.22
(1,2704)	1:398:A:LYS:HA	1:416:A:LEU:HD12	15	0.22
(1,2704)	1:398:A:LYS:HA	1:416:A:LEU:HD13	15	0.22
(1,2574)	1:388:A:GLU:H	1:390:A:PHE:H	18	0.22
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD1	14	0.22
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD2	14	0.22
(1,2488)	1:383:A:LYS:HE2	1:402:A:PHE:HZ	3	0.22
(1,2488)	1:383:A:LYS:HE3	1:402:A:PHE:HZ	3	0.22
(1,2427)	1:380:A:LEU:HD11	1:463:A:ARG:H	20	0.22
(1,2427)	1:380:A:LEU:HD12	1:463:A:ARG:H	20	0.22
(1,2427)	1:380:A:LEU:HD13	1:463:A:ARG:H	20	0.22
(1,2351)	1:375:A:TRP:HE3	1:400:A:LEU:HA	8	0.22
(1,2250)	1:370:A:LYS:HA	1:373:A:THR:HB	2	0.22
(1,2250)	1:370:A:LYS:HA	1:373:A:THR:HB	4	0.22
(1,2199)	1:365:A:LYS:HA	1:368:A:ALA:H	12	0.22
(1,2083)	1:359:A:MET:HA	1:362:A:LYS:HD2	2	0.22
(1,2083)	1:359:A:MET:HA	1:362:A:LYS:HD3	2	0.22
(1,2077)	1:359:A:MET:HG2	1:363:A:LEU:H	5	0.22
(1,2077)	1:359:A:MET:HG3	1:363:A:LEU:H	5	0.22
(1,2041)	1:357:A:LEU:HD21	1:396:A:ILE:H	16	0.22
(1,2041)	1:357:A:LEU:HD22	1:396:A:ILE:H	16	0.22
(1,2041)	1:357:A:LEU:HD23	1:396:A:ILE:H	16	0.22
(1,1945)	1:351:A:ALA:HA	1:355:A:ARG:H	19	0.22
(1,1938)	1:350:A:ASN:HA	1:353:A:THR:HB	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1937)	1:350:A:ASN:HA	1:353:A:THR:H	3	0.22
(1,1843)	1:342:A:SER:HB2	1:343:A:THR:H	7	0.22
(1,1843)	1:342:A:SER:HB3	1:343:A:THR:H	7	0.22
(1,1543)	1:317:A:TYR:HD1	1:389:A:ASP:HB2	9	0.22
(1,1543)	1:317:A:TYR:HD1	1:389:A:ASP:HB3	9	0.22
(1,1543)	1:317:A:TYR:HD2	1:389:A:ASP:HB2	9	0.22
(1,1543)	1:317:A:TYR:HD2	1:389:A:ASP:HB3	9	0.22
(1,1497)	1:315:A:PRO:HG2	1:389:A:ASP:HB2	10	0.22
(1,1497)	1:315:A:PRO:HG2	1:389:A:ASP:HB3	10	0.22
(1,1497)	1:315:A:PRO:HG3	1:389:A:ASP:HB2	10	0.22
(1,1497)	1:315:A:PRO:HG3	1:389:A:ASP:HB3	10	0.22
(1,1452)	1:313:A:PHE:HZ	1:345:A:THR:HA	17	0.22
(1,1443)	1:313:A:PHE:HB2	1:352:A:LEU:HD11	6	0.22
(1,1443)	1:313:A:PHE:HB2	1:352:A:LEU:HD12	6	0.22
(1,1443)	1:313:A:PHE:HB2	1:352:A:LEU:HD13	6	0.22
(1,1443)	1:313:A:PHE:HB3	1:352:A:LEU:HD11	6	0.22
(1,1443)	1:313:A:PHE:HB3	1:352:A:LEU:HD12	6	0.22
(1,1443)	1:313:A:PHE:HB3	1:352:A:LEU:HD13	6	0.22
(1,1420)	1:312:A:GLN:HE21	1:340:A:GLN:H	10	0.22
(1,1420)	1:312:A:GLN:HE22	1:340:A:GLN:H	10	0.22
(1,1324)	1:302:A:GLN:H	1:327:A:SER:H	14	0.22
(1,1318)	1:302:A:GLN:H	1:329:A:ASP:H	4	0.22
(1,1237)	1:300:A:TYR:H	1:326:A:ASP:HA	11	0.22
(1,1219)	1:299:A:LEU:H	1:306:A:ILE:H	4	0.22
(1,1140)	1:297:A:LEU:HA	1:309:A:ASP:HA	9	0.22
(1,1072)	1:295:A:HIS:HE1	1:311:A:GLU:HA	1	0.22
(1,1037)	1:290:A:ASN:HB2	1:292:A:ASP:H	3	0.22
(1,1037)	1:290:A:ASN:HB3	1:292:A:ASP:H	3	0.22
(1,974)	1:286:A:TRP:HE3	1:290:A:ASN:H	18	0.22
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	4	0.22
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	4	0.22
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB2	2	0.22
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB3	2	0.22
(1,620)	1:266:A:ASN:HB2	1:274:A:TYR:HE1	7	0.22
(1,620)	1:266:A:ASN:HB2	1:274:A:TYR:HE2	7	0.22
(1,620)	1:266:A:ASN:HB3	1:274:A:TYR:HE1	7	0.22
(1,620)	1:266:A:ASN:HB3	1:274:A:TYR:HE2	7	0.22
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB2	4	0.22
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB3	4	0.22
(1,447)	1:256:A:ASP:HA	1:258:A:ASN:HD21	16	0.22
(1,447)	1:256:A:ASP:HA	1:258:A:ASN:HD22	16	0.22
(1,376)	1:251:A:LYS:HG2	1:257:A:PHE:HA	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,376)	1:251:A:LYS:HG3	1:257:A:PHE:HA	11	0.22
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB2	19	0.22
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB3	19	0.22
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	18	0.22
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	15	0.22
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	18	0.22
(1,127)	1:236:A:ARG:HB2	1:237:A:ASN:H	13	0.22
(1,127)	1:236:A:ARG:HB3	1:237:A:ASN:H	13	0.22
(1,95)	1:234:A:TRP:HA	1:246:A:TYR:HE2	15	0.22
(1,85)	1:234:A:TRP:HE1	1:275:A:THR:HB	7	0.22
(1,49)	1:233:A:LEU:HA	1:236:A:ARG:H	6	0.22
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	2	0.22
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG11	8	0.21
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG12	8	0.21
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG13	8	0.21
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG11	8	0.21
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG12	8	0.21
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG13	8	0.21
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG11	8	0.21
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG12	8	0.21
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG13	8	0.21
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG21	8	0.21
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG22	8	0.21
(1,3983)	1:455:A:ILE:HD11	2:642:B:VAL:HG23	8	0.21
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG21	8	0.21
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG22	8	0.21
(1,3983)	1:455:A:ILE:HD12	2:642:B:VAL:HG23	8	0.21
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG21	8	0.21
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG22	8	0.21
(1,3983)	1:455:A:ILE:HD13	2:642:B:VAL:HG23	8	0.21
(1,3936)	1:490:A:LEU:HB2	1:494:A:ALA:H	4	0.21
(1,3936)	1:490:A:LEU:HB3	1:494:A:ALA:H	4	0.21
(1,3935)	1:490:A:LEU:HA	1:494:A:ALA:H	3	0.21
(1,3891)	1:486:A:VAL:HG11	1:490:A:LEU:H	6	0.21
(1,3891)	1:486:A:VAL:HG12	1:490:A:LEU:H	6	0.21
(1,3891)	1:486:A:VAL:HG13	1:490:A:LEU:H	6	0.21
(1,3891)	1:486:A:VAL:HG11	1:490:A:LEU:H	15	0.21
(1,3891)	1:486:A:VAL:HG12	1:490:A:LEU:H	15	0.21
(1,3891)	1:486:A:VAL:HG13	1:490:A:LEU:H	15	0.21
(1,3858)	1:482:A:SER:H	1:485:A:LYS:H	17	0.21
(1,3857)	1:481:A:GLN:HE21	1:482:A:SER:H	19	0.21
(1,3857)	1:481:A:GLN:HE22	1:482:A:SER:H	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3848)	1:481:A:GLN:HG2	1:486:A:VAL:HA	19	0.21
(1,3848)	1:481:A:GLN:HG3	1:486:A:VAL:HA	19	0.21
(1,3847)	1:481:A:GLN:HE21	1:486:A:VAL:HA	6	0.21
(1,3847)	1:481:A:GLN:HE22	1:486:A:VAL:HA	6	0.21
(1,3817)	1:475:A:PHE:HD2	1:476:A:ASP:HB2	16	0.21
(1,3708)	1:465:A:ASP:HB2	1:466:A:GLU:H	4	0.21
(1,3708)	1:465:A:ASP:HB3	1:466:A:GLU:H	4	0.21
(1,3598)	1:453:A:LYS:HG2	1:493:A:LEU:HB2	6	0.21
(1,3598)	1:453:A:LYS:HG2	1:493:A:LEU:HB3	6	0.21
(1,3567)	1:450:A:LEU:HA	1:454:A:GLY:H	6	0.21
(1,3562)	1:450:A:LEU:HB2	1:456:A:GLU:HA	8	0.21
(1,3562)	1:450:A:LEU:HB3	1:456:A:GLU:HA	8	0.21
(1,3476)	1:445:A:PRO:HG2	1:446:A:HIS:H	7	0.21
(1,3476)	1:445:A:PRO:HG3	1:446:A:HIS:H	7	0.21
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB2	3	0.21
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB3	3	0.21
(1,3332)	1:435:A:ALA:H	1:460:A:LEU:H	11	0.21
(1,3255)	1:433:A:ILE:HB	1:484:A:SER:H	20	0.21
(1,3248)	1:432:A:TYR:HA	1:457:A:VAL:HA	4	0.21
(1,3231)	1:432:A:TYR:H	1:483:A:VAL:H	20	0.21
(1,3147)	1:429:A:LYS:HD2	1:488:A:GLU:HG2	9	0.21
(1,3147)	1:429:A:LYS:HD2	1:488:A:GLU:HG3	9	0.21
(1,3147)	1:429:A:LYS:HD3	1:488:A:GLU:HG2	9	0.21
(1,3147)	1:429:A:LYS:HD3	1:488:A:GLU:HG3	9	0.21
(1,3099)	1:424:A:LYS:HG2	1:427:A:GLN:HE21	14	0.21
(1,3099)	1:424:A:LYS:HG2	1:427:A:GLN:HE22	14	0.21
(1,3099)	1:424:A:LYS:HG3	1:427:A:GLN:HE21	14	0.21
(1,3099)	1:424:A:LYS:HG3	1:427:A:GLN:HE22	14	0.21
(1,3094)	1:424:A:LYS:HG2	1:454:A:GLY:HA2	4	0.21
(1,3094)	1:424:A:LYS:HG2	1:454:A:GLY:HA3	4	0.21
(1,3094)	1:424:A:LYS:HG3	1:454:A:GLY:HA2	4	0.21
(1,3094)	1:424:A:LYS:HG3	1:454:A:GLY:HA3	4	0.21
(1,3028)	1:419:A:TYR:HA	1:422:A:ARG:HD2	6	0.21
(1,3028)	1:419:A:TYR:HA	1:422:A:ARG:HD3	6	0.21
(1,2892)	1:408:A:ASP:HA	1:442:A:LYS:HE2	2	0.21
(1,2892)	1:408:A:ASP:HA	1:442:A:LYS:HE3	2	0.21
(1,2880)	1:407:A:THR:H	1:409:A:SER:H	9	0.21
(1,2880)	1:407:A:THR:H	1:409:A:SER:H	10	0.21
(1,2871)	1:406:A:HIS:HA	1:456:A:GLU:HG2	12	0.21
(1,2871)	1:406:A:HIS:HA	1:456:A:GLU:HG3	12	0.21
(1,2824)	1:404:A:SER:H	1:414:A:VAL:HB	20	0.21
(1,2810)	1:404:A:SER:HA	1:459:A:LEU:HD11	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2810)	1:404:A:SER:HA	1:459:A:LEU:HD12	6	0.21
(1,2810)	1:404:A:SER:HA	1:459:A:LEU:HD13	6	0.21
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG11	6	0.21
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG12	6	0.21
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG13	6	0.21
(1,2781)	1:403:A:ALA:H	1:459:A:LEU:H	5	0.21
(1,2755)	1:402:A:PHE:HD2	1:460:A:LEU:HD13	12	0.21
(1,2631)	1:393:A:GLN:HA	1:396:A:ILE:H	17	0.21
(1,2619)	1:393:A:GLN:HE21	1:474:A:GLU:H	14	0.21
(1,2619)	1:393:A:GLN:HE22	1:474:A:GLU:H	14	0.21
(1,2613)	1:392:A:ASN:HD21	1:395:A:ALA:HB1	15	0.21
(1,2613)	1:392:A:ASN:HD21	1:395:A:ALA:HB2	15	0.21
(1,2613)	1:392:A:ASN:HD21	1:395:A:ALA:HB3	15	0.21
(1,2613)	1:392:A:ASN:HD22	1:395:A:ALA:HB1	15	0.21
(1,2613)	1:392:A:ASN:HD22	1:395:A:ALA:HB2	15	0.21
(1,2613)	1:392:A:ASN:HD22	1:395:A:ALA:HB3	15	0.21
(1,2594)	1:390:A:PHE:HA	1:393:A:GLN:HA	12	0.21
(1,2433)	1:380:A:LEU:H	1:383:A:LYS:H	6	0.21
(1,2382)	1:376:A:GLN:HG2	1:412:A:GLN:HE21	7	0.21
(1,2382)	1:376:A:GLN:HG2	1:412:A:GLN:HE22	7	0.21
(1,2382)	1:376:A:GLN:HG3	1:412:A:GLN:HE21	7	0.21
(1,2382)	1:376:A:GLN:HG3	1:412:A:GLN:HE22	7	0.21
(1,2351)	1:375:A:TRP:HE3	1:400:A:LEU:HA	12	0.21
(1,2290)	1:372:A:GLN:HG2	1:376:A:GLN:HE21	18	0.21
(1,2290)	1:372:A:GLN:HG2	1:376:A:GLN:HE22	18	0.21
(1,2290)	1:372:A:GLN:HG3	1:376:A:GLN:HE21	18	0.21
(1,2290)	1:372:A:GLN:HG3	1:376:A:GLN:HE22	18	0.21
(1,2196)	1:365:A:LYS:HE2	1:398:A:LYS:HE2	20	0.21
(1,2196)	1:365:A:LYS:HE2	1:398:A:LYS:HE3	20	0.21
(1,2196)	1:365:A:LYS:HE3	1:398:A:LYS:HE2	20	0.21
(1,2196)	1:365:A:LYS:HE3	1:398:A:LYS:HE3	20	0.21
(1,2132)	1:361:A:GLU:HA	1:371:A:TYR:HE1	17	0.21
(1,2123)	1:361:A:GLU:HA	1:399:A:LEU:HA	17	0.21
(1,2108)	1:360:A:LEU:HD21	1:364:A:ALA:H	15	0.21
(1,2108)	1:360:A:LEU:HD22	1:364:A:ALA:H	15	0.21
(1,2108)	1:360:A:LEU:HD23	1:364:A:ALA:H	15	0.21
(1,2041)	1:357:A:LEU:HD21	1:396:A:ILE:H	11	0.21
(1,2041)	1:357:A:LEU:HD22	1:396:A:ILE:H	11	0.21
(1,2041)	1:357:A:LEU:HD23	1:396:A:ILE:H	11	0.21
(1,1946)	1:351:A:ALA:HA	1:355:A:ARG:HD2	17	0.21
(1,1946)	1:351:A:ALA:HA	1:355:A:ARG:HD3	17	0.21
(1,1910)	1:348:A:LEU:HD11	1:352:A:LEU:H	17	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1910)	1:348:A:LEU:HD12	1:352:A:LEU:H	17	0.21
(1,1910)	1:348:A:LEU:HD13	1:352:A:LEU:H	17	0.21
(1,1897)	1:347:A:ASN:HA	1:351:A:ALA:H	8	0.21
(1,1889)	1:346:A:ARG:HA	1:349:A:ARG:HG2	1	0.21
(1,1886)	1:346:A:ARG:HG2	1:350:A:ASN:HD21	10	0.21
(1,1886)	1:346:A:ARG:HG2	1:350:A:ASN:HD22	10	0.21
(1,1886)	1:346:A:ARG:HG3	1:350:A:ASN:HD21	10	0.21
(1,1886)	1:346:A:ARG:HG3	1:350:A:ASN:HD22	10	0.21
(1,1882)	1:345:A:THR:HB	1:346:A:ARG:H	11	0.21
(1,1791)	1:337:A:GLU:H	1:340:A:GLN:H	18	0.21
(1,1762)	1:335:A:SER:H	1:339:A:LEU:H	16	0.21
(1,1676)	1:325:A:ILE:HD11	1:327:A:SER:HB2	18	0.21
(1,1676)	1:325:A:ILE:HD11	1:327:A:SER:HB3	18	0.21
(1,1676)	1:325:A:ILE:HD12	1:327:A:SER:HB2	18	0.21
(1,1676)	1:325:A:ILE:HD12	1:327:A:SER:HB3	18	0.21
(1,1676)	1:325:A:ILE:HD13	1:327:A:SER:HB2	18	0.21
(1,1676)	1:325:A:ILE:HD13	1:327:A:SER:HB3	18	0.21
(1,1626)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	17	0.21
(1,1578)	1:318:A:LEU:HA	1:382:A:LEU:HA	19	0.21
(1,1527)	1:316:A:ASN:H	1:349:A:ARG:HD2	10	0.21
(1,1527)	1:316:A:ASN:H	1:349:A:ARG:HD3	10	0.21
(1,1486)	1:314:A:MET:HB2	1:319:A:ARG:H	11	0.21
(1,1486)	1:314:A:MET:HB3	1:319:A:ARG:H	11	0.21
(1,1378)	1:307:A:MET:HE1	1:310:A:ALA:HB1	18	0.21
(1,1378)	1:307:A:MET:HE1	1:310:A:ALA:HB2	18	0.21
(1,1378)	1:307:A:MET:HE1	1:310:A:ALA:HB3	18	0.21
(1,1378)	1:307:A:MET:HE2	1:310:A:ALA:HB1	18	0.21
(1,1378)	1:307:A:MET:HE2	1:310:A:ALA:HB2	18	0.21
(1,1378)	1:307:A:MET:HE2	1:310:A:ALA:HB3	18	0.21
(1,1378)	1:307:A:MET:HE3	1:310:A:ALA:HB1	18	0.21
(1,1378)	1:307:A:MET:HE3	1:310:A:ALA:HB2	18	0.21
(1,1378)	1:307:A:MET:HE3	1:310:A:ALA:HB3	18	0.21
(1,1320)	1:302:A:GLN:H	1:328:A:SER:HA	11	0.21
(1,1223)	1:299:A:LEU:H	1:305:A:PHE:HA	17	0.21
(1,1139)	1:297:A:LEU:H	1:309:A:ASP:HA	7	0.21
(1,1090)	1:296:A:GLY:H	1:311:A:GLU:HA	2	0.21
(1,1053)	1:293:A:HIS:HB2	1:295:A:HIS:H	19	0.21
(1,1053)	1:293:A:HIS:HB3	1:295:A:HIS:H	19	0.21
(1,1044)	1:291:A:ARG:HA	1:293:A:HIS:HA	2	0.21
(1,877)	1:280:A:ILE:HA	1:322:A:ARG:H	1	0.21
(1,781)	1:277:A:LEU:H	1:324:A:LEU:H	6	0.21
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	12	0.21
(1,704)	1:273:A:GLU:HB2	1:328:A:SER:H	8	0.21
(1,704)	1:273:A:GLU:HB3	1:328:A:SER:H	8	0.21
(1,684)	1:272:A:GLN:HE21	1:351:A:ALA:H	8	0.21
(1,684)	1:272:A:GLN:HE22	1:351:A:ALA:H	8	0.21
(1,648)	1:268:A:VAL:HB	1:274:A:TYR:H	17	0.21
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD21	2	0.21
(1,606)	1:265:A:HIS:H	1:266:A:ASN:HD22	2	0.21
(1,513)	1:261:A:LEU:H	1:281:A:PRO:HA	9	0.21
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	2	0.21
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	2	0.21
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	2	0.21
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	2	0.21
(1,376)	1:251:A:LYS:HG2	1:257:A:PHE:HA	9	0.21
(1,376)	1:251:A:LYS:HG3	1:257:A:PHE:HA	9	0.21
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB2	3	0.21
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB3	3	0.21
(1,174)	1:240:A:GLU:HA	1:242:A:THR:H	15	0.21
(1,158)	1:238:A:LYS:HA	1:241:A:ILE:HB	1	0.21
(1,148)	1:238:A:LYS:HE2	1:266:A:ASN:HD21	15	0.21
(1,148)	1:238:A:LYS:HE2	1:266:A:ASN:HD22	15	0.21
(1,148)	1:238:A:LYS:HE3	1:266:A:ASN:HD21	15	0.21
(1,148)	1:238:A:LYS:HE3	1:266:A:ASN:HD22	15	0.21
(1,110)	1:235:A:THR:HG1	1:267:A:ARG:HD2	17	0.21
(1,110)	1:235:A:THR:HG1	1:267:A:ARG:HD3	17	0.21
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD2	13	0.21
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD3	13	0.21
(1,44)	1:233:A:LEU:HD11	1:242:A:THR:H	17	0.21
(1,44)	1:233:A:LEU:HD12	1:242:A:THR:H	17	0.21
(1,44)	1:233:A:LEU:HD13	1:242:A:THR:H	17	0.21
(1,3943)	1:490:A:LEU:HA	1:492:A:LYS:H	19	0.2
(1,3935)	1:490:A:LEU:HA	1:494:A:ALA:H	8	0.2
(1,3891)	1:486:A:VAL:HG11	1:490:A:LEU:H	10	0.2
(1,3891)	1:486:A:VAL:HG12	1:490:A:LEU:H	10	0.2
(1,3891)	1:486:A:VAL:HG13	1:490:A:LEU:H	10	0.2
(1,3845)	1:481:A:GLN:HG2	1:487:A:ASP:H	12	0.2
(1,3845)	1:481:A:GLN:HG3	1:487:A:ASP:H	12	0.2
(1,3802)	1:475:A:PHE:H	1:480:A:PHE:H	13	0.2
(1,3700)	1:465:A:ASP:HA	1:468:A:MET:H	12	0.2
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	18	0.2
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	18	0.2
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3635)	1:458:A:LEU:HD12	1:480:A:PHE:HE1	12	0.2
(1,3570)	1:450:A:LEU:HA	1:453:A:LYS:H	4	0.2
(1,3492)	1:447:A:LEU:HA	1:483:A:VAL:HB	19	0.2
(1,3231)	1:432:A:TYR:H	1:483:A:VAL:H	17	0.2
(1,3222)	1:431:A:TYR:HD1	1:456:A:GLU:H	19	0.2
(1,3222)	1:431:A:TYR:HD2	1:456:A:GLU:H	19	0.2
(1,3218)	1:431:A:TYR:H	1:457:A:VAL:HA	11	0.2
(1,3214)	1:431:A:TYR:H	1:458:A:LEU:H	1	0.2
(1,3207)	1:431:A:TYR:HA	1:482:A:SER:HA	15	0.2
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD11	3	0.2
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD12	3	0.2
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD13	3	0.2
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB2	13	0.2
(1,3149)	1:429:A:LYS:HB2	1:481:A:GLN:HB3	13	0.2
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB2	13	0.2
(1,3149)	1:429:A:LYS:HB3	1:481:A:GLN:HB3	13	0.2
(1,3143)	1:429:A:LYS:HD2	1:489:A:SER:H	1	0.2
(1,3143)	1:429:A:LYS:HD3	1:489:A:SER:H	1	0.2
(1,3136)	1:428:A:GLU:HG2	1:478:A:LYS:HA	11	0.2
(1,3136)	1:428:A:GLU:HG3	1:478:A:LYS:HA	11	0.2
(1,3113)	1:426:A:GLY:HA2	1:428:A:GLU:HB2	11	0.2
(1,3113)	1:426:A:GLY:HA2	1:428:A:GLU:HB3	11	0.2
(1,3113)	1:426:A:GLY:HA3	1:428:A:GLU:HB2	11	0.2
(1,3113)	1:426:A:GLY:HA3	1:428:A:GLU:HB3	11	0.2
(1,2989)	1:417:A:GLU:HA	1:420:A:VAL:HB	7	0.2
(1,2914)	1:410:A:SER:HA	1:438:A:TYR:HD2	17	0.2
(1,2888)	1:408:A:ASP:HA	1:459:A:LEU:HD11	16	0.2
(1,2888)	1:408:A:ASP:HA	1:459:A:LEU:HD12	16	0.2
(1,2888)	1:408:A:ASP:HA	1:459:A:LEU:HD13	16	0.2
(1,2874)	1:406:A:HIS:HB2	1:422:A:ARG:HD2	5	0.2
(1,2874)	1:406:A:HIS:HB2	1:422:A:ARG:HD3	5	0.2
(1,2874)	1:406:A:HIS:HB3	1:422:A:ARG:HD2	5	0.2
(1,2874)	1:406:A:HIS:HB3	1:422:A:ARG:HD3	5	0.2
(1,2871)	1:406:A:HIS:HA	1:456:A:GLU:HG2	6	0.2
(1,2871)	1:406:A:HIS:HA	1:456:A:GLU:HG3	6	0.2
(1,2831)	1:404:A:SER:H	1:406:A:HIS:H	6	0.2
(1,2789)	1:403:A:ALA:HA	1:414:A:VAL:H	18	0.2
(1,2734)	1:401:A:ARG:HA	1:415:A:SER:HB2	18	0.2
(1,2734)	1:401:A:ARG:HA	1:415:A:SER:HB3	18	0.2
(1,2699)	1:398:A:LYS:HE2	1:417:A:GLU:HG2	4	0.2
(1,2699)	1:398:A:LYS:HE2	1:417:A:GLU:HG3	4	0.2
(1,2699)	1:398:A:LYS:HE3	1:417:A:GLU:HG2	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2699)	1:398:A:LYS:HE3	1:417:A:GLU:HG3	4	0.2
(1,2574)	1:388:A:GLU:H	1:390:A:PHE:H	7	0.2
(1,2445)	1:381:A:VAL:HA	1:385:A:GLY:H	11	0.2
(1,2425)	1:380:A:LEU:HB2	1:464:A:ILE:H	13	0.2
(1,2425)	1:380:A:LEU:HB3	1:464:A:ILE:H	13	0.2
(1,2348)	1:375:A:TRP:HZ3	1:401:A:ARG:H	1	0.2
(1,2323)	1:374:A:PHE:HZ	1:378:A:PHE:HB2	18	0.2
(1,2323)	1:374:A:PHE:HZ	1:378:A:PHE:HB3	18	0.2
(1,2203)	1:365:A:LYS:HA	1:367:A:ASP:H	15	0.2
(1,2108)	1:360:A:LEU:HD21	1:364:A:ALA:H	2	0.2
(1,2108)	1:360:A:LEU:HD22	1:364:A:ALA:H	2	0.2
(1,2108)	1:360:A:LEU:HD23	1:364:A:ALA:H	2	0.2
(1,2107)	1:360:A:LEU:HA	1:364:A:ALA:H	5	0.2
(1,2046)	1:357:A:LEU:HB2	1:395:A:ALA:HB1	13	0.2
(1,2046)	1:357:A:LEU:HB2	1:395:A:ALA:HB2	13	0.2
(1,2046)	1:357:A:LEU:HB2	1:395:A:ALA:HB3	13	0.2
(1,2046)	1:357:A:LEU:HB3	1:395:A:ALA:HB1	13	0.2
(1,2046)	1:357:A:LEU:HB3	1:395:A:ALA:HB2	13	0.2
(1,2046)	1:357:A:LEU:HB3	1:395:A:ALA:HB3	13	0.2
(1,2041)	1:357:A:LEU:HD21	1:396:A:ILE:H	17	0.2
(1,2041)	1:357:A:LEU:HD22	1:396:A:ILE:H	17	0.2
(1,2041)	1:357:A:LEU:HD23	1:396:A:ILE:H	17	0.2
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD11	7	0.2
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD12	7	0.2
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD13	7	0.2
(1,1994)	1:354:A:LYS:HA	1:358:A:GLN:H	14	0.2
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD11	7	0.2
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD12	7	0.2
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD13	7	0.2
(1,1933)	1:350:A:ASN:HA	1:354:A:LYS:H	17	0.2
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD21	10	0.2
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD22	10	0.2
(1,1883)	1:345:A:THR:HB	1:346:A:ARG:HB2	12	0.2
(1,1883)	1:345:A:THR:HB	1:346:A:ARG:HB3	12	0.2
(1,1882)	1:345:A:THR:HB	1:346:A:ARG:H	10	0.2
(1,1871)	1:345:A:THR:HA	1:349:A:ARG:H	8	0.2
(1,1827)	1:340:A:GLN:HA	1:342:A:SER:H	5	0.2
(1,1776)	1:336:A:ARG:HA	1:340:A:GLN:H	2	0.2
(1,1457)	1:313:A:PHE:HE1	1:339:A:LEU:HD11	14	0.2
(1,1457)	1:313:A:PHE:HE1	1:339:A:LEU:HD12	14	0.2
(1,1457)	1:313:A:PHE:HE1	1:339:A:LEU:HD13	14	0.2
(1,1457)	1:313:A:PHE:HE2	1:339:A:LEU:HD11	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1457)	1:313:A:PHE:HE2	1:339:A:LEU:HD12	14	0.2
(1,1457)	1:313:A:PHE:HE2	1:339:A:LEU:HD13	14	0.2
(1,1424)	1:312:A:GLN:HG2	1:340:A:GLN:HB2	20	0.2
(1,1424)	1:312:A:GLN:HG2	1:340:A:GLN:HB3	20	0.2
(1,1424)	1:312:A:GLN:HG3	1:340:A:GLN:HB2	20	0.2
(1,1424)	1:312:A:GLN:HG3	1:340:A:GLN:HB3	20	0.2
(1,1334)	1:303:A:ARG:H	1:327:A:SER:H	9	0.2
(1,1321)	1:302:A:GLN:HA	1:328:A:SER:HA	3	0.2
(1,1318)	1:302:A:GLN:H	1:329:A:ASP:H	3	0.2
(1,1290)	1:301:A:VAL:HA	1:327:A:SER:H	14	0.2
(1,1284)	1:301:A:VAL:HA	1:329:A:ASP:H	15	0.2
(1,1223)	1:299:A:LEU:H	1:305:A:PHE:HA	4	0.2
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD11	17	0.2
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD12	17	0.2
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD13	17	0.2
(1,1161)	1:298:A:LYS:H	1:310:A:ALA:H	9	0.2
(1,1090)	1:296:A:GLY:H	1:311:A:GLU:HA	14	0.2
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD21	19	0.2
(1,1070)	1:295:A:HIS:HE1	1:316:A:ASN:HD22	19	0.2
(1,1024)	1:289:A:TRP:HH2	1:381:A:VAL:HA	7	0.2
(1,1022)	1:289:A:TRP:HH2	1:381:A:VAL:H	16	0.2
(1,958)	1:285:A:PRO:HG2	1:320:A:PHE:HA	9	0.2
(1,958)	1:285:A:PRO:HG3	1:320:A:PHE:HA	9	0.2
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	17	0.2
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	4	0.2
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	4	0.2
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	8	0.2
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	8	0.2
(1,763)	1:276:A:SER:HA	1:326:A:ASP:H	7	0.2
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB2	14	0.2
(1,656)	1:268:A:VAL:HB	1:272:A:GLN:HB3	14	0.2
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	7	0.2
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	7	0.2
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB2	20	0.2
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB3	20	0.2
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	9	0.2
(1,219)	1:244:A:GLU:HA	1:248:A:GLU:H	5	0.2
(1,218)	1:243:A:ASP:HB2	1:244:A:GLU:H	11	0.2
(1,218)	1:243:A:ASP:HB3	1:244:A:GLU:H	11	0.2
(1,174)	1:240:A:GLU:HA	1:242:A:THR:H	6	0.2
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD11	20	0.2
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD12	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD13	20	0.2
(1,3935)	1:490:A:LEU:HA	1:494:A:ALA:H	7	0.19
(1,3915)	1:488:A:GLU:HA	1:492:A:LYS:H	13	0.19
(1,3857)	1:481:A:GLN:HE21	1:482:A:SER:H	8	0.19
(1,3857)	1:481:A:GLN:HE22	1:482:A:SER:H	8	0.19
(1,3807)	1:475:A:PHE:H	1:479:A:PRO:HA	19	0.19
(1,3476)	1:445:A:PRO:HG2	1:446:A:HIS:H	4	0.19
(1,3476)	1:445:A:PRO:HG3	1:446:A:HIS:H	4	0.19
(1,3208)	1:431:A:TYR:HB2	1:482:A:SER:HA	11	0.19
(1,3208)	1:431:A:TYR:HB3	1:482:A:SER:HA	11	0.19
(1,3153)	1:429:A:LYS:HA	1:480:A:PHE:H	7	0.19
(1,3151)	1:429:A:LYS:HG2	1:481:A:GLN:HB2	14	0.19
(1,3151)	1:429:A:LYS:HG2	1:481:A:GLN:HB3	14	0.19
(1,3151)	1:429:A:LYS:HG3	1:481:A:GLN:HB2	14	0.19
(1,3151)	1:429:A:LYS:HG3	1:481:A:GLN:HB3	14	0.19
(1,3147)	1:429:A:LYS:HD2	1:488:A:GLU:HG2	19	0.19
(1,3147)	1:429:A:LYS:HD2	1:488:A:GLU:HG3	19	0.19
(1,3147)	1:429:A:LYS:HD3	1:488:A:GLU:HG2	19	0.19
(1,3147)	1:429:A:LYS:HD3	1:488:A:GLU:HG3	19	0.19
(1,3135)	1:428:A:GLU:HA	1:478:A:LYS:HA	4	0.19
(1,3135)	1:428:A:GLU:HA	1:478:A:LYS:HA	20	0.19
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG2	7	0.19
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG3	7	0.19
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG2	7	0.19
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG3	7	0.19
(1,3113)	1:426:A:GLY:HA2	1:428:A:GLU:HB2	16	0.19
(1,3113)	1:426:A:GLY:HA2	1:428:A:GLU:HB3	16	0.19
(1,3113)	1:426:A:GLY:HA3	1:428:A:GLU:HB2	16	0.19
(1,3113)	1:426:A:GLY:HA3	1:428:A:GLU:HB3	16	0.19
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE21	9	0.19
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE22	9	0.19
(1,3084)	1:423:A:MET:HE1	1:427:A:GLN:HG2	9	0.19
(1,3084)	1:423:A:MET:HE1	1:427:A:GLN:HG3	9	0.19
(1,3084)	1:423:A:MET:HE2	1:427:A:GLN:HG2	9	0.19
(1,3084)	1:423:A:MET:HE2	1:427:A:GLN:HG3	9	0.19
(1,3084)	1:423:A:MET:HE3	1:427:A:GLN:HG2	9	0.19
(1,3084)	1:423:A:MET:HE3	1:427:A:GLN:HG3	9	0.19
(1,2989)	1:417:A:GLU:HA	1:420:A:VAL:HB	2	0.19
(1,2989)	1:417:A:GLU:HA	1:420:A:VAL:HB	15	0.19
(1,2980)	1:417:A:GLU:H	1:475:A:PHE:HZ	11	0.19
(1,2968)	1:416:A:LEU:HA	1:420:A:VAL:H	4	0.19
(1,2892)	1:408:A:ASP:HA	1:442:A:LYS:HE2	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2892)	1:408:A:ASP:HA	1:442:A:LYS:HE3	4	0.19
(1,2862)	1:405:A:THR:HG21	1:408:A:ASP:HA	8	0.19
(1,2862)	1:405:A:THR:HG22	1:408:A:ASP:HA	8	0.19
(1,2862)	1:405:A:THR:HG23	1:408:A:ASP:HA	8	0.19
(1,2855)	1:405:A:THR:HB	1:451:A:ARG:HA	18	0.19
(1,2825)	1:404:A:SER:H	1:414:A:VAL:HG11	1	0.19
(1,2825)	1:404:A:SER:H	1:414:A:VAL:HG12	1	0.19
(1,2825)	1:404:A:SER:H	1:414:A:VAL:HG13	1	0.19
(1,2737)	1:401:A:ARG:HD2	1:414:A:VAL:HA	14	0.19
(1,2737)	1:401:A:ARG:HD3	1:414:A:VAL:HA	14	0.19
(1,2538)	1:386:A:PRO:HA	1:471:A:TYR:HB2	1	0.19
(1,2538)	1:386:A:PRO:HA	1:471:A:TYR:HB3	1	0.19
(1,2426)	1:380:A:LEU:HD22	1:464:A:ILE:H	2	0.19
(1,2380)	1:376:A:GLN:HE21	1:412:A:GLN:H	15	0.19
(1,2380)	1:376:A:GLN:HE22	1:412:A:GLN:H	15	0.19
(1,2365)	1:375:A:TRP:HA	1:379:A:GLY:H	9	0.19
(1,2318)	1:374:A:PHE:HZ	1:382:A:LEU:HB2	6	0.19
(1,2318)	1:374:A:PHE:HZ	1:382:A:LEU:HB3	6	0.19
(1,2250)	1:370:A:LYS:HA	1:373:A:THR:HB	19	0.19
(1,2210)	1:367:A:ASP:H	1:371:A:TYR:H	3	0.19
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	14	0.19
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	14	0.19
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	14	0.19
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	14	0.19
(1,2181)	1:364:A:ALA:HA	1:371:A:TYR:HD1	9	0.19
(1,2181)	1:364:A:ALA:HA	1:371:A:TYR:HD2	9	0.19
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG2	18	0.19
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG3	18	0.19
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG2	18	0.19
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG3	18	0.19
(1,2042)	1:357:A:LEU:HD21	1:396:A:ILE:HA	6	0.19
(1,2042)	1:357:A:LEU:HD22	1:396:A:ILE:HA	6	0.19
(1,2042)	1:357:A:LEU:HD23	1:396:A:ILE:HA	6	0.19
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD11	2	0.19
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD12	2	0.19
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD13	2	0.19
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD21	1	0.19
(1,1991)	1:354:A:LYS:HE2	1:392:A:ASN:HD22	1	0.19
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD21	1	0.19
(1,1991)	1:354:A:LYS:HE3	1:392:A:ASN:HD22	1	0.19
(1,1933)	1:350:A:ASN:HA	1:354:A:LYS:H	13	0.19
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD21	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1885)	1:346:A:ARG:HA	1:350:A:ASN:HD22	1	0.19
(1,1883)	1:345:A:THR:HB	1:346:A:ARG:HB2	19	0.19
(1,1883)	1:345:A:THR:HB	1:346:A:ARG:HB3	19	0.19
(1,1882)	1:345:A:THR:HB	1:346:A:ARG:H	2	0.19
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	9	0.19
(1,1779)	1:336:A:ARG:HG2	1:340:A:GLN:HB2	18	0.19
(1,1779)	1:336:A:ARG:HG2	1:340:A:GLN:HB3	18	0.19
(1,1779)	1:336:A:ARG:HG3	1:340:A:GLN:HB2	18	0.19
(1,1779)	1:336:A:ARG:HG3	1:340:A:GLN:HB3	18	0.19
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE1	20	0.19
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE2	20	0.19
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE3	20	0.19
(1,1610)	1:319:A:ARG:HA	1:321:A:VAL:HB	17	0.19
(1,1373)	1:307:A:MET:HE1	1:335:A:SER:H	2	0.19
(1,1373)	1:307:A:MET:HE2	1:335:A:SER:H	2	0.19
(1,1373)	1:307:A:MET:HE3	1:335:A:SER:H	2	0.19
(1,1354)	1:305:A:PHE:HE2	1:307:A:MET:HA	11	0.19
(1,1278)	1:301:A:VAL:HG11	1:332:A:LEU:HD11	4	0.19
(1,1278)	1:301:A:VAL:HG11	1:332:A:LEU:HD12	4	0.19
(1,1278)	1:301:A:VAL:HG11	1:332:A:LEU:HD13	4	0.19
(1,1278)	1:301:A:VAL:HG12	1:332:A:LEU:HD11	4	0.19
(1,1278)	1:301:A:VAL:HG12	1:332:A:LEU:HD12	4	0.19
(1,1278)	1:301:A:VAL:HG12	1:332:A:LEU:HD13	4	0.19
(1,1278)	1:301:A:VAL:HG13	1:332:A:LEU:HD11	4	0.19
(1,1278)	1:301:A:VAL:HG13	1:332:A:LEU:HD12	4	0.19
(1,1278)	1:301:A:VAL:HG13	1:332:A:LEU:HD13	4	0.19
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE1	17	0.19
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE2	17	0.19
(1,1197)	1:299:A:LEU:HA	1:325:A:ILE:H	11	0.19
(1,1074)	1:295:A:HIS:HA	1:309:A:ASP:HA	11	0.19
(1,966)	1:285:A:PRO:HD2	1:288:A:MET:HE1	10	0.19
(1,966)	1:285:A:PRO:HD2	1:288:A:MET:HE2	10	0.19
(1,966)	1:285:A:PRO:HD2	1:288:A:MET:HE3	10	0.19
(1,966)	1:285:A:PRO:HD3	1:288:A:MET:HE1	10	0.19
(1,966)	1:285:A:PRO:HD3	1:288:A:MET:HE2	10	0.19
(1,966)	1:285:A:PRO:HD3	1:288:A:MET:HE3	10	0.19
(1,963)	1:285:A:PRO:HG2	1:288:A:MET:H	6	0.19
(1,963)	1:285:A:PRO:HG3	1:288:A:MET:H	6	0.19
(1,960)	1:285:A:PRO:HB2	1:294:A:LYS:HB2	17	0.19
(1,960)	1:285:A:PRO:HB2	1:294:A:LYS:HB3	17	0.19
(1,960)	1:285:A:PRO:HB3	1:294:A:LYS:HB2	17	0.19
(1,960)	1:285:A:PRO:HB3	1:294:A:LYS:HB3	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,876)	1:280:A:ILE:H	1:322:A:ARG:H	1	0.19
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	8	0.19
(1,740)	1:275:A:THR:H	1:328:A:SER:H	15	0.19
(1,673)	1:270:A:GLY:H	1:273:A:GLU:HA	9	0.19
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	17	0.19
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	17	0.19
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD1	4	0.19
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD2	4	0.19
(1,473)	1:260:A:PRO:HA	1:281:A:PRO:HA	8	0.19
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	3	0.19
(1,335)	1:250:A:TYR:HE1	1:281:A:PRO:HA	13	0.19
(1,335)	1:250:A:TYR:HE2	1:281:A:PRO:HA	13	0.19
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	8	0.19
(1,294)	1:248:A:GLU:HA	1:251:A:LYS:HB2	5	0.19
(1,294)	1:248:A:GLU:HA	1:251:A:LYS:HB3	5	0.19
(1,269)	1:247:A:LYS:HG2	1:263:A:TRP:HZ3	20	0.19
(1,269)	1:247:A:LYS:HG3	1:263:A:TRP:HZ3	20	0.19
(1,251)	1:246:A:TYR:HE1	1:263:A:TRP:HE1	12	0.19
(1,251)	1:246:A:TYR:HE2	1:263:A:TRP:HE1	12	0.19
(1,180)	1:241:A:ILE:HB	1:246:A:TYR:HD1	16	0.19
(1,180)	1:241:A:ILE:HB	1:246:A:TYR:HD2	16	0.19
(1,158)	1:238:A:LYS:HA	1:241:A:ILE:HB	18	0.19
(1,89)	1:234:A:TRP:HA	1:265:A:HIS:HE1	14	0.19
(1,52)	1:233:A:LEU:HA	1:235:A:THR:H	15	0.19
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	15	0.18
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	15	0.18
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	15	0.18
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	15	0.18
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	15	0.18
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	15	0.18
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	15	0.18
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	15	0.18
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	15	0.18
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	18	0.18
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	18	0.18
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	18	0.18
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	18	0.18
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	18	0.18
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	18	0.18
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	18	0.18
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	18	0.18
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3938)	1:490:A:LEU:HA	1:493:A:LEU:H	5	0.18
(1,3896)	1:486:A:VAL:HA	1:489:A:SER:HB2	4	0.18
(1,3896)	1:486:A:VAL:HA	1:489:A:SER:HB3	4	0.18
(1,3749)	1:469:A:MET:HA	1:471:A:TYR:H	2	0.18
(1,3519)	1:448:A:GLU:HB2	1:452:A:LYS:H	14	0.18
(1,3519)	1:448:A:GLU:HB3	1:452:A:LYS:H	14	0.18
(1,3499)	1:447:A:LEU:HD21	1:457:A:VAL:HB	5	0.18
(1,3499)	1:447:A:LEU:HD22	1:457:A:VAL:HB	5	0.18
(1,3499)	1:447:A:LEU:HD23	1:457:A:VAL:HB	5	0.18
(1,3353)	1:436:A:ASP:HA	1:461:A:SER:HA	19	0.18
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG2	9	0.18
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG3	9	0.18
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG2	9	0.18
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG3	9	0.18
(1,3098)	1:424:A:LYS:HB2	1:427:A:GLN:HE21	5	0.18
(1,3098)	1:424:A:LYS:HB2	1:427:A:GLN:HE22	5	0.18
(1,3098)	1:424:A:LYS:HB3	1:427:A:GLN:HE21	5	0.18
(1,3098)	1:424:A:LYS:HB3	1:427:A:GLN:HE22	5	0.18
(1,2989)	1:417:A:GLU:HA	1:420:A:VAL:HB	1	0.18
(1,2985)	1:417:A:GLU:HB2	1:421:A:SER:H	4	0.18
(1,2985)	1:417:A:GLU:HB3	1:421:A:SER:H	4	0.18
(1,2824)	1:404:A:SER:H	1:414:A:VAL:HB	15	0.18
(1,2793)	1:403:A:ALA:H	1:413:A:THR:H	12	0.18
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG11	19	0.18
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG12	19	0.18
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG13	19	0.18
(1,2736)	1:401:A:ARG:HD2	1:414:A:VAL:H	14	0.18
(1,2736)	1:401:A:ARG:HD3	1:414:A:VAL:H	14	0.18
(1,2566)	1:387:A:ALA:H	1:468:A:MET:HA	13	0.18
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD1	15	0.18
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD2	15	0.18
(1,2538)	1:386:A:PRO:HA	1:471:A:TYR:HB2	4	0.18
(1,2538)	1:386:A:PRO:HA	1:471:A:TYR:HB3	4	0.18
(1,2380)	1:376:A:GLN:HE21	1:412:A:GLN:H	11	0.18
(1,2380)	1:376:A:GLN:HE22	1:412:A:GLN:H	11	0.18
(1,2196)	1:365:A:LYS:HE2	1:398:A:LYS:HE2	8	0.18
(1,2196)	1:365:A:LYS:HE2	1:398:A:LYS:HE3	8	0.18
(1,2196)	1:365:A:LYS:HE3	1:398:A:LYS:HE2	8	0.18
(1,2196)	1:365:A:LYS:HE3	1:398:A:LYS:HE3	8	0.18
(1,2181)	1:364:A:ALA:HA	1:371:A:TYR:HD1	5	0.18
(1,2181)	1:364:A:ALA:HA	1:371:A:TYR:HD2	5	0.18
(1,2181)	1:364:A:ALA:HA	1:371:A:TYR:HD1	13	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2181)	1:364:A:ALA:HA	1:371:A:TYR:HD2	13	0.18
(1,2123)	1:361:A:GLU:HA	1:399:A:LEU:HA	7	0.18
(1,2108)	1:360:A:LEU:HD21	1:364:A:ALA:H	9	0.18
(1,2108)	1:360:A:LEU:HD22	1:364:A:ALA:H	9	0.18
(1,2108)	1:360:A:LEU:HD23	1:364:A:ALA:H	9	0.18
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD11	4	0.18
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD12	4	0.18
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD13	4	0.18
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB1	10	0.18
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB2	10	0.18
(1,1993)	1:354:A:LYS:HE2	1:391:A:ALA:HB3	10	0.18
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB1	10	0.18
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB2	10	0.18
(1,1993)	1:354:A:LYS:HE3	1:391:A:ALA:HB3	10	0.18
(1,1859)	1:344:A:VAL:HB	1:348:A:LEU:H	9	0.18
(1,1847)	1:343:A:THR:HG21	1:347:A:ASN:HD21	6	0.18
(1,1847)	1:343:A:THR:HG21	1:347:A:ASN:HD22	6	0.18
(1,1847)	1:343:A:THR:HG22	1:347:A:ASN:HD21	6	0.18
(1,1847)	1:343:A:THR:HG22	1:347:A:ASN:HD22	6	0.18
(1,1847)	1:343:A:THR:HG23	1:347:A:ASN:HD21	6	0.18
(1,1847)	1:343:A:THR:HG23	1:347:A:ASN:HD22	6	0.18
(1,1843)	1:342:A:SER:HB2	1:343:A:THR:H	15	0.18
(1,1843)	1:342:A:SER:HB3	1:343:A:THR:H	15	0.18
(1,1528)	1:316:A:ASN:HA	1:319:A:ARG:H	12	0.18
(1,1375)	1:307:A:MET:HE1	1:335:A:SER:HB2	7	0.18
(1,1375)	1:307:A:MET:HE1	1:335:A:SER:HB3	7	0.18
(1,1375)	1:307:A:MET:HE2	1:335:A:SER:HB2	7	0.18
(1,1375)	1:307:A:MET:HE2	1:335:A:SER:HB3	7	0.18
(1,1375)	1:307:A:MET:HE3	1:335:A:SER:HB2	7	0.18
(1,1375)	1:307:A:MET:HE3	1:335:A:SER:HB3	7	0.18
(1,1334)	1:303:A:ARG:H	1:327:A:SER:H	3	0.18
(1,1334)	1:303:A:ARG:H	1:327:A:SER:H	18	0.18
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD11	19	0.18
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD12	19	0.18
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD13	19	0.18
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD11	19	0.18
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD12	19	0.18
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD13	19	0.18
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD11	19	0.18
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD12	19	0.18
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD13	19	0.18
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD11	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD12	4	0.18
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD13	4	0.18
(1,1167)	1:298:A:LYS:HA	1:309:A:ASP:HA	2	0.18
(1,1060)	1:294:A:LYS:HD2	1:309:A:ASP:HB2	19	0.18
(1,1060)	1:294:A:LYS:HD2	1:309:A:ASP:HB3	19	0.18
(1,1060)	1:294:A:LYS:HD3	1:309:A:ASP:HB2	19	0.18
(1,1060)	1:294:A:LYS:HD3	1:309:A:ASP:HB3	19	0.18
(1,1053)	1:293:A:HIS:HB2	1:295:A:HIS:H	3	0.18
(1,1053)	1:293:A:HIS:HB3	1:295:A:HIS:H	3	0.18
(1,1023)	1:289:A:TRP:HZ2	1:381:A:VAL:H	3	0.18
(1,877)	1:280:A:ILE:HA	1:322:A:ARG:H	9	0.18
(1,700)	1:273:A:GLU:HB2	1:329:A:ASP:H	15	0.18
(1,700)	1:273:A:GLU:HB3	1:329:A:ASP:H	15	0.18
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	10	0.18
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	14	0.18
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	14	0.18
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	15	0.18
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	15	0.18
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD1	1	0.18
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD2	1	0.18
(1,509)	1:261:A:LEU:H	1:282:A:SER:H	15	0.18
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	2	0.18
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	4	0.18
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	11	0.18
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD2	4	0.18
(1,406)	1:253:A:ILE:HB	1:322:A:ARG:HD3	4	0.18
(1,382)	1:251:A:LYS:HA	1:255:A:HIS:HA	17	0.18
(1,368)	1:251:A:LYS:HE2	1:260:A:PRO:HD2	1	0.18
(1,368)	1:251:A:LYS:HE2	1:260:A:PRO:HD3	1	0.18
(1,368)	1:251:A:LYS:HE3	1:260:A:PRO:HD2	1	0.18
(1,368)	1:251:A:LYS:HE3	1:260:A:PRO:HD3	1	0.18
(1,320)	1:249:A:PHE:H	1:252:A:HIS:H	5	0.18
(1,306)	1:249:A:PHE:HD1	1:323:A:GLY:HA2	2	0.18
(1,306)	1:249:A:PHE:HD1	1:323:A:GLY:HA3	2	0.18
(1,306)	1:249:A:PHE:HD2	1:323:A:GLY:HA2	2	0.18
(1,306)	1:249:A:PHE:HD2	1:323:A:GLY:HA3	2	0.18
(1,153)	1:238:A:LYS:HE2	1:264:A:SER:HA	9	0.18
(1,153)	1:238:A:LYS:HE3	1:264:A:SER:HA	9	0.18
(1,120)	1:236:A:ARG:HB2	1:241:A:ILE:H	13	0.18
(1,120)	1:236:A:ARG:HB3	1:241:A:ILE:H	13	0.18
(1,111)	1:235:A:THR:H	1:265:A:HIS:HE1	4	0.18
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD2	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:235:A:THR:HB	1:303:A:ARG:HD3	14	0.18
(1,84)	1:234:A:TRP:HD1	1:275:A:THR:HB	12	0.18
(1,75)	1:234:A:TRP:HZ2	1:300:A:TYR:HE1	18	0.18
(1,75)	1:234:A:TRP:HZ2	1:300:A:TYR:HE2	18	0.18
(1,2)	1:230:A:ALA:H	1:231:A:GLN:H	20	0.18
(2,14)	1:442:A:LYS:H	1:461:A:SER:HB2	17	0.17
(2,14)	1:442:A:LYS:H	1:461:A:SER:HB3	17	0.17
(1,3749)	1:469:A:MET:HA	1:471:A:TYR:H	7	0.17
(1,3749)	1:469:A:MET:HA	1:471:A:TYR:H	10	0.17
(1,3536)	1:449:A:LEU:HA	1:453:A:LYS:H	12	0.17
(1,3519)	1:448:A:GLU:HB2	1:452:A:LYS:H	7	0.17
(1,3519)	1:448:A:GLU:HB3	1:452:A:LYS:H	7	0.17
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB2	13	0.17
(1,3363)	1:437:A:SER:H	1:461:A:SER:HB3	13	0.17
(1,3309)	1:434:A:THR:HB	1:466:A:GLU:H	16	0.17
(1,3248)	1:432:A:TYR:HA	1:457:A:VAL:HA	3	0.17
(1,3248)	1:432:A:TYR:HA	1:457:A:VAL:HA	14	0.17
(1,3207)	1:431:A:TYR:HA	1:482:A:SER:HA	11	0.17
(1,3135)	1:428:A:GLU:HA	1:478:A:LYS:HA	5	0.17
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD11	15	0.17
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD12	15	0.17
(1,3117)	1:427:A:GLN:HA	1:493:A:LEU:HD13	15	0.17
(1,3007)	1:419:A:TYR:HE2	1:478:A:LYS:HG2	15	0.17
(1,3007)	1:419:A:TYR:HE2	1:478:A:LYS:HG3	15	0.17
(1,2989)	1:417:A:GLU:HA	1:420:A:VAL:HB	4	0.17
(1,2988)	1:417:A:GLU:HA	1:420:A:VAL:H	14	0.17
(1,2911)	1:410:A:SER:HA	1:438:A:TYR:HD1	1	0.17
(1,2911)	1:410:A:SER:HA	1:438:A:TYR:HD2	1	0.17
(1,2876)	1:406:A:HIS:HB2	1:414:A:VAL:HG21	15	0.17
(1,2876)	1:406:A:HIS:HB2	1:414:A:VAL:HG22	15	0.17
(1,2876)	1:406:A:HIS:HB2	1:414:A:VAL:HG23	15	0.17
(1,2876)	1:406:A:HIS:HB3	1:414:A:VAL:HG21	15	0.17
(1,2876)	1:406:A:HIS:HB3	1:414:A:VAL:HG22	15	0.17
(1,2876)	1:406:A:HIS:HB3	1:414:A:VAL:HG23	15	0.17
(1,2831)	1:404:A:SER:H	1:406:A:HIS:H	8	0.17
(1,2830)	1:404:A:SER:H	1:407:A:THR:HB	19	0.17
(1,2828)	1:404:A:SER:H	1:412:A:GLN:HA	20	0.17
(1,2813)	1:404:A:SER:HB2	1:458:A:LEU:HA	17	0.17
(1,2813)	1:404:A:SER:HB3	1:458:A:LEU:HA	17	0.17
(1,2796)	1:403:A:ALA:H	1:412:A:GLN:HA	14	0.17
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG11	9	0.17
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG12	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG13	9	0.17
(1,2739)	1:401:A:ARG:HD2	1:413:A:THR:HA	10	0.17
(1,2739)	1:401:A:ARG:HD3	1:413:A:THR:HA	10	0.17
(1,2701)	1:398:A:LYS:HA	1:416:A:LEU:H	10	0.17
(1,2590)	1:390:A:PHE:HD1	1:471:A:TYR:HB2	8	0.17
(1,2590)	1:390:A:PHE:HD1	1:471:A:TYR:HB3	8	0.17
(1,2590)	1:390:A:PHE:HD2	1:471:A:TYR:HB2	8	0.17
(1,2590)	1:390:A:PHE:HD2	1:471:A:TYR:HB3	8	0.17
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD1	10	0.17
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD2	10	0.17
(1,2398)	1:378:A:PHE:HA	1:382:A:LEU:H	10	0.17
(1,2337)	1:375:A:TRP:HD1	1:413:A:THR:HA	20	0.17
(1,2317)	1:374:A:PHE:HZ	1:382:A:LEU:H	11	0.17
(1,2199)	1:365:A:LYS:HA	1:368:A:ALA:H	16	0.17
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG2	15	0.17
(1,2197)	1:365:A:LYS:HE2	1:398:A:LYS:HG3	15	0.17
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG2	15	0.17
(1,2197)	1:365:A:LYS:HE3	1:398:A:LYS:HG3	15	0.17
(1,2196)	1:365:A:LYS:HE2	1:398:A:LYS:HE2	19	0.17
(1,2196)	1:365:A:LYS:HE2	1:398:A:LYS:HE3	19	0.17
(1,2196)	1:365:A:LYS:HE3	1:398:A:LYS:HE2	19	0.17
(1,2196)	1:365:A:LYS:HE3	1:398:A:LYS:HE3	19	0.17
(1,2181)	1:364:A:ALA:HA	1:371:A:TYR:HD1	15	0.17
(1,2181)	1:364:A:ALA:HA	1:371:A:TYR:HD2	15	0.17
(1,2122)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	14	0.17
(1,2122)	1:361:A:GLU:HG3	1:401:A:ARG:HH22	15	0.17
(1,2107)	1:360:A:LEU:HA	1:364:A:ALA:H	2	0.17
(1,2107)	1:360:A:LEU:HA	1:364:A:ALA:H	9	0.17
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD11	9	0.17
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD12	9	0.17
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD13	9	0.17
(1,1945)	1:351:A:ALA:HA	1:355:A:ARG:H	3	0.17
(1,1938)	1:350:A:ASN:HA	1:353:A:THR:HB	15	0.17
(1,1858)	1:344:A:VAL:HA	1:348:A:LEU:H	9	0.17
(1,1816)	1:339:A:LEU:HA	1:342:A:SER:H	10	0.17
(1,1349)	1:305:A:PHE:HZ	1:308:A:ASP:HA	4	0.17
(1,1278)	1:301:A:VAL:HG11	1:332:A:LEU:HD11	10	0.17
(1,1278)	1:301:A:VAL:HG11	1:332:A:LEU:HD12	10	0.17
(1,1278)	1:301:A:VAL:HG11	1:332:A:LEU:HD13	10	0.17
(1,1278)	1:301:A:VAL:HG12	1:332:A:LEU:HD11	10	0.17
(1,1278)	1:301:A:VAL:HG12	1:332:A:LEU:HD12	10	0.17
(1,1278)	1:301:A:VAL:HG12	1:332:A:LEU:HD13	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1278)	1:301:A:VAL:HG13	1:332:A:LEU:HD11	10	0.17
(1,1278)	1:301:A:VAL:HG13	1:332:A:LEU:HD12	10	0.17
(1,1278)	1:301:A:VAL:HG13	1:332:A:LEU:HD13	10	0.17
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD11	18	0.17
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD12	18	0.17
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD13	18	0.17
(1,1197)	1:299:A:LEU:HA	1:325:A:ILE:H	16	0.17
(1,1167)	1:298:A:LYS:HA	1:309:A:ASP:HA	7	0.17
(1,1162)	1:298:A:LYS:HA	1:310:A:ALA:H	9	0.17
(1,1132)	1:297:A:LEU:H	1:310:A:ALA:H	16	0.17
(1,1074)	1:295:A:HIS:HA	1:309:A:ASP:HA	8	0.17
(1,1037)	1:290:A:ASN:HB2	1:292:A:ASP:H	4	0.17
(1,1037)	1:290:A:ASN:HB3	1:292:A:ASP:H	4	0.17
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	12	0.17
(1,941)	1:284:A:ALA:H	1:377:A:GLN:HA	8	0.17
(1,876)	1:280:A:ILE:H	1:322:A:ARG:H	2	0.17
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	10	0.17
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	3	0.17
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	3	0.17
(1,763)	1:276:A:SER:HA	1:326:A:ASP:H	19	0.17
(1,673)	1:270:A:GLY:H	1:273:A:GLU:HA	8	0.17
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	17	0.17
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	17	0.17
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	19	0.17
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	19	0.17
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	7	0.17
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	10	0.17
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD21	14	0.17
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD22	14	0.17
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB2	10	0.17
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB3	10	0.17
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB2	19	0.17
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB3	19	0.17
(1,513)	1:261:A:LEU:H	1:281:A:PRO:HA	4	0.17
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD2	4	0.17
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD3	4	0.17
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD2	4	0.17
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD3	4	0.17
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD2	4	0.17
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD3	4	0.17
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	7	0.17
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	7	0.17
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	7	0.17
(1,372)	1:251:A:LYS:HG2	1:259:A:ASP:HA	13	0.17
(1,372)	1:251:A:LYS:HG3	1:259:A:ASP:HA	13	0.17
(1,353)	1:250:A:TYR:HE1	1:256:A:ASP:HB2	16	0.17
(1,353)	1:250:A:TYR:HE1	1:256:A:ASP:HB3	16	0.17
(1,353)	1:250:A:TYR:HE2	1:256:A:ASP:HB2	16	0.17
(1,353)	1:250:A:TYR:HE2	1:256:A:ASP:HB3	16	0.17
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	13	0.17
(1,127)	1:236:A:ARG:HB2	1:237:A:ASN:H	15	0.17
(1,127)	1:236:A:ARG:HB3	1:237:A:ASN:H	15	0.17
(1,95)	1:234:A:TRP:HA	1:246:A:TYR:HE2	13	0.17
(1,21)	1:232:A:ALA:H	1:235:A:THR:H	13	0.17
(1,19)	1:232:A:ALA:HA	1:249:A:PHE:HE1	5	0.17
(1,19)	1:232:A:ALA:HA	1:249:A:PHE:HE2	5	0.17
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG21	16	0.16
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG22	16	0.16
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG23	16	0.16
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG21	16	0.16
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG22	16	0.16
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG23	16	0.16
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG21	16	0.16
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG22	16	0.16
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG23	16	0.16
(1,3891)	1:486:A:VAL:HG11	1:490:A:LEU:H	3	0.16
(1,3891)	1:486:A:VAL:HG12	1:490:A:LEU:H	3	0.16
(1,3891)	1:486:A:VAL:HG13	1:490:A:LEU:H	3	0.16
(1,3869)	1:483:A:VAL:HB	1:490:A:LEU:HD11	14	0.16
(1,3869)	1:483:A:VAL:HB	1:490:A:LEU:HD12	14	0.16
(1,3869)	1:483:A:VAL:HB	1:490:A:LEU:HD13	14	0.16
(1,3848)	1:481:A:GLN:HG2	1:486:A:VAL:HA	9	0.16
(1,3848)	1:481:A:GLN:HG3	1:486:A:VAL:HA	9	0.16
(1,3841)	1:481:A:GLN:HG2	1:489:A:SER:HA	3	0.16
(1,3841)	1:481:A:GLN:HG3	1:489:A:SER:HA	3	0.16
(1,3772)	1:472:A:LEU:HD21	1:474:A:GLU:HA	4	0.16
(1,3772)	1:472:A:LEU:HD22	1:474:A:GLU:HA	4	0.16
(1,3772)	1:472:A:LEU:HD23	1:474:A:GLU:HA	4	0.16
(1,3744)	1:469:A:MET:HA	1:472:A:LEU:H	4	0.16
(1,3567)	1:450:A:LEU:HA	1:454:A:GLY:H	14	0.16
(1,3540)	1:449:A:LEU:HA	1:452:A:LYS:H	13	0.16
(1,3492)	1:447:A:LEU:HA	1:483:A:VAL:HB	4	0.16
(1,3478)	1:446:A:HIS:HD2	1:486:A:VAL:HG21	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3478)	1:446:A:HIS:HD2	1:486:A:VAL:HG22	11	0.16
(1,3478)	1:446:A:HIS:HD2	1:486:A:VAL:HG23	11	0.16
(1,3477)	1:446:A:HIS:HD2	1:490:A:LEU:HD11	11	0.16
(1,3477)	1:446:A:HIS:HD2	1:490:A:LEU:HD12	11	0.16
(1,3477)	1:446:A:HIS:HD2	1:490:A:LEU:HD13	11	0.16
(1,3372)	1:437:A:SER:H	1:439:A:ALA:H	11	0.16
(1,3365)	1:437:A:SER:H	1:441:A:ALA:H	4	0.16
(1,3262)	1:433:A:ILE:H	1:482:A:SER:HA	3	0.16
(1,3242)	1:432:A:TYR:HA	1:459:A:LEU:HA	18	0.16
(1,3222)	1:431:A:TYR:HD1	1:456:A:GLU:H	4	0.16
(1,3222)	1:431:A:TYR:HD2	1:456:A:GLU:H	4	0.16
(1,3218)	1:431:A:TYR:H	1:457:A:VAL:HA	13	0.16
(1,3208)	1:431:A:TYR:HB2	1:482:A:SER:HA	15	0.16
(1,3208)	1:431:A:TYR:HB3	1:482:A:SER:HA	15	0.16
(1,3176)	1:430:A:ILE:HB	1:480:A:PHE:HD2	10	0.16
(1,3170)	1:430:A:ILE:H	1:481:A:GLN:H	14	0.16
(1,3164)	1:429:A:LYS:HB2	1:431:A:TYR:HE1	16	0.16
(1,3164)	1:429:A:LYS:HB2	1:431:A:TYR:HE2	16	0.16
(1,3164)	1:429:A:LYS:HB3	1:431:A:TYR:HE1	16	0.16
(1,3164)	1:429:A:LYS:HB3	1:431:A:TYR:HE2	16	0.16
(1,3163)	1:429:A:LYS:H	1:431:A:TYR:HE1	6	0.16
(1,3163)	1:429:A:LYS:H	1:431:A:TYR:HE2	6	0.16
(1,3154)	1:429:A:LYS:HA	1:480:A:PHE:HA	2	0.16
(1,3154)	1:429:A:LYS:HA	1:480:A:PHE:HA	9	0.16
(1,3147)	1:429:A:LYS:HD2	1:488:A:GLU:HG2	13	0.16
(1,3147)	1:429:A:LYS:HD2	1:488:A:GLU:HG3	13	0.16
(1,3147)	1:429:A:LYS:HD3	1:488:A:GLU:HG2	13	0.16
(1,3147)	1:429:A:LYS:HD3	1:488:A:GLU:HG3	13	0.16
(1,3143)	1:429:A:LYS:HD2	1:489:A:SER:H	7	0.16
(1,3143)	1:429:A:LYS:HD3	1:489:A:SER:H	7	0.16
(1,2984)	1:417:A:GLU:HA	1:421:A:SER:H	1	0.16
(1,2913)	1:410:A:SER:HA	1:438:A:TYR:HE1	17	0.16
(1,2913)	1:410:A:SER:HA	1:438:A:TYR:HE2	17	0.16
(1,2912)	1:410:A:SER:HB2	1:438:A:TYR:HD1	15	0.16
(1,2912)	1:410:A:SER:HB2	1:438:A:TYR:HD2	15	0.16
(1,2912)	1:410:A:SER:HB3	1:438:A:TYR:HD1	15	0.16
(1,2912)	1:410:A:SER:HB3	1:438:A:TYR:HD2	15	0.16
(1,2816)	1:404:A:SER:HA	1:457:A:VAL:HB	5	0.16
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG11	18	0.16
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG12	18	0.16
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG13	18	0.16
(1,2696)	1:398:A:LYS:HA	1:475:A:PHE:HE1	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2696)	1:398:A:LYS:HA	1:475:A:PHE:HE2	6	0.16
(1,2658)	1:395:A:ALA:HA	1:398:A:LYS:HB2	6	0.16
(1,2658)	1:395:A:ALA:HA	1:398:A:LYS:HB3	6	0.16
(1,2640)	1:394:A:GLU:HA	1:475:A:PHE:HA	9	0.16
(1,2632)	1:393:A:GLN:HA	1:396:A:ILE:HB	1	0.16
(1,2574)	1:388:A:GLU:H	1:390:A:PHE:H	5	0.16
(1,2574)	1:388:A:GLU:H	1:390:A:PHE:H	19	0.16
(1,2544)	1:386:A:PRO:HG2	1:397:A:ALA:H	13	0.16
(1,2544)	1:386:A:PRO:HG3	1:397:A:ALA:H	13	0.16
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD11	7	0.16
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD12	7	0.16
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD13	7	0.16
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD11	14	0.16
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD12	14	0.16
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD13	14	0.16
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD11	16	0.16
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD12	16	0.16
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD13	16	0.16
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD11	17	0.16
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD12	17	0.16
(1,2507)	1:384:A:GLU:H	1:464:A:ILE:HD13	17	0.16
(1,2445)	1:381:A:VAL:HA	1:385:A:GLY:H	14	0.16
(1,2335)	1:375:A:TRP:HH2	1:468:A:MET:HE1	9	0.16
(1,2335)	1:375:A:TRP:HH2	1:468:A:MET:HE2	9	0.16
(1,2335)	1:375:A:TRP:HH2	1:468:A:MET:HE3	9	0.16
(1,2317)	1:374:A:PHE:HZ	1:382:A:LEU:H	5	0.16
(1,2290)	1:372:A:GLN:HG2	1:376:A:GLN:HE21	3	0.16
(1,2290)	1:372:A:GLN:HG2	1:376:A:GLN:HE22	3	0.16
(1,2290)	1:372:A:GLN:HG3	1:376:A:GLN:HE21	3	0.16
(1,2290)	1:372:A:GLN:HG3	1:376:A:GLN:HE22	3	0.16
(1,2290)	1:372:A:GLN:HG2	1:376:A:GLN:HE21	17	0.16
(1,2290)	1:372:A:GLN:HG2	1:376:A:GLN:HE22	17	0.16
(1,2290)	1:372:A:GLN:HG3	1:376:A:GLN:HE21	17	0.16
(1,2290)	1:372:A:GLN:HG3	1:376:A:GLN:HE22	17	0.16
(1,2053)	1:357:A:LEU:HA	1:361:A:GLU:H	13	0.16
(1,2041)	1:357:A:LEU:HD21	1:396:A:ILE:H	6	0.16
(1,2041)	1:357:A:LEU:HD22	1:396:A:ILE:H	6	0.16
(1,2041)	1:357:A:LEU:HD23	1:396:A:ILE:H	6	0.16
(1,1954)	1:351:A:ALA:HA	1:353:A:THR:HB	19	0.16
(1,1938)	1:350:A:ASN:HA	1:353:A:THR:HB	3	0.16
(1,1933)	1:350:A:ASN:HA	1:354:A:LYS:H	15	0.16
(1,1882)	1:345:A:THR:HB	1:346:A:ARG:H	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1843)	1:342:A:SER:HB2	1:343:A:THR:H	8	0.16
(1,1843)	1:342:A:SER:HB3	1:343:A:THR:H	8	0.16
(1,1810)	1:339:A:LEU:HA	1:345:A:THR:H	16	0.16
(1,1768)	1:335:A:SER:H	1:338:A:ILE:HD11	8	0.16
(1,1768)	1:335:A:SER:H	1:338:A:ILE:HD12	8	0.16
(1,1768)	1:335:A:SER:H	1:338:A:ILE:HD13	8	0.16
(1,1578)	1:318:A:LEU:HA	1:382:A:LEU:HA	17	0.16
(1,1420)	1:312:A:GLN:HE21	1:340:A:GLN:H	5	0.16
(1,1420)	1:312:A:GLN:HE22	1:340:A:GLN:H	5	0.16
(1,1419)	1:312:A:GLN:HB2	1:345:A:THR:HG21	16	0.16
(1,1419)	1:312:A:GLN:HB2	1:345:A:THR:HG22	16	0.16
(1,1419)	1:312:A:GLN:HB2	1:345:A:THR:HG23	16	0.16
(1,1419)	1:312:A:GLN:HB3	1:345:A:THR:HG21	16	0.16
(1,1419)	1:312:A:GLN:HB3	1:345:A:THR:HG22	16	0.16
(1,1419)	1:312:A:GLN:HB3	1:345:A:THR:HG23	16	0.16
(1,1374)	1:307:A:MET:HE1	1:335:A:SER:HA	6	0.16
(1,1374)	1:307:A:MET:HE2	1:335:A:SER:HA	6	0.16
(1,1374)	1:307:A:MET:HE3	1:335:A:SER:HA	6	0.16
(1,1354)	1:305:A:PHE:HE2	1:307:A:MET:HA	4	0.16
(1,1353)	1:305:A:PHE:HE1	1:307:A:MET:HA	4	0.16
(1,1353)	1:305:A:PHE:HE2	1:307:A:MET:HA	4	0.16
(1,1320)	1:302:A:GLN:H	1:328:A:SER:HA	20	0.16
(1,1223)	1:299:A:LEU:H	1:305:A:PHE:HA	1	0.16
(1,1223)	1:299:A:LEU:H	1:305:A:PHE:HA	3	0.16
(1,1219)	1:299:A:LEU:H	1:306:A:ILE:H	20	0.16
(1,1139)	1:297:A:LEU:H	1:309:A:ASP:HA	3	0.16
(1,1044)	1:291:A:ARG:HA	1:293:A:HIS:HA	20	0.16
(1,997)	1:287:A:ASP:HA	1:289:A:TRP:H	8	0.16
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	5	0.16
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	9	0.16
(1,707)	1:273:A:GLU:H	1:327:A:SER:HA	19	0.16
(1,701)	1:273:A:GLU:H	1:329:A:ASP:HA	15	0.16
(1,665)	1:269:A:GLU:HA	1:274:A:TYR:H	1	0.16
(1,570)	1:264:A:SER:HB2	1:359:A:MET:HA	2	0.16
(1,570)	1:264:A:SER:HB3	1:359:A:MET:HA	2	0.16
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	17	0.16
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	19	0.16
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	19	0.16
(1,509)	1:261:A:LEU:H	1:282:A:SER:H	12	0.16
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	11	0.16
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	2	0.16
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:255:A:HIS:HE1	1:308:A:ASP:HB2	16	0.16
(1,439)	1:255:A:HIS:HE1	1:308:A:ASP:HB3	16	0.16
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD2	9	0.16
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD3	9	0.16
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD2	9	0.16
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD3	9	0.16
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD2	9	0.16
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD3	9	0.16
(1,376)	1:251:A:LYS:HG2	1:257:A:PHE:HA	2	0.16
(1,376)	1:251:A:LYS:HG3	1:257:A:PHE:HA	2	0.16
(1,376)	1:251:A:LYS:HG2	1:257:A:PHE:HA	15	0.16
(1,376)	1:251:A:LYS:HG3	1:257:A:PHE:HA	15	0.16
(1,347)	1:250:A:TYR:HE1	1:260:A:PRO:HA	7	0.16
(1,347)	1:250:A:TYR:HE2	1:260:A:PRO:HA	7	0.16
(1,319)	1:249:A:PHE:HE1	1:253:A:ILE:HD11	7	0.16
(1,319)	1:249:A:PHE:HE1	1:253:A:ILE:HD12	7	0.16
(1,319)	1:249:A:PHE:HE1	1:253:A:ILE:HD13	7	0.16
(1,319)	1:249:A:PHE:HE2	1:253:A:ILE:HD11	7	0.16
(1,319)	1:249:A:PHE:HE2	1:253:A:ILE:HD12	7	0.16
(1,319)	1:249:A:PHE:HE2	1:253:A:ILE:HD13	7	0.16
(1,307)	1:249:A:PHE:HE1	1:323:A:GLY:HA2	2	0.16
(1,307)	1:249:A:PHE:HE1	1:323:A:GLY:HA3	2	0.16
(1,307)	1:249:A:PHE:HE2	1:323:A:GLY:HA2	2	0.16
(1,307)	1:249:A:PHE:HE2	1:323:A:GLY:HA3	2	0.16
(1,251)	1:246:A:TYR:HE1	1:263:A:TRP:HE1	4	0.16
(1,251)	1:246:A:TYR:HE2	1:263:A:TRP:HE1	4	0.16
(1,218)	1:243:A:ASP:HB2	1:244:A:GLU:H	7	0.16
(1,218)	1:243:A:ASP:HB3	1:244:A:GLU:H	7	0.16
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	6	0.16
(1,161)	1:238:A:LYS:H	1:240:A:GLU:H	19	0.16
(2,3)	1:257:A:PHE:HA	1:259:A:ASP:HA	3	0.15
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD11	1	0.15
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD12	1	0.15
(1,3980)	1:423:A:MET:HE1	2:639:B:LEU:HD13	1	0.15
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD11	1	0.15
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD12	1	0.15
(1,3980)	1:423:A:MET:HE2	2:639:B:LEU:HD13	1	0.15
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD11	1	0.15
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD12	1	0.15
(1,3980)	1:423:A:MET:HE3	2:639:B:LEU:HD13	1	0.15
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG11	17	0.15
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG12	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3979)	1:483:A:VAL:HG11	2:635:B:VAL:HG13	17	0.15
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG11	17	0.15
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG12	17	0.15
(1,3979)	1:483:A:VAL:HG12	2:635:B:VAL:HG13	17	0.15
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG11	17	0.15
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG12	17	0.15
(1,3979)	1:483:A:VAL:HG13	2:635:B:VAL:HG13	17	0.15
(1,3972)	1:318:A:LEU:HD11	2:622:B:TYR:HE1	7	0.15
(1,3972)	1:318:A:LEU:HD12	2:622:B:TYR:HE1	7	0.15
(1,3972)	1:318:A:LEU:HD13	2:622:B:TYR:HE1	7	0.15
(1,3935)	1:490:A:LEU:HA	1:494:A:ALA:H	16	0.15
(1,3911)	1:487:A:ASP:H	1:489:A:SER:HB2	2	0.15
(1,3911)	1:487:A:ASP:H	1:489:A:SER:HB3	2	0.15
(1,3749)	1:469:A:MET:HA	1:471:A:TYR:H	13	0.15
(1,3744)	1:469:A:MET:HA	1:472:A:LEU:H	19	0.15
(1,3742)	1:469:A:MET:HE1	1:473:A:THR:HA	3	0.15
(1,3742)	1:469:A:MET:HE2	1:473:A:THR:HA	3	0.15
(1,3742)	1:469:A:MET:HE3	1:473:A:THR:HA	3	0.15
(1,3730)	1:468:A:MET:HA	1:471:A:TYR:HD1	14	0.15
(1,3730)	1:468:A:MET:HA	1:471:A:TYR:HD2	14	0.15
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	16	0.15
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	16	0.15
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	16	0.15
(1,3561)	1:450:A:LEU:HD11	1:456:A:GLU:H	15	0.15
(1,3561)	1:450:A:LEU:HD12	1:456:A:GLU:H	15	0.15
(1,3561)	1:450:A:LEU:HD13	1:456:A:GLU:H	15	0.15
(1,3541)	1:449:A:LEU:HA	1:452:A:LYS:HB2	12	0.15
(1,3541)	1:449:A:LEU:HA	1:452:A:LYS:HB3	12	0.15
(1,3540)	1:449:A:LEU:HA	1:452:A:LYS:H	1	0.15
(1,3530)	1:449:A:LEU:HD11	1:494:A:ALA:HA	14	0.15
(1,3530)	1:449:A:LEU:HD12	1:494:A:ALA:HA	14	0.15
(1,3530)	1:449:A:LEU:HD13	1:494:A:ALA:HA	14	0.15
(1,3530)	1:449:A:LEU:HD21	1:494:A:ALA:HA	14	0.15
(1,3530)	1:449:A:LEU:HD22	1:494:A:ALA:HA	14	0.15
(1,3530)	1:449:A:LEU:HD23	1:494:A:ALA:HA	14	0.15
(1,3364)	1:437:A:SER:HA	1:461:A:SER:HB2	20	0.15
(1,3364)	1:437:A:SER:HA	1:461:A:SER:HB3	20	0.15
(1,3341)	1:435:A:ALA:HB1	1:440:A:ALA:HA	18	0.15
(1,3341)	1:435:A:ALA:HB2	1:440:A:ALA:HA	18	0.15
(1,3341)	1:435:A:ALA:HB3	1:440:A:ALA:HA	18	0.15
(1,3294)	1:433:A:ILE:HB	1:441:A:ALA:HA	18	0.15
(1,3218)	1:431:A:TYR:H	1:457:A:VAL:HA	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3218)	1:431:A:TYR:H	1:457:A:VAL:HA	19	0.15
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD11	14	0.15
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD12	14	0.15
(1,3169)	1:429:A:LYS:HA	1:430:A:ILE:HD13	14	0.15
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG2	16	0.15
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG3	16	0.15
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG2	16	0.15
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG3	16	0.15
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE21	10	0.15
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE22	10	0.15
(1,3084)	1:423:A:MET:HE1	1:427:A:GLN:HG2	4	0.15
(1,3084)	1:423:A:MET:HE1	1:427:A:GLN:HG3	4	0.15
(1,3084)	1:423:A:MET:HE2	1:427:A:GLN:HG2	4	0.15
(1,3084)	1:423:A:MET:HE2	1:427:A:GLN:HG3	4	0.15
(1,3084)	1:423:A:MET:HE3	1:427:A:GLN:HG2	4	0.15
(1,3084)	1:423:A:MET:HE3	1:427:A:GLN:HG3	4	0.15
(1,3007)	1:419:A:TYR:HE2	1:478:A:LYS:HG2	12	0.15
(1,3007)	1:419:A:TYR:HE2	1:478:A:LYS:HG3	12	0.15
(1,2997)	1:418:A:ASP:HA	1:422:A:ARG:HG2	19	0.15
(1,2997)	1:418:A:ASP:HA	1:422:A:ARG:HG3	19	0.15
(1,2988)	1:417:A:GLU:HA	1:420:A:VAL:H	1	0.15
(1,2985)	1:417:A:GLU:HB2	1:421:A:SER:H	2	0.15
(1,2985)	1:417:A:GLU:HB3	1:421:A:SER:H	2	0.15
(1,2961)	1:416:A:LEU:HB2	1:475:A:PHE:HZ	3	0.15
(1,2961)	1:416:A:LEU:HB3	1:475:A:PHE:HZ	3	0.15
(1,2845)	1:405:A:THR:H	1:457:A:VAL:H	13	0.15
(1,2827)	1:404:A:SER:H	1:413:A:THR:H	11	0.15
(1,2808)	1:404:A:SER:HB2	1:459:A:LEU:H	3	0.15
(1,2808)	1:404:A:SER:HB3	1:459:A:LEU:H	3	0.15
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG11	2	0.15
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG12	2	0.15
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG13	2	0.15
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG11	2	0.15
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG12	2	0.15
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG13	2	0.15
(1,2621)	1:393:A:GLN:HE21	1:473:A:THR:H	12	0.15
(1,2621)	1:393:A:GLN:HE22	1:473:A:THR:H	12	0.15
(1,2565)	1:387:A:ALA:HB2	1:471:A:TYR:HD1	7	0.15
(1,2508)	1:384:A:GLU:HA	1:464:A:ILE:HD11	7	0.15
(1,2508)	1:384:A:GLU:HA	1:464:A:ILE:HD12	7	0.15
(1,2508)	1:384:A:GLU:HA	1:464:A:ILE:HD13	7	0.15
(1,2484)	1:383:A:LYS:HB2	1:464:A:ILE:HD11	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2484)	1:383:A:LYS:HB2	1:464:A:ILE:HD12	15	0.15
(1,2484)	1:383:A:LYS:HB2	1:464:A:ILE:HD13	15	0.15
(1,2484)	1:383:A:LYS:HB3	1:464:A:ILE:HD11	15	0.15
(1,2484)	1:383:A:LYS:HB3	1:464:A:ILE:HD12	15	0.15
(1,2484)	1:383:A:LYS:HB3	1:464:A:ILE:HD13	15	0.15
(1,2448)	1:381:A:VAL:HA	1:384:A:GLU:H	17	0.15
(1,2437)	1:380:A:LEU:H	1:382:A:LEU:H	7	0.15
(1,2346)	1:375:A:TRP:HH2	1:401:A:ARG:H	9	0.15
(1,2340)	1:375:A:TRP:HD1	1:412:A:GLN:HE21	9	0.15
(1,2340)	1:375:A:TRP:HD1	1:412:A:GLN:HE22	9	0.15
(1,2340)	1:375:A:TRP:HD1	1:412:A:GLN:HE21	19	0.15
(1,2340)	1:375:A:TRP:HD1	1:412:A:GLN:HE22	19	0.15
(1,2337)	1:375:A:TRP:HD1	1:413:A:THR:HA	12	0.15
(1,2314)	1:374:A:PHE:HZ	1:399:A:LEU:HD11	19	0.15
(1,2314)	1:374:A:PHE:HZ	1:399:A:LEU:HD12	19	0.15
(1,2314)	1:374:A:PHE:HZ	1:399:A:LEU:HD13	19	0.15
(1,2250)	1:370:A:LYS:HA	1:373:A:THR:HB	7	0.15
(1,2250)	1:370:A:LYS:HA	1:373:A:THR:HB	13	0.15
(1,2203)	1:365:A:LYS:HA	1:367:A:ASP:H	14	0.15
(1,2196)	1:365:A:LYS:HE2	1:398:A:LYS:HE2	6	0.15
(1,2196)	1:365:A:LYS:HE2	1:398:A:LYS:HE3	6	0.15
(1,2196)	1:365:A:LYS:HE3	1:398:A:LYS:HE2	6	0.15
(1,2196)	1:365:A:LYS:HE3	1:398:A:LYS:HE3	6	0.15
(1,2045)	1:357:A:LEU:HD21	1:395:A:ALA:H	5	0.15
(1,2045)	1:357:A:LEU:HD22	1:395:A:ALA:H	5	0.15
(1,2045)	1:357:A:LEU:HD23	1:395:A:ALA:H	5	0.15
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE21	12	0.15
(1,2015)	1:355:A:ARG:HA	1:358:A:GLN:HE22	12	0.15
(1,2013)	1:355:A:ARG:HA	1:358:A:GLN:H	13	0.15
(1,1994)	1:354:A:LYS:HA	1:358:A:GLN:H	10	0.15
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD11	2	0.15
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD12	2	0.15
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD13	2	0.15
(1,1958)	1:352:A:LEU:HA	1:356:A:VAL:H	3	0.15
(1,1910)	1:348:A:LEU:HD11	1:352:A:LEU:H	13	0.15
(1,1910)	1:348:A:LEU:HD12	1:352:A:LEU:H	13	0.15
(1,1910)	1:348:A:LEU:HD13	1:352:A:LEU:H	13	0.15
(1,1858)	1:344:A:VAL:HA	1:348:A:LEU:H	10	0.15
(1,1790)	1:337:A:GLU:HG2	1:341:A:ASP:HB2	12	0.15
(1,1790)	1:337:A:GLU:HG2	1:341:A:ASP:HB3	12	0.15
(1,1790)	1:337:A:GLU:HG3	1:341:A:ASP:HB2	12	0.15
(1,1790)	1:337:A:GLU:HG3	1:341:A:ASP:HB3	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1621)	1:320:A:PHE:HE1	1:378:A:PHE:HB2	17	0.15
(1,1621)	1:320:A:PHE:HE1	1:378:A:PHE:HB3	17	0.15
(1,1621)	1:320:A:PHE:HE2	1:378:A:PHE:HB2	17	0.15
(1,1621)	1:320:A:PHE:HE2	1:378:A:PHE:HB3	17	0.15
(1,1505)	1:315:A:PRO:HD2	1:350:A:ASN:HA	18	0.15
(1,1505)	1:315:A:PRO:HD3	1:350:A:ASN:HA	18	0.15
(1,1353)	1:305:A:PHE:HE1	1:307:A:MET:HA	9	0.15
(1,1353)	1:305:A:PHE:HE2	1:307:A:MET:HA	9	0.15
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD11	16	0.15
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD12	16	0.15
(1,1244)	1:300:A:TYR:H	1:325:A:ILE:HD13	16	0.15
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD11	16	0.15
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD12	16	0.15
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD13	16	0.15
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD11	16	0.15
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD12	16	0.15
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD13	16	0.15
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD11	16	0.15
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD12	16	0.15
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD13	16	0.15
(1,1140)	1:297:A:LEU:HA	1:309:A:ASP:HA	20	0.15
(1,1053)	1:293:A:HIS:HB2	1:295:A:HIS:H	2	0.15
(1,1053)	1:293:A:HIS:HB3	1:295:A:HIS:H	2	0.15
(1,1053)	1:293:A:HIS:HB2	1:295:A:HIS:H	16	0.15
(1,1053)	1:293:A:HIS:HB3	1:295:A:HIS:H	16	0.15
(1,988)	1:287:A:ASP:HB2	1:293:A:HIS:HA	12	0.15
(1,988)	1:287:A:ASP:HB3	1:293:A:HIS:HA	12	0.15
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	3	0.15
(1,764)	1:276:A:SER:HB2	1:326:A:ASP:H	15	0.15
(1,764)	1:276:A:SER:HB3	1:326:A:ASP:H	15	0.15
(1,763)	1:276:A:SER:HA	1:326:A:ASP:H	11	0.15
(1,675)	1:270:A:GLY:H	1:272:A:GLN:H	13	0.15
(1,671)	1:269:A:GLU:HB2	1:270:A:GLY:H	15	0.15
(1,671)	1:269:A:GLU:HB3	1:270:A:GLY:H	15	0.15
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	1	0.15
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	9	0.15
(1,550)	1:263:A:TRP:HA	1:359:A:MET:HG2	7	0.15
(1,550)	1:263:A:TRP:HA	1:359:A:MET:HG3	7	0.15
(1,549)	1:263:A:TRP:H	1:359:A:MET:HG2	13	0.15
(1,549)	1:263:A:TRP:H	1:359:A:MET:HG3	13	0.15
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB2	6	0.15
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB3	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,525)	1:262:A:THR:HB	1:370:A:LYS:HD2	12	0.15
(1,525)	1:262:A:THR:HB	1:370:A:LYS:HD3	12	0.15
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD1	15	0.15
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD2	15	0.15
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	7	0.15
(1,376)	1:251:A:LYS:HG2	1:257:A:PHE:HA	4	0.15
(1,376)	1:251:A:LYS:HG3	1:257:A:PHE:HA	4	0.15
(1,291)	1:248:A:GLU:HA	1:252:A:HIS:H	13	0.15
(1,251)	1:246:A:TYR:HE1	1:263:A:TRP:HE1	15	0.15
(1,251)	1:246:A:TYR:HE2	1:263:A:TRP:HE1	15	0.15
(1,207)	1:243:A:ASP:HA	1:247:A:LYS:H	17	0.15
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	6	0.15
(1,174)	1:240:A:GLU:HA	1:242:A:THR:H	4	0.15
(1,123)	1:236:A:ARG:HB2	1:240:A:GLU:H	15	0.15
(1,123)	1:236:A:ARG:HB3	1:240:A:GLU:H	15	0.15
(1,23)	1:232:A:ALA:HB1	1:235:A:THR:HB	13	0.15
(1,23)	1:232:A:ALA:HB2	1:235:A:THR:HB	13	0.15
(1,23)	1:232:A:ALA:HB3	1:235:A:THR:HB	13	0.15
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD11	10	0.14
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD12	10	0.14
(1,3978)	1:460:A:LEU:HD21	2:634:B:LEU:HD13	10	0.14
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD11	10	0.14
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD12	10	0.14
(1,3978)	1:460:A:LEU:HD22	2:634:B:LEU:HD13	10	0.14
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD11	10	0.14
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD12	10	0.14
(1,3978)	1:460:A:LEU:HD23	2:634:B:LEU:HD13	10	0.14
(1,3807)	1:475:A:PHE:H	1:479:A:PRO:HA	3	0.14
(1,3785)	1:474:A:GLU:HA	1:480:A:PHE:H	5	0.14
(1,3740)	1:469:A:MET:HE1	1:473:A:THR:H	4	0.14
(1,3740)	1:469:A:MET:HE2	1:473:A:THR:H	4	0.14
(1,3740)	1:469:A:MET:HE3	1:473:A:THR:H	4	0.14
(1,3637)	1:458:A:LEU:HB2	1:460:A:LEU:H	12	0.14
(1,3637)	1:458:A:LEU:HB3	1:460:A:LEU:H	12	0.14
(1,3567)	1:450:A:LEU:HA	1:454:A:GLY:H	12	0.14
(1,3563)	1:450:A:LEU:HA	1:455:A:ILE:H	20	0.14
(1,3531)	1:449:A:LEU:HD11	1:493:A:LEU:HB2	1	0.14
(1,3531)	1:449:A:LEU:HD11	1:493:A:LEU:HB3	1	0.14
(1,3531)	1:449:A:LEU:HD12	1:493:A:LEU:HB2	1	0.14
(1,3531)	1:449:A:LEU:HD12	1:493:A:LEU:HB3	1	0.14
(1,3531)	1:449:A:LEU:HD13	1:493:A:LEU:HB2	1	0.14
(1,3531)	1:449:A:LEU:HD13	1:493:A:LEU:HB3	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3531)	1:449:A:LEU:HD21	1:493:A:LEU:HB2	1	0.14
(1,3531)	1:449:A:LEU:HD21	1:493:A:LEU:HB3	1	0.14
(1,3531)	1:449:A:LEU:HD22	1:493:A:LEU:HB2	1	0.14
(1,3531)	1:449:A:LEU:HD22	1:493:A:LEU:HB3	1	0.14
(1,3531)	1:449:A:LEU:HD23	1:493:A:LEU:HB2	1	0.14
(1,3531)	1:449:A:LEU:HD23	1:493:A:LEU:HB3	1	0.14
(1,3522)	1:448:A:GLU:HA	1:451:A:ARG:H	15	0.14
(1,3517)	1:447:A:LEU:HB2	1:448:A:GLU:H	16	0.14
(1,3517)	1:447:A:LEU:HB3	1:448:A:GLU:H	16	0.14
(1,3501)	1:447:A:LEU:HD21	1:457:A:VAL:HG11	1	0.14
(1,3501)	1:447:A:LEU:HD21	1:457:A:VAL:HG12	1	0.14
(1,3501)	1:447:A:LEU:HD21	1:457:A:VAL:HG13	1	0.14
(1,3501)	1:447:A:LEU:HD22	1:457:A:VAL:HG11	1	0.14
(1,3501)	1:447:A:LEU:HD22	1:457:A:VAL:HG12	1	0.14
(1,3501)	1:447:A:LEU:HD22	1:457:A:VAL:HG13	1	0.14
(1,3501)	1:447:A:LEU:HD23	1:457:A:VAL:HG11	1	0.14
(1,3501)	1:447:A:LEU:HD23	1:457:A:VAL:HG12	1	0.14
(1,3501)	1:447:A:LEU:HD23	1:457:A:VAL:HG13	1	0.14
(1,3231)	1:432:A:TYR:H	1:483:A:VAL:H	13	0.14
(1,3195)	1:431:A:TYR:HE2	1:493:A:LEU:HD12	15	0.14
(1,3171)	1:430:A:ILE:HA	1:481:A:GLN:H	4	0.14
(1,3164)	1:429:A:LYS:HB2	1:431:A:TYR:HE1	14	0.14
(1,3164)	1:429:A:LYS:HB2	1:431:A:TYR:HE2	14	0.14
(1,3164)	1:429:A:LYS:HB3	1:431:A:TYR:HE1	14	0.14
(1,3164)	1:429:A:LYS:HB3	1:431:A:TYR:HE2	14	0.14
(1,3153)	1:429:A:LYS:HA	1:480:A:PHE:H	17	0.14
(1,3076)	1:423:A:MET:HE1	1:429:A:LYS:H	5	0.14
(1,3076)	1:423:A:MET:HE2	1:429:A:LYS:H	5	0.14
(1,3076)	1:423:A:MET:HE3	1:429:A:LYS:H	5	0.14
(1,3028)	1:419:A:TYR:HA	1:422:A:ARG:HD2	4	0.14
(1,3028)	1:419:A:TYR:HA	1:422:A:ARG:HD3	4	0.14
(1,2940)	1:414:A:VAL:HG21	1:418:A:ASP:HB2	16	0.14
(1,2940)	1:414:A:VAL:HG21	1:418:A:ASP:HB3	16	0.14
(1,2940)	1:414:A:VAL:HG22	1:418:A:ASP:HB2	16	0.14
(1,2940)	1:414:A:VAL:HG22	1:418:A:ASP:HB3	16	0.14
(1,2940)	1:414:A:VAL:HG23	1:418:A:ASP:HB2	16	0.14
(1,2940)	1:414:A:VAL:HG23	1:418:A:ASP:HB3	16	0.14
(1,2940)	1:414:A:VAL:HG21	1:418:A:ASP:HB2	18	0.14
(1,2940)	1:414:A:VAL:HG21	1:418:A:ASP:HB3	18	0.14
(1,2940)	1:414:A:VAL:HG22	1:418:A:ASP:HB2	18	0.14
(1,2940)	1:414:A:VAL:HG22	1:418:A:ASP:HB3	18	0.14
(1,2940)	1:414:A:VAL:HG23	1:418:A:ASP:HB2	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2940)	1:414:A:VAL:HG23	1:418:A:ASP:HB3	18	0.14
(1,2914)	1:410:A:SER:HA	1:438:A:TYR:HE2	7	0.14
(1,2910)	1:410:A:SER:HA	1:459:A:LEU:HD11	6	0.14
(1,2910)	1:410:A:SER:HA	1:459:A:LEU:HD12	6	0.14
(1,2910)	1:410:A:SER:HA	1:459:A:LEU:HD13	6	0.14
(1,2855)	1:405:A:THR:HB	1:451:A:ARG:HA	9	0.14
(1,2824)	1:404:A:SER:H	1:414:A:VAL:HB	17	0.14
(1,2790)	1:403:A:ALA:HA	1:414:A:VAL:HB	20	0.14
(1,2755)	1:402:A:PHE:HD1	1:460:A:LEU:HD12	13	0.14
(1,2593)	1:390:A:PHE:HA	1:393:A:GLN:H	5	0.14
(1,2562)	1:387:A:ALA:HB1	1:471:A:TYR:HD1	18	0.14
(1,2562)	1:387:A:ALA:HB1	1:471:A:TYR:HD2	18	0.14
(1,2562)	1:387:A:ALA:HB2	1:471:A:TYR:HD1	18	0.14
(1,2562)	1:387:A:ALA:HB2	1:471:A:TYR:HD2	18	0.14
(1,2562)	1:387:A:ALA:HB3	1:471:A:TYR:HD1	18	0.14
(1,2562)	1:387:A:ALA:HB3	1:471:A:TYR:HD2	18	0.14
(1,2488)	1:383:A:LYS:HE2	1:402:A:PHE:HZ	2	0.14
(1,2488)	1:383:A:LYS:HE3	1:402:A:PHE:HZ	2	0.14
(1,2433)	1:380:A:LEU:H	1:383:A:LYS:H	3	0.14
(1,2405)	1:378:A:PHE:H	1:380:A:LEU:H	17	0.14
(1,2353)	1:375:A:TRP:HZ3	1:400:A:LEU:HA	12	0.14
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA2	15	0.14
(1,2321)	1:374:A:PHE:HZ	1:379:A:GLY:HA3	15	0.14
(1,2319)	1:374:A:PHE:HZ	1:382:A:LEU:HD11	9	0.14
(1,2319)	1:374:A:PHE:HZ	1:382:A:LEU:HD12	9	0.14
(1,2319)	1:374:A:PHE:HZ	1:382:A:LEU:HD13	9	0.14
(1,2227)	1:368:A:ALA:HA	1:371:A:TYR:H	6	0.14
(1,2166)	1:363:A:LEU:HA	1:367:A:ASP:HB2	2	0.14
(1,2166)	1:363:A:LEU:HA	1:367:A:ASP:HB3	2	0.14
(1,2146)	1:362:A:LYS:HG2	1:366:A:ASP:H	14	0.14
(1,2146)	1:362:A:LYS:HG3	1:366:A:ASP:H	14	0.14
(1,2134)	1:361:A:GLU:HG2	1:365:A:LYS:HE2	6	0.14
(1,2134)	1:361:A:GLU:HG2	1:365:A:LYS:HE3	6	0.14
(1,2134)	1:361:A:GLU:HG3	1:365:A:LYS:HE2	6	0.14
(1,2134)	1:361:A:GLU:HG3	1:365:A:LYS:HE3	6	0.14
(1,2052)	1:357:A:LEU:HD21	1:382:A:LEU:HD11	20	0.14
(1,2052)	1:357:A:LEU:HD21	1:382:A:LEU:HD12	20	0.14
(1,2052)	1:357:A:LEU:HD21	1:382:A:LEU:HD13	20	0.14
(1,2052)	1:357:A:LEU:HD22	1:382:A:LEU:HD11	20	0.14
(1,2052)	1:357:A:LEU:HD22	1:382:A:LEU:HD12	20	0.14
(1,2052)	1:357:A:LEU:HD22	1:382:A:LEU:HD13	20	0.14
(1,2052)	1:357:A:LEU:HD23	1:382:A:LEU:HD11	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2052)	1:357:A:LEU:HD23	1:382:A:LEU:HD12	20	0.14
(1,2052)	1:357:A:LEU:HD23	1:382:A:LEU:HD13	20	0.14
(1,2052)	1:357:A:LEU:HD21	1:382:A:LEU:HD21	20	0.14
(1,2052)	1:357:A:LEU:HD21	1:382:A:LEU:HD22	20	0.14
(1,2052)	1:357:A:LEU:HD21	1:382:A:LEU:HD23	20	0.14
(1,2052)	1:357:A:LEU:HD22	1:382:A:LEU:HD21	20	0.14
(1,2052)	1:357:A:LEU:HD22	1:382:A:LEU:HD22	20	0.14
(1,2052)	1:357:A:LEU:HD22	1:382:A:LEU:HD23	20	0.14
(1,2052)	1:357:A:LEU:HD23	1:382:A:LEU:HD21	20	0.14
(1,2052)	1:357:A:LEU:HD23	1:382:A:LEU:HD22	20	0.14
(1,2052)	1:357:A:LEU:HD23	1:382:A:LEU:HD23	20	0.14
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD11	3	0.14
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD12	3	0.14
(1,2001)	1:354:A:LYS:HA	1:357:A:LEU:HD13	3	0.14
(1,1954)	1:351:A:ALA:HA	1:353:A:THR:HB	14	0.14
(1,1882)	1:345:A:THR:HB	1:346:A:ARG:H	9	0.14
(1,1882)	1:345:A:THR:HB	1:346:A:ARG:H	15	0.14
(1,1882)	1:345:A:THR:HB	1:346:A:ARG:H	17	0.14
(1,1843)	1:342:A:SER:HB2	1:343:A:THR:H	13	0.14
(1,1843)	1:342:A:SER:HB3	1:343:A:THR:H	13	0.14
(1,1843)	1:342:A:SER:HB2	1:343:A:THR:H	18	0.14
(1,1843)	1:342:A:SER:HB3	1:343:A:THR:H	18	0.14
(1,1791)	1:337:A:GLU:H	1:340:A:GLN:H	14	0.14
(1,1762)	1:335:A:SER:H	1:339:A:LEU:H	11	0.14
(1,1674)	1:325:A:ILE:HD11	1:327:A:SER:H	18	0.14
(1,1674)	1:325:A:ILE:HD12	1:327:A:SER:H	18	0.14
(1,1674)	1:325:A:ILE:HD13	1:327:A:SER:H	18	0.14
(1,1674)	1:325:A:ILE:HD11	1:327:A:SER:H	19	0.14
(1,1674)	1:325:A:ILE:HD12	1:327:A:SER:H	19	0.14
(1,1674)	1:325:A:ILE:HD13	1:327:A:SER:H	19	0.14
(1,1506)	1:315:A:PRO:HA	1:349:A:ARG:HD2	10	0.14
(1,1506)	1:315:A:PRO:HA	1:349:A:ARG:HD3	10	0.14
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG21	15	0.14
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG22	15	0.14
(1,1418)	1:312:A:GLN:HA	1:345:A:THR:HG23	15	0.14
(1,1382)	1:307:A:MET:HB2	1:308:A:ASP:H	4	0.14
(1,1382)	1:307:A:MET:HB3	1:308:A:ASP:H	4	0.14
(1,1382)	1:307:A:MET:HB2	1:308:A:ASP:H	9	0.14
(1,1382)	1:307:A:MET:HB3	1:308:A:ASP:H	9	0.14
(1,1219)	1:299:A:LEU:H	1:306:A:ILE:H	1	0.14
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD11	1	0.14
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD12	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1200)	1:299:A:LEU:HD11	1:325:A:ILE:HD13	1	0.14
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD11	1	0.14
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD12	1	0.14
(1,1200)	1:299:A:LEU:HD12	1:325:A:ILE:HD13	1	0.14
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD11	1	0.14
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD12	1	0.14
(1,1200)	1:299:A:LEU:HD13	1:325:A:ILE:HD13	1	0.14
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD11	6	0.14
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD12	6	0.14
(1,1199)	1:299:A:LEU:HA	1:325:A:ILE:HD13	6	0.14
(1,1167)	1:298:A:LYS:HA	1:309:A:ASP:HA	13	0.14
(1,1159)	1:298:A:LYS:H	1:322:A:ARG:HD2	18	0.14
(1,1159)	1:298:A:LYS:H	1:322:A:ARG:HD3	18	0.14
(1,1060)	1:294:A:LYS:HD2	1:309:A:ASP:HB2	16	0.14
(1,1060)	1:294:A:LYS:HD2	1:309:A:ASP:HB3	16	0.14
(1,1060)	1:294:A:LYS:HD3	1:309:A:ASP:HB2	16	0.14
(1,1060)	1:294:A:LYS:HD3	1:309:A:ASP:HB3	16	0.14
(1,879)	1:280:A:ILE:HA	1:321:A:VAL:HA	16	0.14
(1,763)	1:276:A:SER:HA	1:326:A:ASP:H	15	0.14
(1,763)	1:276:A:SER:HA	1:326:A:ASP:H	18	0.14
(1,723)	1:274:A:TYR:H	1:328:A:SER:H	12	0.14
(1,685)	1:272:A:GLN:HE21	1:351:A:ALA:HB1	7	0.14
(1,685)	1:272:A:GLN:HE21	1:351:A:ALA:HB2	7	0.14
(1,685)	1:272:A:GLN:HE21	1:351:A:ALA:HB3	7	0.14
(1,685)	1:272:A:GLN:HE22	1:351:A:ALA:HB1	7	0.14
(1,685)	1:272:A:GLN:HE22	1:351:A:ALA:HB2	7	0.14
(1,685)	1:272:A:GLN:HE22	1:351:A:ALA:HB3	7	0.14
(1,634)	1:267:A:ARG:HG2	1:274:A:TYR:H	14	0.14
(1,634)	1:267:A:ARG:HG3	1:274:A:TYR:H	14	0.14
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD1	3	0.14
(1,543)	1:262:A:THR:HA	1:279:A:TYR:HD2	3	0.14
(1,456)	1:258:A:ASN:HB2	1:283:A:GLN:HB2	3	0.14
(1,456)	1:258:A:ASN:HB2	1:283:A:GLN:HB3	3	0.14
(1,456)	1:258:A:ASN:HB3	1:283:A:GLN:HB2	3	0.14
(1,456)	1:258:A:ASN:HB3	1:283:A:GLN:HB3	3	0.14
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB2	5	0.14
(1,405)	1:253:A:ILE:HD11	1:322:A:ARG:HB3	5	0.14
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB2	5	0.14
(1,405)	1:253:A:ILE:HD12	1:322:A:ARG:HB3	5	0.14
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB2	5	0.14
(1,405)	1:253:A:ILE:HD13	1:322:A:ARG:HB3	5	0.14
(1,339)	1:250:A:TYR:HE1	1:280:A:ILE:HA	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:250:A:TYR:HE2	1:280:A:ILE:HA	6	0.14
(1,210)	1:243:A:ASP:H	1:246:A:TYR:H	12	0.14
(1,180)	1:241:A:ILE:HB	1:246:A:TYR:HD1	13	0.14
(1,180)	1:241:A:ILE:HB	1:246:A:TYR:HD2	13	0.14
(1,149)	1:238:A:LYS:HA	1:265:A:HIS:HE1	7	0.14
(1,82)	1:234:A:TRP:HD1	1:276:A:SER:HA	6	0.14
(1,24)	1:232:A:ALA:H	1:235:A:THR:HG21	20	0.14
(1,24)	1:232:A:ALA:H	1:235:A:THR:HG22	20	0.14
(1,24)	1:232:A:ALA:H	1:235:A:THR:HG23	20	0.14
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD11	10	0.13
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD12	10	0.13
(1,3968)	1:396:A:ILE:HD11	2:620:B:LEU:HD13	10	0.13
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD11	10	0.13
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD12	10	0.13
(1,3968)	1:396:A:ILE:HD12	2:620:B:LEU:HD13	10	0.13
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD11	10	0.13
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD12	10	0.13
(1,3968)	1:396:A:ILE:HD13	2:620:B:LEU:HD13	10	0.13
(1,3935)	1:490:A:LEU:HA	1:494:A:ALA:H	14	0.13
(1,3896)	1:486:A:VAL:HA	1:489:A:SER:HB2	18	0.13
(1,3896)	1:486:A:VAL:HA	1:489:A:SER:HB3	18	0.13
(1,3858)	1:482:A:SER:H	1:485:A:LYS:H	8	0.13
(1,3857)	1:481:A:GLN:HE21	1:482:A:SER:H	7	0.13
(1,3857)	1:481:A:GLN:HE22	1:482:A:SER:H	7	0.13
(1,3730)	1:468:A:MET:HA	1:471:A:TYR:HD1	18	0.13
(1,3730)	1:468:A:MET:HA	1:471:A:TYR:HD2	18	0.13
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	11	0.13
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	11	0.13
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	11	0.13
(1,3689)	1:464:A:ILE:HD11	1:467:A:TRP:HZ3	19	0.13
(1,3689)	1:464:A:ILE:HD12	1:467:A:TRP:HZ3	19	0.13
(1,3689)	1:464:A:ILE:HD13	1:467:A:TRP:HZ3	19	0.13
(1,3679)	1:463:A:ARG:HA	1:466:A:GLU:H	5	0.13
(1,3649)	1:460:A:LEU:HD21	1:472:A:LEU:HD11	3	0.13
(1,3649)	1:460:A:LEU:HD21	1:472:A:LEU:HD12	3	0.13
(1,3649)	1:460:A:LEU:HD21	1:472:A:LEU:HD13	3	0.13
(1,3649)	1:460:A:LEU:HD22	1:472:A:LEU:HD11	3	0.13
(1,3649)	1:460:A:LEU:HD22	1:472:A:LEU:HD12	3	0.13
(1,3649)	1:460:A:LEU:HD22	1:472:A:LEU:HD13	3	0.13
(1,3649)	1:460:A:LEU:HD23	1:472:A:LEU:HD11	3	0.13
(1,3649)	1:460:A:LEU:HD23	1:472:A:LEU:HD12	3	0.13
(1,3649)	1:460:A:LEU:HD23	1:472:A:LEU:HD13	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3622)	1:456:A:GLU:HG2	1:457:A:VAL:H	8	0.13
(1,3622)	1:456:A:GLU:HG3	1:457:A:VAL:H	8	0.13
(1,3598)	1:453:A:LYS:HG2	1:493:A:LEU:HB2	15	0.13
(1,3598)	1:453:A:LYS:HG2	1:493:A:LEU:HB3	15	0.13
(1,3536)	1:449:A:LEU:HA	1:453:A:LYS:H	6	0.13
(1,3519)	1:448:A:GLU:HB2	1:452:A:LYS:H	11	0.13
(1,3519)	1:448:A:GLU:HB3	1:452:A:LYS:H	11	0.13
(1,3505)	1:447:A:LEU:HB2	1:451:A:ARG:H	18	0.13
(1,3505)	1:447:A:LEU:HB3	1:451:A:ARG:H	18	0.13
(1,3405)	1:439:A:ALA:HA	1:442:A:LYS:HB2	1	0.13
(1,3405)	1:439:A:ALA:HA	1:442:A:LYS:HB3	1	0.13
(1,3390)	1:438:A:TYR:HE1	1:442:A:LYS:HD2	7	0.13
(1,3362)	1:437:A:SER:HA	1:461:A:SER:HA	5	0.13
(1,3353)	1:436:A:ASP:HA	1:461:A:SER:HA	10	0.13
(1,3207)	1:431:A:TYR:HA	1:482:A:SER:HA	9	0.13
(1,3185)	1:430:A:ILE:HD11	1:475:A:PHE:H	12	0.13
(1,3185)	1:430:A:ILE:HD12	1:475:A:PHE:H	12	0.13
(1,3185)	1:430:A:ILE:HD13	1:475:A:PHE:H	12	0.13
(1,3153)	1:429:A:LYS:HA	1:480:A:PHE:H	20	0.13
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG2	20	0.13
(1,3134)	1:428:A:GLU:HG2	1:479:A:PRO:HG3	20	0.13
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG2	20	0.13
(1,3134)	1:428:A:GLU:HG3	1:479:A:PRO:HG3	20	0.13
(1,3133)	1:428:A:GLU:HG2	1:479:A:PRO:HD2	18	0.13
(1,3133)	1:428:A:GLU:HG2	1:479:A:PRO:HD3	18	0.13
(1,3133)	1:428:A:GLU:HG3	1:479:A:PRO:HD2	18	0.13
(1,3133)	1:428:A:GLU:HG3	1:479:A:PRO:HD3	18	0.13
(1,3112)	1:426:A:GLY:HA2	1:428:A:GLU:HA	16	0.13
(1,3112)	1:426:A:GLY:HA3	1:428:A:GLU:HA	16	0.13
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE21	20	0.13
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE22	20	0.13
(1,3078)	1:423:A:MET:HE1	1:428:A:GLU:H	6	0.13
(1,3078)	1:423:A:MET:HE2	1:428:A:GLU:H	6	0.13
(1,3078)	1:423:A:MET:HE3	1:428:A:GLU:H	6	0.13
(1,2986)	1:417:A:GLU:HA	1:421:A:SER:HB2	2	0.13
(1,2986)	1:417:A:GLU:HA	1:421:A:SER:HB3	2	0.13
(1,2985)	1:417:A:GLU:HB2	1:421:A:SER:H	17	0.13
(1,2985)	1:417:A:GLU:HB3	1:421:A:SER:H	17	0.13
(1,2940)	1:414:A:VAL:HG21	1:418:A:ASP:HB2	12	0.13
(1,2940)	1:414:A:VAL:HG21	1:418:A:ASP:HB3	12	0.13
(1,2940)	1:414:A:VAL:HG22	1:418:A:ASP:HB2	12	0.13
(1,2940)	1:414:A:VAL:HG22	1:418:A:ASP:HB3	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2940)	1:414:A:VAL:HG23	1:418:A:ASP:HB2	12	0.13
(1,2940)	1:414:A:VAL:HG23	1:418:A:ASP:HB3	12	0.13
(1,2940)	1:414:A:VAL:HG21	1:418:A:ASP:HB2	19	0.13
(1,2940)	1:414:A:VAL:HG21	1:418:A:ASP:HB3	19	0.13
(1,2940)	1:414:A:VAL:HG22	1:418:A:ASP:HB2	19	0.13
(1,2940)	1:414:A:VAL:HG22	1:418:A:ASP:HB3	19	0.13
(1,2940)	1:414:A:VAL:HG23	1:418:A:ASP:HB2	19	0.13
(1,2940)	1:414:A:VAL:HG23	1:418:A:ASP:HB3	19	0.13
(1,2927)	1:412:A:GLN:HA	1:414:A:VAL:HB	1	0.13
(1,2912)	1:410:A:SER:HB2	1:438:A:TYR:HD1	18	0.13
(1,2912)	1:410:A:SER:HB2	1:438:A:TYR:HD2	18	0.13
(1,2912)	1:410:A:SER:HB3	1:438:A:TYR:HD1	18	0.13
(1,2912)	1:410:A:SER:HB3	1:438:A:TYR:HD2	18	0.13
(1,2848)	1:405:A:THR:H	1:457:A:VAL:HB	13	0.13
(1,2824)	1:404:A:SER:H	1:414:A:VAL:HB	5	0.13
(1,2811)	1:404:A:SER:HB2	1:458:A:LEU:H	8	0.13
(1,2811)	1:404:A:SER:HB3	1:458:A:LEU:H	8	0.13
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG11	3	0.13
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG12	3	0.13
(1,2792)	1:403:A:ALA:HA	1:414:A:VAL:HG13	3	0.13
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG11	5	0.13
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG12	5	0.13
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG13	5	0.13
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG11	19	0.13
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG12	19	0.13
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG13	19	0.13
(1,2761)	1:402:A:PHE:H	1:415:A:SER:HA	18	0.13
(1,2697)	1:398:A:LYS:HA	1:475:A:PHE:HE1	6	0.13
(1,2574)	1:388:A:GLU:H	1:390:A:PHE:H	6	0.13
(1,2574)	1:388:A:GLU:H	1:390:A:PHE:H	8	0.13
(1,2574)	1:388:A:GLU:H	1:390:A:PHE:H	12	0.13
(1,2566)	1:387:A:ALA:H	1:468:A:MET:HA	6	0.13
(1,2564)	1:387:A:ALA:HA	1:471:A:TYR:HD1	18	0.13
(1,2547)	1:386:A:PRO:HA	1:396:A:ILE:HB	5	0.13
(1,2524)	1:385:A:GLY:HA2	1:389:A:ASP:H	1	0.13
(1,2524)	1:385:A:GLY:HA3	1:389:A:ASP:H	1	0.13
(1,2434)	1:380:A:LEU:HA	1:383:A:LYS:H	11	0.13
(1,2379)	1:376:A:GLN:HE21	1:413:A:THR:HG21	20	0.13
(1,2379)	1:376:A:GLN:HE21	1:413:A:THR:HG22	20	0.13
(1,2379)	1:376:A:GLN:HE21	1:413:A:THR:HG23	20	0.13
(1,2379)	1:376:A:GLN:HE22	1:413:A:THR:HG21	20	0.13
(1,2379)	1:376:A:GLN:HE22	1:413:A:THR:HG22	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2379)	1:376:A:GLN:HE22	1:413:A:THR:HG23	20	0.13
(1,2344)	1:375:A:TRP:HZ2	1:402:A:PHE:HA	10	0.13
(1,2012)	1:355:A:ARG:H	1:358:A:GLN:H	12	0.13
(1,1938)	1:350:A:ASN:HA	1:353:A:THR:HB	7	0.13
(1,1937)	1:350:A:ASN:HA	1:353:A:THR:H	11	0.13
(1,1889)	1:346:A:ARG:HA	1:349:A:ARG:HG2	12	0.13
(1,1843)	1:342:A:SER:HB2	1:343:A:THR:H	2	0.13
(1,1843)	1:342:A:SER:HB3	1:343:A:THR:H	2	0.13
(1,1810)	1:339:A:LEU:HA	1:345:A:THR:H	18	0.13
(1,1790)	1:337:A:GLU:HG2	1:341:A:ASP:HB2	10	0.13
(1,1790)	1:337:A:GLU:HG2	1:341:A:ASP:HB3	10	0.13
(1,1790)	1:337:A:GLU:HG3	1:341:A:ASP:HB2	10	0.13
(1,1790)	1:337:A:GLU:HG3	1:341:A:ASP:HB3	10	0.13
(1,1788)	1:337:A:GLU:HA	1:341:A:ASP:H	5	0.13
(1,1762)	1:335:A:SER:H	1:339:A:LEU:H	18	0.13
(1,1451)	1:313:A:PHE:HB2	1:348:A:LEU:HD11	19	0.13
(1,1451)	1:313:A:PHE:HB2	1:348:A:LEU:HD12	19	0.13
(1,1451)	1:313:A:PHE:HB2	1:348:A:LEU:HD13	19	0.13
(1,1451)	1:313:A:PHE:HB3	1:348:A:LEU:HD11	19	0.13
(1,1451)	1:313:A:PHE:HB3	1:348:A:LEU:HD12	19	0.13
(1,1451)	1:313:A:PHE:HB3	1:348:A:LEU:HD13	19	0.13
(1,1432)	1:312:A:GLN:HE21	1:336:A:ARG:HG2	12	0.13
(1,1432)	1:312:A:GLN:HE21	1:336:A:ARG:HG3	12	0.13
(1,1432)	1:312:A:GLN:HE22	1:336:A:ARG:HG2	12	0.13
(1,1432)	1:312:A:GLN:HE22	1:336:A:ARG:HG3	12	0.13
(1,1431)	1:312:A:GLN:HE21	1:336:A:ARG:HD2	9	0.13
(1,1431)	1:312:A:GLN:HE21	1:336:A:ARG:HD3	9	0.13
(1,1431)	1:312:A:GLN:HE22	1:336:A:ARG:HD2	9	0.13
(1,1431)	1:312:A:GLN:HE22	1:336:A:ARG:HD3	9	0.13
(1,1367)	1:307:A:MET:HE1	1:339:A:LEU:H	1	0.13
(1,1367)	1:307:A:MET:HE2	1:339:A:LEU:H	1	0.13
(1,1367)	1:307:A:MET:HE3	1:339:A:LEU:H	1	0.13
(1,1325)	1:302:A:GLN:H	1:327:A:SER:HA	16	0.13
(1,1277)	1:301:A:VAL:HB	1:332:A:LEU:HD11	16	0.13
(1,1277)	1:301:A:VAL:HB	1:332:A:LEU:HD12	16	0.13
(1,1277)	1:301:A:VAL:HB	1:332:A:LEU:HD13	16	0.13
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE1	3	0.13
(1,1249)	1:300:A:TYR:H	1:313:A:PHE:HE2	3	0.13
(1,1223)	1:299:A:LEU:H	1:305:A:PHE:HA	15	0.13
(1,1215)	1:299:A:LEU:H	1:307:A:MET:H	3	0.13
(1,1096)	1:296:A:GLY:HA2	1:309:A:ASP:H	11	0.13
(1,1096)	1:296:A:GLY:HA3	1:309:A:ASP:H	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1053)	1:293:A:HIS:HB2	1:295:A:HIS:H	18	0.13
(1,1053)	1:293:A:HIS:HB3	1:295:A:HIS:H	18	0.13
(1,1051)	1:293:A:HIS:HE1	1:309:A:ASP:HB2	19	0.13
(1,1051)	1:293:A:HIS:HE1	1:309:A:ASP:HB3	19	0.13
(1,1035)	1:290:A:ASN:H	1:292:A:ASP:H	15	0.13
(1,1007)	1:288:A:MET:HE1	1:320:A:PHE:HA	2	0.13
(1,1007)	1:288:A:MET:HE2	1:320:A:PHE:HA	2	0.13
(1,1007)	1:288:A:MET:HE3	1:320:A:PHE:HA	2	0.13
(1,978)	1:286:A:TRP:HA	1:289:A:TRP:H	14	0.13
(1,966)	1:285:A:PRO:HD2	1:288:A:MET:HE1	2	0.13
(1,966)	1:285:A:PRO:HD2	1:288:A:MET:HE2	2	0.13
(1,966)	1:285:A:PRO:HD2	1:288:A:MET:HE3	2	0.13
(1,966)	1:285:A:PRO:HD3	1:288:A:MET:HE1	2	0.13
(1,966)	1:285:A:PRO:HD3	1:288:A:MET:HE2	2	0.13
(1,966)	1:285:A:PRO:HD3	1:288:A:MET:HE3	2	0.13
(1,961)	1:285:A:PRO:HG2	1:294:A:LYS:HB2	3	0.13
(1,961)	1:285:A:PRO:HG2	1:294:A:LYS:HB3	3	0.13
(1,961)	1:285:A:PRO:HG3	1:294:A:LYS:HB2	3	0.13
(1,961)	1:285:A:PRO:HG3	1:294:A:LYS:HB3	3	0.13
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	10	0.13
(1,803)	1:278:A:LEU:HB2	1:356:A:VAL:HA	20	0.13
(1,803)	1:278:A:LEU:HB3	1:356:A:VAL:HA	20	0.13
(1,764)	1:276:A:SER:HB2	1:326:A:ASP:H	12	0.13
(1,764)	1:276:A:SER:HB3	1:326:A:ASP:H	12	0.13
(1,763)	1:276:A:SER:HA	1:326:A:ASP:H	14	0.13
(1,690)	1:272:A:GLN:HG2	1:344:A:VAL:HG11	10	0.13
(1,690)	1:272:A:GLN:HG2	1:344:A:VAL:HG12	10	0.13
(1,690)	1:272:A:GLN:HG2	1:344:A:VAL:HG13	10	0.13
(1,690)	1:272:A:GLN:HG3	1:344:A:VAL:HG11	10	0.13
(1,690)	1:272:A:GLN:HG3	1:344:A:VAL:HG12	10	0.13
(1,690)	1:272:A:GLN:HG3	1:344:A:VAL:HG13	10	0.13
(1,680)	1:271:A:LYS:HA	1:273:A:GLU:H	8	0.13
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	2	0.13
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	2	0.13
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	5	0.13
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	5	0.13
(1,620)	1:266:A:ASN:HB2	1:274:A:TYR:HE1	8	0.13
(1,620)	1:266:A:ASN:HB2	1:274:A:TYR:HE2	8	0.13
(1,620)	1:266:A:ASN:HB3	1:274:A:TYR:HE1	8	0.13
(1,620)	1:266:A:ASN:HB3	1:274:A:TYR:HE2	8	0.13
(1,565)	1:263:A:TRP:HD1	1:265:A:HIS:HA	5	0.13
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB2	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:262:A:THR:H	1:279:A:TYR:HB3	7	0.13
(1,471)	1:260:A:PRO:HA	1:282:A:SER:H	16	0.13
(1,455)	1:258:A:ASN:HB2	1:283:A:GLN:H	3	0.13
(1,455)	1:258:A:ASN:HB3	1:283:A:GLN:H	3	0.13
(1,382)	1:251:A:LYS:HA	1:255:A:HIS:HA	11	0.13
(1,293)	1:248:A:GLU:HA	1:251:A:LYS:H	12	0.13
(1,210)	1:243:A:ASP:H	1:246:A:TYR:H	4	0.13
(1,210)	1:243:A:ASP:H	1:246:A:TYR:H	10	0.13
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	9	0.13
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	5	0.13
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	14	0.13
(1,153)	1:238:A:LYS:HE2	1:264:A:SER:HA	15	0.13
(1,153)	1:238:A:LYS:HE3	1:264:A:SER:HA	15	0.13
(1,137)	1:237:A:ASN:H	1:239:A:SER:H	12	0.13
(1,135)	1:237:A:ASN:HD21	1:240:A:GLU:H	6	0.13
(1,135)	1:237:A:ASN:HD22	1:240:A:GLU:H	6	0.13
(1,95)	1:234:A:TRP:HA	1:246:A:TYR:HE2	7	0.13
(1,86)	1:234:A:TRP:HD1	1:275:A:THR:HG21	5	0.13
(1,86)	1:234:A:TRP:HD1	1:275:A:THR:HG22	5	0.13
(1,86)	1:234:A:TRP:HD1	1:275:A:THR:HG23	5	0.13
(1,86)	1:234:A:TRP:HD1	1:275:A:THR:HG21	12	0.13
(1,86)	1:234:A:TRP:HD1	1:275:A:THR:HG22	12	0.13
(1,86)	1:234:A:TRP:HD1	1:275:A:THR:HG23	12	0.13
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG21	6	0.12
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG22	6	0.12
(2,8)	1:338:A:ILE:HD11	1:344:A:VAL:HG23	6	0.12
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG21	6	0.12
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG22	6	0.12
(2,8)	1:338:A:ILE:HD12	1:344:A:VAL:HG23	6	0.12
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG21	6	0.12
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG22	6	0.12
(2,8)	1:338:A:ILE:HD13	1:344:A:VAL:HG23	6	0.12
(1,3943)	1:490:A:LEU:HA	1:492:A:LYS:H	4	0.12
(1,3903)	1:487:A:ASP:H	1:491:A:GLU:H	14	0.12
(1,3767)	1:472:A:LEU:HD22	1:480:A:PHE:HE2	17	0.12
(1,3636)	1:458:A:LEU:HD11	1:469:A:MET:HE1	1	0.12
(1,3636)	1:458:A:LEU:HD11	1:469:A:MET:HE2	1	0.12
(1,3636)	1:458:A:LEU:HD11	1:469:A:MET:HE3	1	0.12
(1,3636)	1:458:A:LEU:HD12	1:469:A:MET:HE1	1	0.12
(1,3636)	1:458:A:LEU:HD12	1:469:A:MET:HE2	1	0.12
(1,3636)	1:458:A:LEU:HD12	1:469:A:MET:HE3	1	0.12
(1,3636)	1:458:A:LEU:HD13	1:469:A:MET:HE1	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3636)	1:458:A:LEU:HD13	1:469:A:MET:HE2	1	0.12
(1,3636)	1:458:A:LEU:HD13	1:469:A:MET:HE3	1	0.12
(1,3622)	1:456:A:GLU:HG2	1:457:A:VAL:H	6	0.12
(1,3622)	1:456:A:GLU:HG3	1:457:A:VAL:H	6	0.12
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD11	6	0.12
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD12	6	0.12
(1,3509)	1:447:A:LEU:HD21	1:450:A:LEU:HD13	6	0.12
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD11	6	0.12
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD12	6	0.12
(1,3509)	1:447:A:LEU:HD22	1:450:A:LEU:HD13	6	0.12
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD11	6	0.12
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD12	6	0.12
(1,3509)	1:447:A:LEU:HD23	1:450:A:LEU:HD13	6	0.12
(1,3492)	1:447:A:LEU:HA	1:483:A:VAL:HB	18	0.12
(1,3248)	1:432:A:TYR:HA	1:457:A:VAL:HA	16	0.12
(1,3232)	1:432:A:TYR:HA	1:483:A:VAL:H	14	0.12
(1,3214)	1:431:A:TYR:H	1:458:A:LEU:H	8	0.12
(1,3214)	1:431:A:TYR:H	1:458:A:LEU:H	13	0.12
(1,3208)	1:431:A:TYR:HB2	1:482:A:SER:HA	2	0.12
(1,3208)	1:431:A:TYR:HB3	1:482:A:SER:HA	2	0.12
(1,3207)	1:431:A:TYR:HA	1:482:A:SER:HA	7	0.12
(1,3171)	1:430:A:ILE:HA	1:481:A:GLN:H	17	0.12
(1,3160)	1:429:A:LYS:HA	1:478:A:LYS:HA	19	0.12
(1,3155)	1:429:A:LYS:HB2	1:480:A:PHE:HA	4	0.12
(1,3155)	1:429:A:LYS:HB3	1:480:A:PHE:HA	4	0.12
(1,3155)	1:429:A:LYS:HB2	1:480:A:PHE:HA	18	0.12
(1,3155)	1:429:A:LYS:HB3	1:480:A:PHE:HA	18	0.12
(1,3143)	1:429:A:LYS:HD2	1:489:A:SER:H	9	0.12
(1,3143)	1:429:A:LYS:HD3	1:489:A:SER:H	9	0.12
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE21	4	0.12
(1,3097)	1:424:A:LYS:H	1:427:A:GLN:HE22	4	0.12
(1,3082)	1:423:A:MET:HA	1:427:A:GLN:HE21	8	0.12
(1,3082)	1:423:A:MET:HA	1:427:A:GLN:HE22	8	0.12
(1,3073)	1:423:A:MET:HE1	1:430:A:ILE:H	18	0.12
(1,3073)	1:423:A:MET:HE2	1:430:A:ILE:H	18	0.12
(1,3073)	1:423:A:MET:HE3	1:430:A:ILE:H	18	0.12
(1,3017)	1:419:A:TYR:HE1	1:431:A:TYR:H	3	0.12
(1,3017)	1:419:A:TYR:HE2	1:431:A:TYR:H	3	0.12
(1,2968)	1:416:A:LEU:HA	1:420:A:VAL:H	17	0.12
(1,2940)	1:414:A:VAL:HG21	1:418:A:ASP:HB2	17	0.12
(1,2940)	1:414:A:VAL:HG21	1:418:A:ASP:HB3	17	0.12
(1,2940)	1:414:A:VAL:HG22	1:418:A:ASP:HB2	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2940)	1:414:A:VAL:HG22	1:418:A:ASP:HB3	17	0.12
(1,2940)	1:414:A:VAL:HG23	1:418:A:ASP:HB2	17	0.12
(1,2940)	1:414:A:VAL:HG23	1:418:A:ASP:HB3	17	0.12
(1,2926)	1:412:A:GLN:HA	1:414:A:VAL:H	8	0.12
(1,2911)	1:410:A:SER:HA	1:438:A:TYR:HD1	12	0.12
(1,2911)	1:410:A:SER:HA	1:438:A:TYR:HD2	12	0.12
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG11	3	0.12
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG12	3	0.12
(1,2765)	1:402:A:PHE:H	1:414:A:VAL:HG13	3	0.12
(1,2544)	1:386:A:PRO:HG2	1:397:A:ALA:H	18	0.12
(1,2544)	1:386:A:PRO:HG3	1:397:A:ALA:H	18	0.12
(1,2487)	1:383:A:LYS:HE2	1:402:A:PHE:HA	3	0.12
(1,2487)	1:383:A:LYS:HE3	1:402:A:PHE:HA	3	0.12
(1,2427)	1:380:A:LEU:HD11	1:463:A:ARG:H	7	0.12
(1,2427)	1:380:A:LEU:HD12	1:463:A:ARG:H	7	0.12
(1,2427)	1:380:A:LEU:HD13	1:463:A:ARG:H	7	0.12
(1,2427)	1:380:A:LEU:HD11	1:463:A:ARG:H	14	0.12
(1,2427)	1:380:A:LEU:HD12	1:463:A:ARG:H	14	0.12
(1,2427)	1:380:A:LEU:HD13	1:463:A:ARG:H	14	0.12
(1,2353)	1:375:A:TRP:HZ3	1:400:A:LEU:HA	10	0.12
(1,2344)	1:375:A:TRP:HZ2	1:402:A:PHE:HA	3	0.12
(1,2318)	1:374:A:PHE:HZ	1:382:A:LEU:HB2	20	0.12
(1,2318)	1:374:A:PHE:HZ	1:382:A:LEU:HB3	20	0.12
(1,2300)	1:373:A:THR:HG21	1:378:A:PHE:HE1	6	0.12
(1,2300)	1:373:A:THR:HG21	1:378:A:PHE:HE2	6	0.12
(1,2300)	1:373:A:THR:HG22	1:378:A:PHE:HE1	6	0.12
(1,2300)	1:373:A:THR:HG22	1:378:A:PHE:HE2	6	0.12
(1,2300)	1:373:A:THR:HG23	1:378:A:PHE:HE1	6	0.12
(1,2300)	1:373:A:THR:HG23	1:378:A:PHE:HE2	6	0.12
(1,2200)	1:365:A:LYS:HA	1:368:A:ALA:HA	13	0.12
(1,2181)	1:364:A:ALA:HA	1:371:A:TYR:HD1	19	0.12
(1,2181)	1:364:A:ALA:HA	1:371:A:TYR:HD2	19	0.12
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG2	5	0.12
(1,2129)	1:361:A:GLU:HG2	1:398:A:LYS:HG3	5	0.12
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG2	5	0.12
(1,2129)	1:361:A:GLU:HG3	1:398:A:LYS:HG3	5	0.12
(1,2107)	1:360:A:LEU:HA	1:364:A:ALA:H	15	0.12
(1,2049)	1:357:A:LEU:HD11	1:392:A:ASN:HB2	1	0.12
(1,2049)	1:357:A:LEU:HD11	1:392:A:ASN:HB3	1	0.12
(1,2049)	1:357:A:LEU:HD12	1:392:A:ASN:HB2	1	0.12
(1,2049)	1:357:A:LEU:HD12	1:392:A:ASN:HB3	1	0.12
(1,2049)	1:357:A:LEU:HD13	1:392:A:ASN:HB2	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2049)	1:357:A:LEU:HD13	1:392:A:ASN:HB3	1	0.12
(1,2049)	1:357:A:LEU:HD21	1:392:A:ASN:HB2	1	0.12
(1,2049)	1:357:A:LEU:HD21	1:392:A:ASN:HB3	1	0.12
(1,2049)	1:357:A:LEU:HD22	1:392:A:ASN:HB2	1	0.12
(1,2049)	1:357:A:LEU:HD22	1:392:A:ASN:HB3	1	0.12
(1,2049)	1:357:A:LEU:HD23	1:392:A:ASN:HB2	1	0.12
(1,2049)	1:357:A:LEU:HD23	1:392:A:ASN:HB3	1	0.12
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD11	9	0.12
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD12	9	0.12
(1,2038)	1:357:A:LEU:HA	1:399:A:LEU:HD13	9	0.12
(1,2013)	1:355:A:ARG:HA	1:358:A:GLN:H	3	0.12
(1,1954)	1:351:A:ALA:HA	1:353:A:THR:HB	20	0.12
(1,1933)	1:350:A:ASN:HA	1:354:A:LYS:H	19	0.12
(1,1854)	1:343:A:THR:HA	1:345:A:THR:HB	7	0.12
(1,1843)	1:342:A:SER:HB2	1:343:A:THR:H	6	0.12
(1,1843)	1:342:A:SER:HB3	1:343:A:THR:H	6	0.12
(1,1843)	1:342:A:SER:HB2	1:343:A:THR:H	12	0.12
(1,1843)	1:342:A:SER:HB3	1:343:A:THR:H	12	0.12
(1,1843)	1:342:A:SER:HB2	1:343:A:THR:H	17	0.12
(1,1843)	1:342:A:SER:HB3	1:343:A:THR:H	17	0.12
(1,1827)	1:340:A:GLN:HA	1:342:A:SER:H	10	0.12
(1,1810)	1:339:A:LEU:HA	1:345:A:THR:H	4	0.12
(1,1765)	1:335:A:SER:H	1:338:A:ILE:H	14	0.12
(1,1762)	1:335:A:SER:H	1:339:A:LEU:H	6	0.12
(1,1717)	1:330:A:LEU:HD21	1:334:A:VAL:HB	2	0.12
(1,1717)	1:330:A:LEU:HD22	1:334:A:VAL:HB	2	0.12
(1,1717)	1:330:A:LEU:HD23	1:334:A:VAL:HB	2	0.12
(1,1382)	1:307:A:MET:HB2	1:308:A:ASP:H	8	0.12
(1,1382)	1:307:A:MET:HB3	1:308:A:ASP:H	8	0.12
(1,1349)	1:305:A:PHE:HZ	1:308:A:ASP:HA	3	0.12
(1,1130)	1:297:A:LEU:H	1:311:A:GLU:HA	10	0.12
(1,1090)	1:296:A:GLY:H	1:311:A:GLU:HA	5	0.12
(1,1060)	1:294:A:LYS:HD2	1:309:A:ASP:HB2	8	0.12
(1,1060)	1:294:A:LYS:HD2	1:309:A:ASP:HB3	8	0.12
(1,1060)	1:294:A:LYS:HD3	1:309:A:ASP:HB2	8	0.12
(1,1060)	1:294:A:LYS:HD3	1:309:A:ASP:HB3	8	0.12
(1,1037)	1:290:A:ASN:HB2	1:292:A:ASP:H	14	0.12
(1,1037)	1:290:A:ASN:HB3	1:292:A:ASP:H	14	0.12
(1,1036)	1:290:A:ASN:HA	1:292:A:ASP:H	12	0.12
(1,1024)	1:289:A:TRP:HH2	1:381:A:VAL:HA	13	0.12
(1,1023)	1:289:A:TRP:HZ2	1:381:A:VAL:H	6	0.12
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD21	10	0.12
(1,976)	1:286:A:TRP:HE3	1:290:A:ASN:HD22	10	0.12
(1,917)	1:282:A:SER:HA	1:374:A:PHE:HA	14	0.12
(1,916)	1:282:A:SER:HA	1:377:A:GLN:HB2	14	0.12
(1,916)	1:282:A:SER:HA	1:377:A:GLN:HB3	14	0.12
(1,915)	1:282:A:SER:HA	1:378:A:PHE:HZ	18	0.12
(1,848)	1:279:A:TYR:H	1:322:A:ARG:H	9	0.12
(1,764)	1:276:A:SER:HB2	1:326:A:ASP:H	3	0.12
(1,764)	1:276:A:SER:HB3	1:326:A:ASP:H	3	0.12
(1,708)	1:273:A:GLU:HB2	1:327:A:SER:HA	8	0.12
(1,708)	1:273:A:GLU:HB3	1:327:A:SER:HA	8	0.12
(1,700)	1:273:A:GLU:HB2	1:329:A:ASP:H	1	0.12
(1,700)	1:273:A:GLU:HB3	1:329:A:ASP:H	1	0.12
(1,680)	1:271:A:LYS:HA	1:273:A:GLU:H	2	0.12
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD1	9	0.12
(1,635)	1:267:A:ARG:HA	1:274:A:TYR:HD2	9	0.12
(1,614)	1:266:A:ASN:H	1:276:A:SER:H	8	0.12
(1,525)	1:262:A:THR:HB	1:370:A:LYS:HD2	2	0.12
(1,525)	1:262:A:THR:HB	1:370:A:LYS:HD3	2	0.12
(1,513)	1:261:A:LEU:H	1:281:A:PRO:HA	15	0.12
(1,513)	1:261:A:LEU:H	1:281:A:PRO:HA	17	0.12
(1,509)	1:261:A:LEU:H	1:282:A:SER:H	17	0.12
(1,470)	1:260:A:PRO:HA	1:283:A:GLN:H	7	0.12
(1,452)	1:257:A:PHE:H	1:258:A:ASN:H	17	0.12
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	17	0.12
(1,409)	1:253:A:ILE:HA	1:298:A:LYS:HD2	6	0.12
(1,409)	1:253:A:ILE:HA	1:298:A:LYS:HD3	6	0.12
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD2	13	0.12
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD3	13	0.12
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD2	13	0.12
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD3	13	0.12
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD2	13	0.12
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD3	13	0.12
(1,316)	1:249:A:PHE:HA	1:253:A:ILE:H	1	0.12
(1,310)	1:249:A:PHE:HZ	1:298:A:LYS:HD3	16	0.12
(1,295)	1:248:A:GLU:HA	1:251:A:LYS:HD2	13	0.12
(1,295)	1:248:A:GLU:HA	1:251:A:LYS:HD3	13	0.12
(1,234)	1:245:A:GLU:HA	1:248:A:GLU:H	16	0.12
(1,210)	1:243:A:ASP:H	1:246:A:TYR:H	9	0.12
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	17	0.12
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	20	0.12
(1,112)	1:235:A:THR:HA	1:265:A:HIS:HE1	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:235:A:THR:H	1:265:A:HIS:HE1	10	0.12
(1,111)	1:235:A:THR:H	1:265:A:HIS:HE1	15	0.12
(1,86)	1:234:A:TRP:HD1	1:275:A:THR:HG21	13	0.12
(1,86)	1:234:A:TRP:HD1	1:275:A:THR:HG22	13	0.12
(1,86)	1:234:A:TRP:HD1	1:275:A:THR:HG23	13	0.12
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD11	3	0.12
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD12	3	0.12
(1,61)	1:234:A:TRP:HH2	1:324:A:LEU:HD13	3	0.12
(1,8)	1:231:A:GLN:HG2	1:236:A:ARG:HG2	6	0.12
(1,8)	1:231:A:GLN:HG2	1:236:A:ARG:HG3	6	0.12
(1,8)	1:231:A:GLN:HG3	1:236:A:ARG:HG2	6	0.12
(1,8)	1:231:A:GLN:HG3	1:236:A:ARG:HG3	6	0.12
(1,3942)	1:490:A:LEU:H	1:492:A:LYS:H	13	0.11
(1,3918)	1:488:A:GLU:HA	1:491:A:GLU:HA	2	0.11
(1,3917)	1:488:A:GLU:HA	1:491:A:GLU:H	14	0.11
(1,3785)	1:474:A:GLU:HA	1:480:A:PHE:H	20	0.11
(1,3744)	1:469:A:MET:HA	1:472:A:LEU:H	14	0.11
(1,3742)	1:469:A:MET:HE1	1:473:A:THR:HA	7	0.11
(1,3742)	1:469:A:MET:HE2	1:473:A:THR:HA	7	0.11
(1,3742)	1:469:A:MET:HE3	1:473:A:THR:HA	7	0.11
(1,3703)	1:465:A:ASP:H	1:467:A:TRP:H	5	0.11
(1,3688)	1:464:A:ILE:HD11	1:467:A:TRP:HE3	8	0.11
(1,3688)	1:464:A:ILE:HD12	1:467:A:TRP:HE3	8	0.11
(1,3688)	1:464:A:ILE:HD13	1:467:A:TRP:HE3	8	0.11
(1,3674)	1:462:A:ASP:HB2	1:464:A:ILE:H	5	0.11
(1,3674)	1:462:A:ASP:HB3	1:464:A:ILE:H	5	0.11
(1,3624)	1:457:A:VAL:HA	1:483:A:VAL:HG11	18	0.11
(1,3624)	1:457:A:VAL:HA	1:483:A:VAL:HG12	18	0.11
(1,3624)	1:457:A:VAL:HA	1:483:A:VAL:HG13	18	0.11
(1,3616)	1:455:A:ILE:HB	1:456:A:GLU:H	5	0.11
(1,3598)	1:453:A:LYS:HG2	1:493:A:LEU:HB2	5	0.11
(1,3598)	1:453:A:LYS:HG2	1:493:A:LEU:HB3	5	0.11
(1,3563)	1:450:A:LEU:HA	1:455:A:ILE:H	8	0.11
(1,3553)	1:450:A:LEU:HD11	1:483:A:VAL:HB	14	0.11
(1,3553)	1:450:A:LEU:HD12	1:483:A:VAL:HB	14	0.11
(1,3553)	1:450:A:LEU:HD13	1:483:A:VAL:HB	14	0.11
(1,3405)	1:439:A:ALA:HA	1:442:A:LYS:HB2	19	0.11
(1,3405)	1:439:A:ALA:HA	1:442:A:LYS:HB3	19	0.11
(1,3265)	1:433:A:ILE:H	1:460:A:LEU:H	18	0.11
(1,3248)	1:432:A:TYR:HA	1:457:A:VAL:HA	13	0.11
(1,3238)	1:432:A:TYR:HB2	1:460:A:LEU:H	14	0.11
(1,3238)	1:432:A:TYR:HB3	1:460:A:LEU:H	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3164)	1:429:A:LYS:HB2	1:431:A:TYR:HE1	10	0.11
(1,3164)	1:429:A:LYS:HB2	1:431:A:TYR:HE2	10	0.11
(1,3164)	1:429:A:LYS:HB3	1:431:A:TYR:HE1	10	0.11
(1,3164)	1:429:A:LYS:HB3	1:431:A:TYR:HE2	10	0.11
(1,3155)	1:429:A:LYS:HB2	1:480:A:PHE:HA	2	0.11
(1,3155)	1:429:A:LYS:HB3	1:480:A:PHE:HA	2	0.11
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG2	3	0.11
(1,3148)	1:429:A:LYS:HE2	1:488:A:GLU:HG3	3	0.11
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG2	3	0.11
(1,3148)	1:429:A:LYS:HE3	1:488:A:GLU:HG3	3	0.11
(1,3143)	1:429:A:LYS:HD2	1:489:A:SER:H	13	0.11
(1,3143)	1:429:A:LYS:HD3	1:489:A:SER:H	13	0.11
(1,3093)	1:424:A:LYS:HE2	1:454:A:GLY:HA2	20	0.11
(1,3093)	1:424:A:LYS:HE2	1:454:A:GLY:HA3	20	0.11
(1,3093)	1:424:A:LYS:HE3	1:454:A:GLY:HA2	20	0.11
(1,3093)	1:424:A:LYS:HE3	1:454:A:GLY:HA3	20	0.11
(1,2968)	1:416:A:LEU:HA	1:420:A:VAL:H	18	0.11
(1,2968)	1:416:A:LEU:HA	1:420:A:VAL:H	19	0.11
(1,2961)	1:416:A:LEU:HB2	1:475:A:PHE:HZ	16	0.11
(1,2961)	1:416:A:LEU:HB3	1:475:A:PHE:HZ	16	0.11
(1,2914)	1:410:A:SER:HA	1:438:A:TYR:HE1	3	0.11
(1,2855)	1:405:A:THR:HB	1:451:A:ARG:HA	20	0.11
(1,2816)	1:404:A:SER:HA	1:457:A:VAL:HB	14	0.11
(1,2807)	1:404:A:SER:HA	1:459:A:LEU:H	15	0.11
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG11	19	0.11
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG12	19	0.11
(1,2791)	1:403:A:ALA:H	1:414:A:VAL:HG13	19	0.11
(1,2786)	1:403:A:ALA:H	1:458:A:LEU:HA	13	0.11
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG11	4	0.11
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG12	4	0.11
(1,2766)	1:402:A:PHE:HB2	1:414:A:VAL:HG13	4	0.11
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG11	4	0.11
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG12	4	0.11
(1,2766)	1:402:A:PHE:HB3	1:414:A:VAL:HG13	4	0.11
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD11	4	0.11
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD12	4	0.11
(1,2746)	1:402:A:PHE:HZ	1:472:A:LEU:HD13	4	0.11
(1,2739)	1:401:A:ARG:HD2	1:413:A:THR:HA	14	0.11
(1,2739)	1:401:A:ARG:HD3	1:413:A:THR:HA	14	0.11
(1,2632)	1:393:A:GLN:HA	1:396:A:ILE:HB	2	0.11
(1,2585)	1:389:A:ASP:HA	1:391:A:ALA:H	18	0.11
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD1	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2561)	1:387:A:ALA:HA	1:471:A:TYR:HD2	8	0.11
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB2	20	0.11
(1,2560)	1:387:A:ALA:HA	1:471:A:TYR:HB3	20	0.11
(1,2534)	1:386:A:PRO:HB2	1:472:A:LEU:H	10	0.11
(1,2534)	1:386:A:PRO:HB3	1:472:A:LEU:H	10	0.11
(1,2445)	1:381:A:VAL:HA	1:385:A:GLY:H	2	0.11
(1,2260)	1:371:A:TYR:HE1	1:399:A:LEU:HA	14	0.11
(1,2260)	1:371:A:TYR:HE2	1:399:A:LEU:HA	14	0.11
(1,2200)	1:365:A:LYS:HA	1:368:A:ALA:HA	12	0.11
(1,2137)	1:361:A:GLU:HA	1:364:A:ALA:H	19	0.11
(1,2133)	1:361:A:GLU:HA	1:365:A:LYS:H	2	0.11
(1,1997)	1:354:A:LYS:HB2	1:358:A:GLN:HE21	15	0.11
(1,1997)	1:354:A:LYS:HB2	1:358:A:GLN:HE22	15	0.11
(1,1997)	1:354:A:LYS:HB3	1:358:A:GLN:HE21	15	0.11
(1,1997)	1:354:A:LYS:HB3	1:358:A:GLN:HE22	15	0.11
(1,1988)	1:353:A:THR:HB	1:354:A:LYS:H	3	0.11
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD11	13	0.11
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD12	13	0.11
(1,1978)	1:353:A:THR:HB	1:357:A:LEU:HD13	13	0.11
(1,1937)	1:350:A:ASN:HA	1:353:A:THR:H	20	0.11
(1,1788)	1:337:A:GLU:HA	1:341:A:ASP:H	2	0.11
(1,1768)	1:335:A:SER:H	1:338:A:ILE:HD11	13	0.11
(1,1768)	1:335:A:SER:H	1:338:A:ILE:HD12	13	0.11
(1,1768)	1:335:A:SER:H	1:338:A:ILE:HD13	13	0.11
(1,1676)	1:325:A:ILE:HD11	1:327:A:SER:HB2	16	0.11
(1,1676)	1:325:A:ILE:HD11	1:327:A:SER:HB3	16	0.11
(1,1676)	1:325:A:ILE:HD12	1:327:A:SER:HB2	16	0.11
(1,1676)	1:325:A:ILE:HD12	1:327:A:SER:HB3	16	0.11
(1,1676)	1:325:A:ILE:HD13	1:327:A:SER:HB2	16	0.11
(1,1676)	1:325:A:ILE:HD13	1:327:A:SER:HB3	16	0.11
(1,1452)	1:313:A:PHE:HZ	1:345:A:THR:HA	12	0.11
(1,1452)	1:313:A:PHE:HZ	1:345:A:THR:HA	19	0.11
(1,1382)	1:307:A:MET:HB2	1:308:A:ASP:H	3	0.11
(1,1382)	1:307:A:MET:HB3	1:308:A:ASP:H	3	0.11
(1,1382)	1:307:A:MET:HB2	1:308:A:ASP:H	7	0.11
(1,1382)	1:307:A:MET:HB3	1:308:A:ASP:H	7	0.11
(1,1382)	1:307:A:MET:HB2	1:308:A:ASP:H	16	0.11
(1,1382)	1:307:A:MET:HB3	1:308:A:ASP:H	16	0.11
(1,1324)	1:302:A:GLN:H	1:327:A:SER:H	17	0.11
(1,1320)	1:302:A:GLN:H	1:328:A:SER:HA	18	0.11
(1,1277)	1:301:A:VAL:HB	1:332:A:LEU:HD11	10	0.11
(1,1277)	1:301:A:VAL:HB	1:332:A:LEU:HD12	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1277)	1:301:A:VAL:HB	1:332:A:LEU:HD13	10	0.11
(1,1219)	1:299:A:LEU:H	1:306:A:ILE:H	17	0.11
(1,1167)	1:298:A:LYS:HA	1:309:A:ASP:HA	14	0.11
(1,1167)	1:298:A:LYS:HA	1:309:A:ASP:HA	16	0.11
(1,1124)	1:297:A:LEU:H	1:313:A:PHE:H	6	0.11
(1,1038)	1:290:A:ASN:HB2	1:292:A:ASP:HB2	3	0.11
(1,1038)	1:290:A:ASN:HB2	1:292:A:ASP:HB3	3	0.11
(1,1038)	1:290:A:ASN:HB3	1:292:A:ASP:HB2	3	0.11
(1,1038)	1:290:A:ASN:HB3	1:292:A:ASP:HB3	3	0.11
(1,1023)	1:289:A:TRP:HZ2	1:381:A:VAL:H	11	0.11
(1,979)	1:286:A:TRP:HE3	1:289:A:TRP:H	17	0.11
(1,848)	1:279:A:TYR:H	1:322:A:ARG:H	6	0.11
(1,848)	1:279:A:TYR:H	1:322:A:ARG:H	8	0.11
(1,821)	1:278:A:LEU:HA	1:322:A:ARG:H	7	0.11
(1,800)	1:278:A:LEU:HB2	1:359:A:MET:HE1	18	0.11
(1,800)	1:278:A:LEU:HB2	1:359:A:MET:HE2	18	0.11
(1,800)	1:278:A:LEU:HB2	1:359:A:MET:HE3	18	0.11
(1,800)	1:278:A:LEU:HB3	1:359:A:MET:HE1	18	0.11
(1,800)	1:278:A:LEU:HB3	1:359:A:MET:HE2	18	0.11
(1,800)	1:278:A:LEU:HB3	1:359:A:MET:HE3	18	0.11
(1,769)	1:276:A:SER:HB2	1:325:A:ILE:HB	15	0.11
(1,769)	1:276:A:SER:HB3	1:325:A:ILE:HB	15	0.11
(1,767)	1:276:A:SER:HB2	1:325:A:ILE:HA	11	0.11
(1,767)	1:276:A:SER:HB3	1:325:A:ILE:HA	11	0.11
(1,764)	1:276:A:SER:HB2	1:326:A:ASP:H	10	0.11
(1,764)	1:276:A:SER:HB3	1:326:A:ASP:H	10	0.11
(1,764)	1:276:A:SER:HB2	1:326:A:ASP:H	19	0.11
(1,764)	1:276:A:SER:HB3	1:326:A:ASP:H	19	0.11
(1,763)	1:276:A:SER:HA	1:326:A:ASP:H	10	0.11
(1,752)	1:275:A:THR:HG21	1:324:A:LEU:HD21	2	0.11
(1,752)	1:275:A:THR:HG21	1:324:A:LEU:HD22	2	0.11
(1,752)	1:275:A:THR:HG21	1:324:A:LEU:HD23	2	0.11
(1,752)	1:275:A:THR:HG22	1:324:A:LEU:HD21	2	0.11
(1,752)	1:275:A:THR:HG22	1:324:A:LEU:HD22	2	0.11
(1,752)	1:275:A:THR:HG22	1:324:A:LEU:HD23	2	0.11
(1,752)	1:275:A:THR:HG23	1:324:A:LEU:HD21	2	0.11
(1,752)	1:275:A:THR:HG23	1:324:A:LEU:HD22	2	0.11
(1,752)	1:275:A:THR:HG23	1:324:A:LEU:HD23	2	0.11
(1,740)	1:275:A:THR:H	1:328:A:SER:H	18	0.11
(1,724)	1:274:A:TYR:HA	1:328:A:SER:H	15	0.11
(1,700)	1:273:A:GLU:HB2	1:329:A:ASP:H	6	0.11
(1,700)	1:273:A:GLU:HB3	1:329:A:ASP:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,699)	1:273:A:GLU:H	1:329:A:ASP:H	6	0.11
(1,653)	1:268:A:VAL:HB	1:273:A:GLU:HA	17	0.11
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD21	16	0.11
(1,588)	1:264:A:SER:HA	1:266:A:ASN:HD22	16	0.11
(1,564)	1:263:A:TRP:HE1	1:265:A:HIS:H	7	0.11
(1,452)	1:257:A:PHE:H	1:258:A:ASN:H	3	0.11
(1,451)	1:257:A:PHE:HA	1:259:A:ASP:H	2	0.11
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD2	8	0.11
(1,407)	1:253:A:ILE:HD11	1:322:A:ARG:HD3	8	0.11
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD2	8	0.11
(1,407)	1:253:A:ILE:HD12	1:322:A:ARG:HD3	8	0.11
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD2	8	0.11
(1,407)	1:253:A:ILE:HD13	1:322:A:ARG:HD3	8	0.11
(1,379)	1:251:A:LYS:HG2	1:256:A:ASP:H	16	0.11
(1,379)	1:251:A:LYS:HG3	1:256:A:ASP:H	16	0.11
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	20	0.11
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	20	0.11
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	20	0.11
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	20	0.11
(1,347)	1:250:A:TYR:HE1	1:260:A:PRO:HA	13	0.11
(1,347)	1:250:A:TYR:HE2	1:260:A:PRO:HA	13	0.11
(1,309)	1:249:A:PHE:HE2	1:298:A:LYS:HD3	12	0.11
(1,282)	1:247:A:LYS:HA	1:250:A:TYR:H	10	0.11
(1,251)	1:246:A:TYR:HE1	1:263:A:TRP:HE1	10	0.11
(1,251)	1:246:A:TYR:HE2	1:263:A:TRP:HE1	10	0.11
(1,250)	1:246:A:TYR:HD1	1:263:A:TRP:HE1	11	0.11
(1,250)	1:246:A:TYR:HD2	1:263:A:TRP:HE1	11	0.11
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB2	4	0.11
(1,221)	1:244:A:GLU:HA	1:248:A:GLU:HB3	4	0.11
(1,218)	1:243:A:ASP:HB2	1:244:A:GLU:H	19	0.11
(1,218)	1:243:A:ASP:HB3	1:244:A:GLU:H	19	0.11
(1,204)	1:243:A:ASP:HA	1:263:A:TRP:HH2	20	0.11
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	8	0.11
(1,190)	1:242:A:THR:HA	1:246:A:TYR:H	20	0.11
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	5	0.11
(1,189)	1:242:A:THR:H	1:246:A:TYR:H	16	0.11
(1,127)	1:236:A:ARG:HB2	1:237:A:ASN:H	2	0.11
(1,127)	1:236:A:ARG:HB3	1:237:A:ASN:H	2	0.11
(1,111)	1:235:A:THR:H	1:265:A:HIS:HE1	16	0.11
(1,52)	1:233:A:LEU:HA	1:235:A:THR:H	13	0.11
(1,24)	1:232:A:ALA:H	1:235:A:THR:HG21	4	0.11
(1,24)	1:232:A:ALA:H	1:235:A:THR:HG22	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:232:A:ALA:H	1:235:A:THR:HG23	4	0.11
(1,3807)	1:475:A:PHE:H	1:479:A:PRO:HA	20	0.1
(1,3777)	1:473:A:THR:HB	1:480:A:PHE:H	13	0.1
(1,3439)	1:442:A:LYS:H	1:459:A:LEU:HD11	16	0.1
(1,3439)	1:442:A:LYS:H	1:459:A:LEU:HD12	16	0.1
(1,3439)	1:442:A:LYS:H	1:459:A:LEU:HD13	16	0.1
(1,3353)	1:436:A:ASP:HA	1:461:A:SER:HA	14	0.1
(1,3309)	1:434:A:THR:HB	1:466:A:GLU:H	19	0.1
(1,3174)	1:430:A:ILE:H	1:480:A:PHE:HA	10	0.1
(1,2945)	1:415:A:SER:H	1:419:A:TYR:H	19	0.1
(1,2893)	1:408:A:ASP:HB2	1:442:A:LYS:HE2	16	0.1
(1,2893)	1:408:A:ASP:HB2	1:442:A:LYS:HE3	16	0.1
(1,2893)	1:408:A:ASP:HB3	1:442:A:LYS:HE2	16	0.1
(1,2893)	1:408:A:ASP:HB3	1:442:A:LYS:HE3	16	0.1
(1,2827)	1:404:A:SER:H	1:413:A:THR:H	6	0.1
(1,2824)	1:404:A:SER:H	1:414:A:VAL:HB	3	0.1
(1,2566)	1:387:A:ALA:H	1:468:A:MET:HA	4	0.1
(1,2548)	1:386:A:PRO:HG2	1:396:A:ILE:HB	18	0.1
(1,2548)	1:386:A:PRO:HG3	1:396:A:ILE:HB	18	0.1
(1,2540)	1:386:A:PRO:HB2	1:468:A:MET:HA	10	0.1
(1,2540)	1:386:A:PRO:HB3	1:468:A:MET:HA	10	0.1
(1,2416)	1:379:A:GLY:H	1:382:A:LEU:H	12	0.1
(1,2398)	1:378:A:PHE:HA	1:382:A:LEU:H	7	0.1
(1,2360)	1:375:A:TRP:HZ2	1:383:A:LYS:HG2	7	0.1
(1,2360)	1:375:A:TRP:HZ2	1:383:A:LYS:HG3	7	0.1
(1,2358)	1:375:A:TRP:HZ2	1:383:A:LYS:HE2	15	0.1
(1,2358)	1:375:A:TRP:HZ2	1:383:A:LYS:HE3	15	0.1
(1,2305)	1:373:A:THR:HA	1:376:A:GLN:H	11	0.1
(1,2267)	1:371:A:TYR:HE1	1:375:A:TRP:HE3	9	0.1
(1,2267)	1:371:A:TYR:HE2	1:375:A:TRP:HE3	9	0.1
(1,2203)	1:365:A:LYS:HA	1:367:A:ASP:H	10	0.1
(1,2133)	1:361:A:GLU:HA	1:365:A:LYS:H	4	0.1
(1,2041)	1:357:A:LEU:HD21	1:396:A:ILE:H	3	0.1
(1,2041)	1:357:A:LEU:HD22	1:396:A:ILE:H	3	0.1
(1,2041)	1:357:A:LEU:HD23	1:396:A:ILE:H	3	0.1
(1,2014)	1:355:A:ARG:HA	1:358:A:GLN:HB2	9	0.1
(1,2014)	1:355:A:ARG:HA	1:358:A:GLN:HB3	9	0.1
(1,2014)	1:355:A:ARG:HA	1:358:A:GLN:HB2	18	0.1
(1,2014)	1:355:A:ARG:HA	1:358:A:GLN:HB3	18	0.1
(1,2013)	1:355:A:ARG:HA	1:358:A:GLN:H	5	0.1
(1,1897)	1:347:A:ASN:HA	1:351:A:ALA:H	18	0.1
(1,1790)	1:337:A:GLU:HG2	1:341:A:ASP:HB2	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1790)	1:337:A:GLU:HG2	1:341:A:ASP:HB3	14	0.1
(1,1790)	1:337:A:GLU:HG3	1:341:A:ASP:HB2	14	0.1
(1,1790)	1:337:A:GLU:HG3	1:341:A:ASP:HB3	14	0.1
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE1	7	0.1
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE2	7	0.1
(1,1654)	1:322:A:ARG:H	1:359:A:MET:HE3	7	0.1
(1,1626)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	8	0.1
(1,1626)	1:320:A:PHE:HZ	1:374:A:PHE:HZ	20	0.1
(1,1610)	1:319:A:ARG:HA	1:321:A:VAL:HB	8	0.1
(1,1570)	1:317:A:TYR:HA	1:320:A:PHE:HE1	6	0.1
(1,1570)	1:317:A:TYR:HA	1:320:A:PHE:HE2	6	0.1
(1,1479)	1:314:A:MET:H	1:349:A:ARG:HD2	17	0.1
(1,1479)	1:314:A:MET:H	1:349:A:ARG:HD3	17	0.1
(1,1219)	1:299:A:LEU:H	1:306:A:ILE:H	8	0.1
(1,1051)	1:293:A:HIS:HE1	1:309:A:ASP:HB2	17	0.1
(1,1051)	1:293:A:HIS:HE1	1:309:A:ASP:HB3	17	0.1
(1,960)	1:285:A:PRO:HB2	1:294:A:LYS:HB2	15	0.1
(1,960)	1:285:A:PRO:HB2	1:294:A:LYS:HB3	15	0.1
(1,960)	1:285:A:PRO:HB3	1:294:A:LYS:HB2	15	0.1
(1,960)	1:285:A:PRO:HB3	1:294:A:LYS:HB3	15	0.1
(1,879)	1:280:A:ILE:HA	1:321:A:VAL:HA	17	0.1
(1,770)	1:276:A:SER:HA	1:324:A:LEU:H	6	0.1
(1,763)	1:276:A:SER:HA	1:326:A:ASP:H	16	0.1
(1,676)	1:270:A:GLY:HA2	1:272:A:GLN:H	17	0.1
(1,676)	1:270:A:GLY:HA3	1:272:A:GLN:H	17	0.1
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD1	18	0.1
(1,520)	1:261:A:LEU:H	1:279:A:TYR:HD2	18	0.1
(1,513)	1:261:A:LEU:H	1:281:A:PRO:HA	18	0.1
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB2	17	0.1
(1,377)	1:251:A:LYS:HG2	1:257:A:PHE:HB3	17	0.1
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB2	17	0.1
(1,377)	1:251:A:LYS:HG3	1:257:A:PHE:HB3	17	0.1
(1,222)	1:244:A:GLU:H	1:247:A:LYS:H	9	0.1
(1,211)	1:243:A:ASP:HA	1:246:A:TYR:H	12	0.1
(1,144)	1:237:A:ASN:HD21	1:238:A:LYS:H	16	0.1
(1,144)	1:237:A:ASN:HD22	1:238:A:LYS:H	16	0.1
(1,111)	1:235:A:THR:H	1:265:A:HIS:HE1	18	0.1
(1,48)	1:233:A:LEU:H	1:236:A:ARG:H	6	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found