



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 07:31 AM UTC

PDB ID : 2MQ3 / pdb_00002mq3
BMRB ID : 25010
Title : NMR structure of the c3 domain of human cardiac myosin binding protein-c with a hypertrophic cardiomyopathy-related mutation R502W.
Authors : Zhang, X.; De, S.; McIntosh, L.P.; Paetzel, M.
Deposited on : 2014-06-12

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

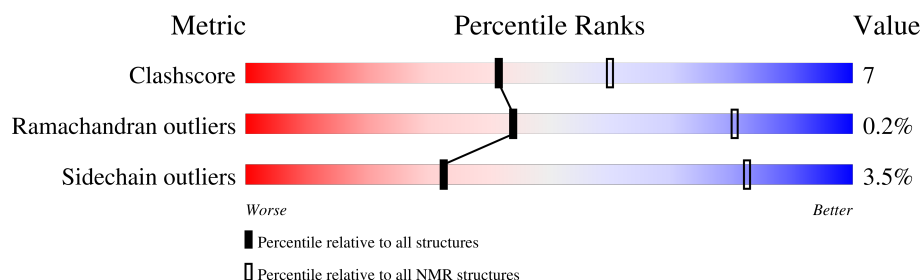
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	95	 89% 6% .

2 Ensemble composition and analysis

This entry contains 10 models. Model 2 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:453-A:543 (91)	0.95	2

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 1 clusters and 7 single-model clusters were found.

Cluster number	Models
1	2, 5, 10
Single-model clusters	1; 3; 4; 6; 7; 8; 9

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1511 atoms, of which 750 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Myosin-binding protein C, cardiac-type.

Mol	Chain	Residues	Atoms						Trace
1	A	95	Total	C	H	N	O	S	0
			1511	480	750	130	146	5	

There are 5 discrepancies between the modelled and reference sequences:

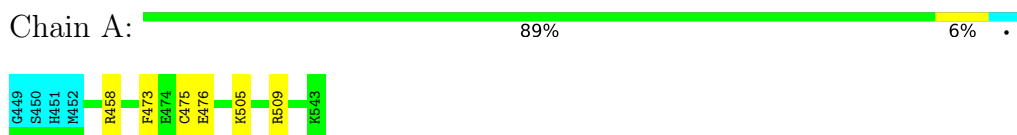
Chain	Residue	Modelled	Actual	Comment	Reference
A	449	GLY	-	expression tag	UNP Q14896
A	450	SER	-	expression tag	UNP Q14896
A	451	HIS	-	expression tag	UNP Q14896
A	452	MET	-	expression tag	UNP Q14896
A	502	TRP	ARG	engineered mutation	UNP Q14896

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Myosin-binding protein C, cardiac-type

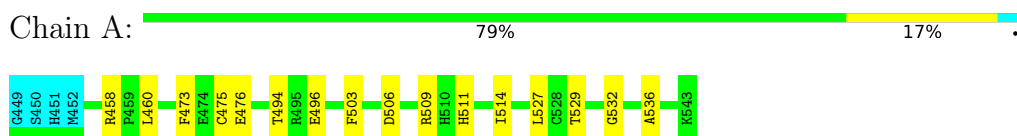


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

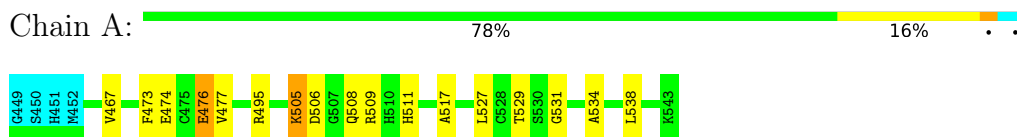
4.2.1 Score per residue for model 1

- Molecule 1: Myosin-binding protein C, cardiac-type



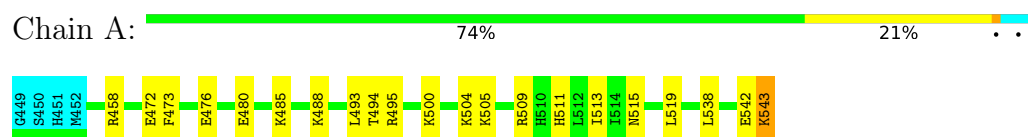
4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Myosin-binding protein C, cardiac-type



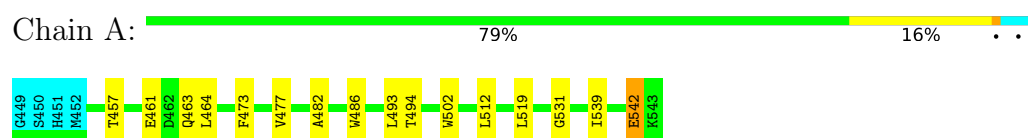
4.2.3 Score per residue for model 3

- Molecule 1: Myosin-binding protein C, cardiac-type



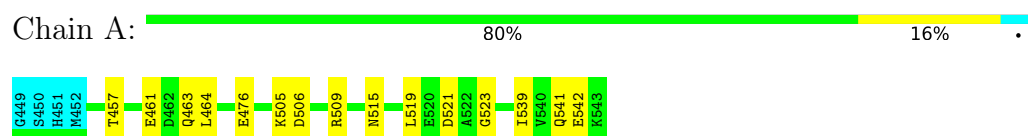
4.2.4 Score per residue for model 4

- Molecule 1: Myosin-binding protein C, cardiac-type



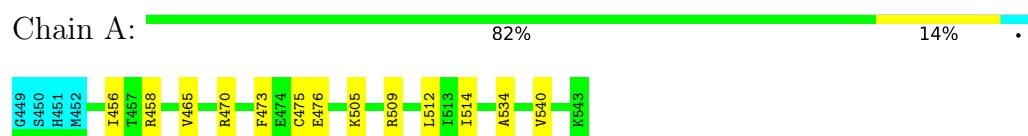
4.2.5 Score per residue for model 5

- Molecule 1: Myosin-binding protein C, cardiac-type



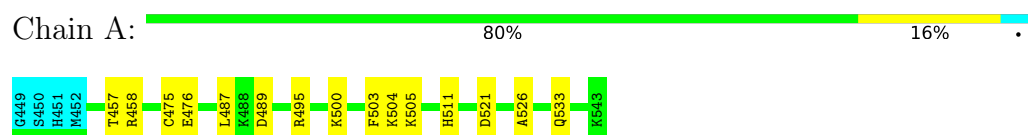
4.2.6 Score per residue for model 6

- Molecule 1: Myosin-binding protein C, cardiac-type



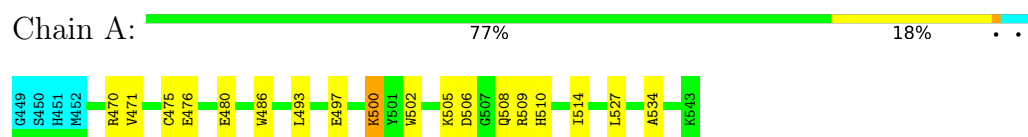
4.2.7 Score per residue for model 7

- Molecule 1: Myosin-binding protein C, cardiac-type



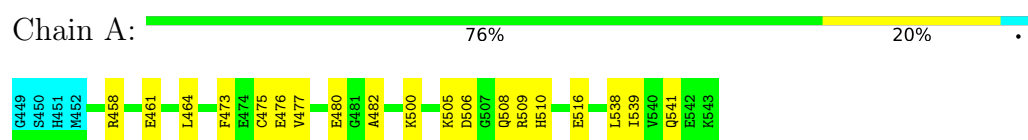
4.2.8 Score per residue for model 8

- Molecule 1: Myosin-binding protein C, cardiac-type



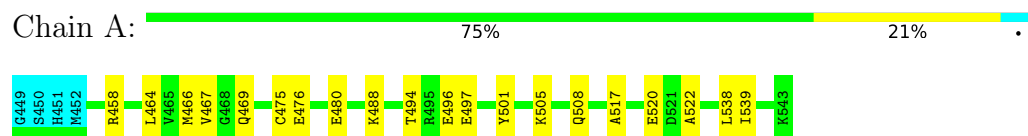
4.2.9 Score per residue for model 9

- Molecule 1: Myosin-binding protein C, cardiac-type



4.2.10 Score per residue for model 10

- Molecule 1: Myosin-binding protein C, cardiac-type



5 Refinement protocol and experimental data overview

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

Of the 10 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1084
Number of shifts mapped to atoms	1084
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	733	724	721	10±2
All	All	7330	7240	7210	99

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:519:LEU:HG	1:A:542:GLU:HG2	0.83	1.50	4	1
1:A:504:LYS:HG2	1:A:511:HIS:HB2	0.81	1.52	3	1
1:A:464:LEU:HG	1:A:539:ILE:HB	0.66	1.66	5	3
1:A:461:GLU:HG3	1:A:538:LEU:HD13	0.65	1.67	9	1
1:A:458:ARG:HG2	1:A:476:GLU:HG2	0.65	1.67	7	2
1:A:458:ARG:HB2	1:A:475:CYS:HA	0.64	1.67	10	5
1:A:456:ILE:HG13	1:A:534:ALA:HB2	0.61	1.73	6	1
1:A:457:THR:HB	1:A:476:GLU:HG3	0.60	1.72	7	1
1:A:504:LYS:HE2	1:A:513:ILE:HD11	0.58	1.75	3	1
1:A:542:GLU:HG2	1:A:543:LYS:HD3	0.58	1.75	3	1
1:A:519:LEU:HD11	1:A:542:GLU:HB2	0.57	1.76	3	1
1:A:476:GLU:CB	1:A:509:ARG:HA	0.56	2.30	1	1
1:A:476:GLU:HB2	1:A:509:ARG:HA	0.56	1.78	1	2
1:A:471:VAL:HG23	1:A:514:ILE:HB	0.55	1.78	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:475:CYS:O	1:A:510:HIS:HB2	0.55	2.01	8	2
1:A:461:GLU:HB2	1:A:463:GLN:OE1	0.54	2.03	5	1
1:A:473:PHE:HB2	1:A:512:LEU:HB3	0.53	1.80	6	1
1:A:458:ARG:CB	1:A:475:CYS:HA	0.53	2.33	9	1
1:A:543:LYS:HD3	1:A:543:LYS:H	0.53	1.64	3	1
1:A:495:ARG:HD3	1:A:503:PHE:CE2	0.52	2.38	7	1
1:A:473:PHE:HD2	1:A:512:LEU:HD23	0.51	1.65	4	1
1:A:519:LEU:HD21	1:A:542:GLU:HB3	0.51	1.82	5	1
1:A:475:CYS:SG	1:A:527:LEU:HD13	0.50	2.46	1	1
1:A:503:PHE:HA	1:A:511:HIS:O	0.49	2.06	1	2
1:A:458:ARG:CG	1:A:476:GLU:HG2	0.49	2.37	10	2
1:A:500:LYS:HE3	1:A:516:GLU:HB2	0.49	1.83	9	1
1:A:504:LYS:CE	1:A:513:ILE:HD11	0.49	2.37	3	1
1:A:505:LYS:NZ	1:A:505:LYS:HB3	0.49	2.22	2	1
1:A:506:ASP:HB2	1:A:509:ARG:HG2	0.49	1.85	2	1
1:A:519:LEU:HG	1:A:542:GLU:CG	0.49	2.31	4	1
1:A:506:ASP:HB3	1:A:509:ARG:HB2	0.48	1.84	8	2
1:A:480:GLU:HA	1:A:508:GLN:HB3	0.48	1.84	8	3
1:A:461:GLU:HB3	1:A:473:PHE:CE1	0.48	2.43	9	1
1:A:522:ALA:HA	1:A:538:LEU:O	0.48	2.08	10	1
1:A:494:THR:HG23	1:A:496:GLU:HG2	0.48	1.85	1	1
1:A:527:LEU:HB3	1:A:534:ALA:HB3	0.48	1.86	8	2
1:A:466:MET:H	1:A:469:GLN:NE2	0.47	2.07	10	1
1:A:504:LYS:HB3	1:A:504:LYS:NZ	0.47	2.24	7	1
1:A:457:THR:CG2	1:A:476:GLU:HB2	0.46	2.39	5	1
1:A:472:GLU:HG2	1:A:513:ILE:HG12	0.46	1.87	3	1
1:A:461:GLU:HB3	1:A:463:GLN:NE2	0.46	2.24	4	1
1:A:458:ARG:HG3	1:A:476:GLU:HG2	0.46	1.87	9	1
1:A:476:GLU:CB	1:A:509:ARG:HG2	0.46	2.41	3	1
1:A:464:LEU:CD2	1:A:541:GLN:HG3	0.46	2.41	5	1
1:A:476:GLU:HG3	1:A:509:ARG:HG2	0.45	1.88	6	1
1:A:477:VAL:HG21	1:A:482:ALA:HB3	0.45	1.88	9	2
1:A:506:ASP:HB2	1:A:509:ARG:HB2	0.45	1.88	9	1
1:A:529:THR:HB	1:A:532:GLY:O	0.44	2.11	1	1
1:A:461:GLU:HG2	1:A:473:PHE:HD1	0.44	1.72	4	1
1:A:464:LEU:HG	1:A:539:ILE:O	0.44	2.12	4	1
1:A:473:PHE:CD2	1:A:512:LEU:HD23	0.44	2.48	4	1
1:A:473:PHE:HZ	1:A:538:LEU:HD22	0.43	1.72	3	2
1:A:497:GLU:OE2	1:A:500:LYS:HB2	0.43	2.13	8	1
1:A:467:VAL:HA	1:A:517:ALA:O	0.43	2.13	2	2
1:A:464:LEU:HD21	1:A:541:GLN:HG3	0.43	1.89	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:488:LYS:C	1:A:488:LYS:HD3	0.43	2.39	10	2
1:A:500:LYS:O	1:A:515:ASN:HB3	0.43	2.13	3	1
1:A:487:LEU:HB3	1:A:526:ALA:HB3	0.43	1.91	7	1
1:A:457:THR:HG22	1:A:476:GLU:HB2	0.43	1.91	5	1
1:A:474:GLU:HG2	1:A:511:HIS:CE1	0.42	2.49	2	1
1:A:464:LEU:HD22	1:A:541:GLN:HG3	0.42	1.90	5	1
1:A:493:LEU:O	1:A:493:LEU:HD12	0.42	2.14	3	1
1:A:500:LYS:HZ1	1:A:521:ASP:CG	0.42	2.23	7	1
1:A:466:MET:O	1:A:469:GLN:HG2	0.42	2.14	10	1
1:A:497:GLU:HG2	1:A:501:TYR:CZ	0.42	2.49	10	1
1:A:460:LEU:HB2	1:A:536:ALA:HB3	0.42	1.91	1	1
1:A:521:ASP:C	1:A:523:GLY:H	0.42	2.23	5	1
1:A:520:GLU:CD	1:A:520:GLU:H	0.42	2.23	10	1
1:A:476:GLU:OE1	1:A:509:ARG:HB2	0.41	2.15	2	1
1:A:470:ARG:HG3	1:A:514:ILE:O	0.41	2.16	6	1
1:A:505:LYS:O	1:A:505:LYS:HG3	0.41	2.15	7	1
1:A:465:VAL:HG23	1:A:540:VAL:HG23	0.41	1.92	6	1
1:A:494:THR:HG22	1:A:496:GLU:H	0.41	1.74	10	1
1:A:473:PHE:HE2	1:A:514:ILE:HD12	0.41	1.76	1	1
1:A:464:LEU:HG	1:A:539:ILE:CB	0.41	2.41	5	1
1:A:473:PHE:CZ	1:A:538:LEU:HD22	0.40	2.51	3	1
1:A:486:TRP:HB3	1:A:493:LEU:HD12	0.40	1.91	4	1
1:A:486:TRP:HB2	1:A:493:LEU:HD21	0.40	1.93	8	1
1:A:477:VAL:HG22	1:A:508:GLN:O	0.40	2.17	2	1
1:A:506:ASP:HB3	1:A:509:ARG:CG	0.40	2.47	1	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	90/95 (95%)	79±14 (88±16%)	4±1 (4±1%)	0±0 (0±0%)	44	80
All	All	829/950 (87%)	790 (95%)	37 (4%)	2 (0%)	44	80

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	531	GLY	2

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	78/81 (96%)	75±2 (97±3%)	3±2 (3±3%)	32 82
All	All	780/810 (96%)	753 (97%)	27 (3%)	32 82

All 17 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	505	LYS	7
1	A	476	GLU	2
1	A	495	ARG	2
1	A	494	THR	2
1	A	502	TRP	2
1	A	529	THR	1
1	A	458	ARG	1
1	A	480	GLU	1
1	A	485	LYS	1
1	A	543	LYS	1
1	A	457	THR	1
1	A	542	GLU	1
1	A	515	ASN	1
1	A	489	ASP	1
1	A	533	GLN	1
1	A	470	ARG	1
1	A	500	LYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1084
Number of shifts mapped to atoms	1084
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	92	-0.11 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	86	-0.22 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	89	-0.24 ± 0.44	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 84%, i.e. 1068 atoms were assigned a chemical shift out of a possible 1268. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	365/458 (80%)	186/187 (99%)	91/182 (50%)	88/89 (99%)
Sidechain	645/714 (90%)	441/462 (95%)	195/227 (86%)	9/25 (36%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	58/96 (60%)	31/47 (66%)	25/41 (61%)	2/8 (25%)
Overall	1068/1268 (84%)	658/696 (95%)	311/450 (69%)	99/122 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1084 atoms were assigned a chemical shift out of a possible 1313. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	369/479 (77%)	188/196 (96%)	92/190 (48%)	89/93 (96%)
Sidechain	653/730 (89%)	446/473 (94%)	198/232 (85%)	9/25 (36%)
Aromatic	62/104 (60%)	33/51 (65%)	27/43 (63%)	2/10 (20%)
Overall	1084/1313 (83%)	667/720 (93%)	317/465 (68%)	100/128 (78%)

7.1.4 Statistically unusual chemical shifts [i](#)

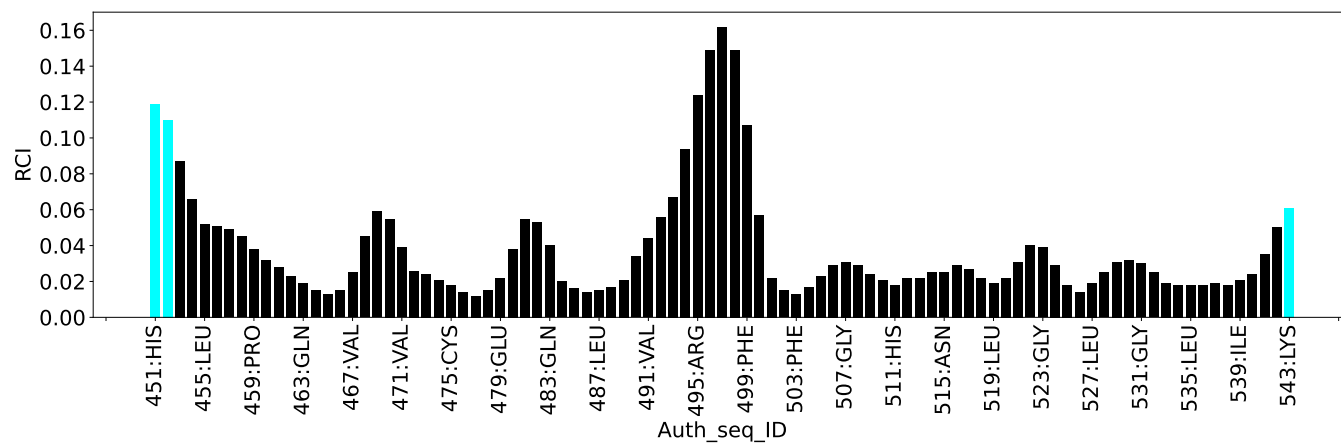
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	512	LEU	HB2	-0.80	-0.07 – 3.30	-7.2

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1314
Intra-residue ($ i-j =0$)	309
Sequential ($ i-j =1$)	365
Medium range ($ i-j >1$ and $ i-j <5$)	147
Long range ($ i-j \geq 5$)	493
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	13.8
Number of long range restraints per residue ¹	5.2

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	26.1	0.2
0.2-0.5 (Medium)	59.9	0.5
>0.5 (Large)	72.1	3.24

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

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

9 Distance violation analysis ⓘ

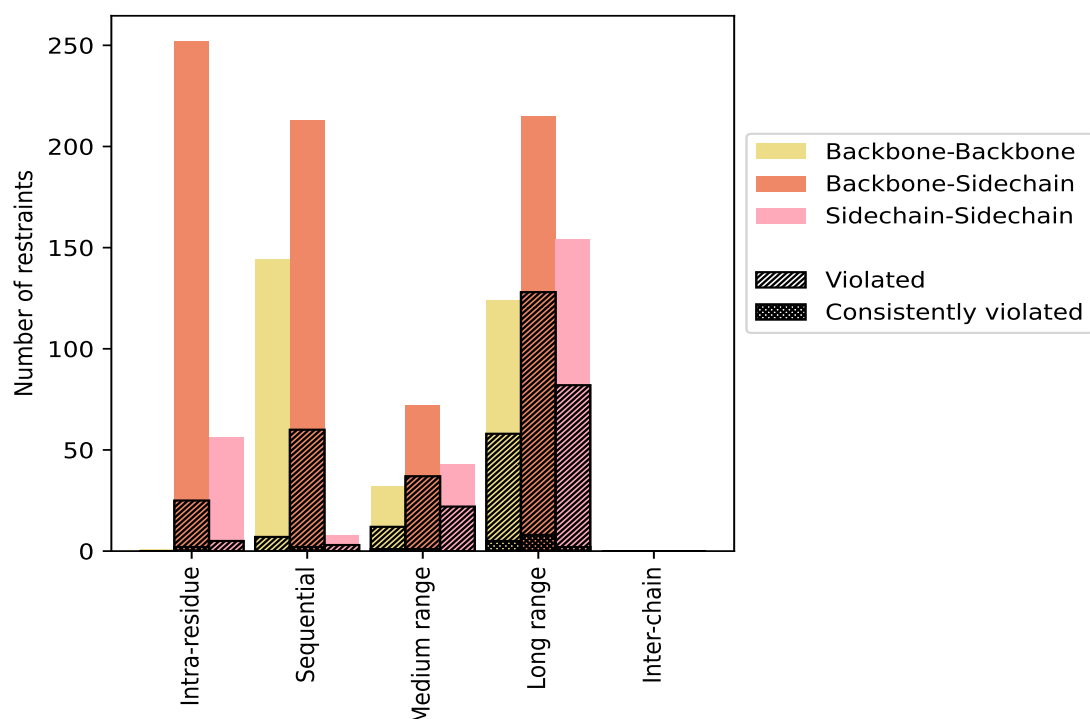
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	309	23.5	30	9.7	2.3	2	0.6	0.2
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	252	19.2	25	9.9	1.9	2	0.8	0.2
Sidechain-Sidechain	56	4.3	5	8.9	0.4	0	0.0	0.0
Sequential ($i-j =1$)	365	27.8	70	19.2	5.3	2	0.5	0.2
Backbone-Backbone	144	11.0	7	4.9	0.5	0	0.0	0.0
Backbone-Sidechain	213	16.2	60	28.2	4.6	2	0.9	0.2
Sidechain-Sidechain	8	0.6	3	37.5	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	147	11.2	71	48.3	5.4	2	1.4	0.2
Backbone-Backbone	32	2.4	12	37.5	0.9	1	3.1	0.1
Backbone-Sidechain	72	5.5	37	51.4	2.8	1	1.4	0.1
Sidechain-Sidechain	43	3.3	22	51.2	1.7	0	0.0	0.0
Long range ($i-j \geq 5$)	493	37.5	268	54.4	20.4	15	3.0	1.1
Backbone-Backbone	124	9.4	58	46.8	4.4	5	4.0	0.4
Backbone-Sidechain	215	16.4	128	59.5	9.7	8	3.7	0.6
Sidechain-Sidechain	154	11.7	82	53.2	6.2	2	1.3	0.2
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1314	100.0	439	33.4	33.4	21	1.6	1.6
Backbone-Backbone	301	22.9	77	25.6	5.9	6	2.0	0.5
Backbone-Sidechain	752	57.2	250	33.2	19.0	13	1.7	1.0
Sidechain-Sidechain	261	19.9	112	42.9	8.5	2	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 [i](#)



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

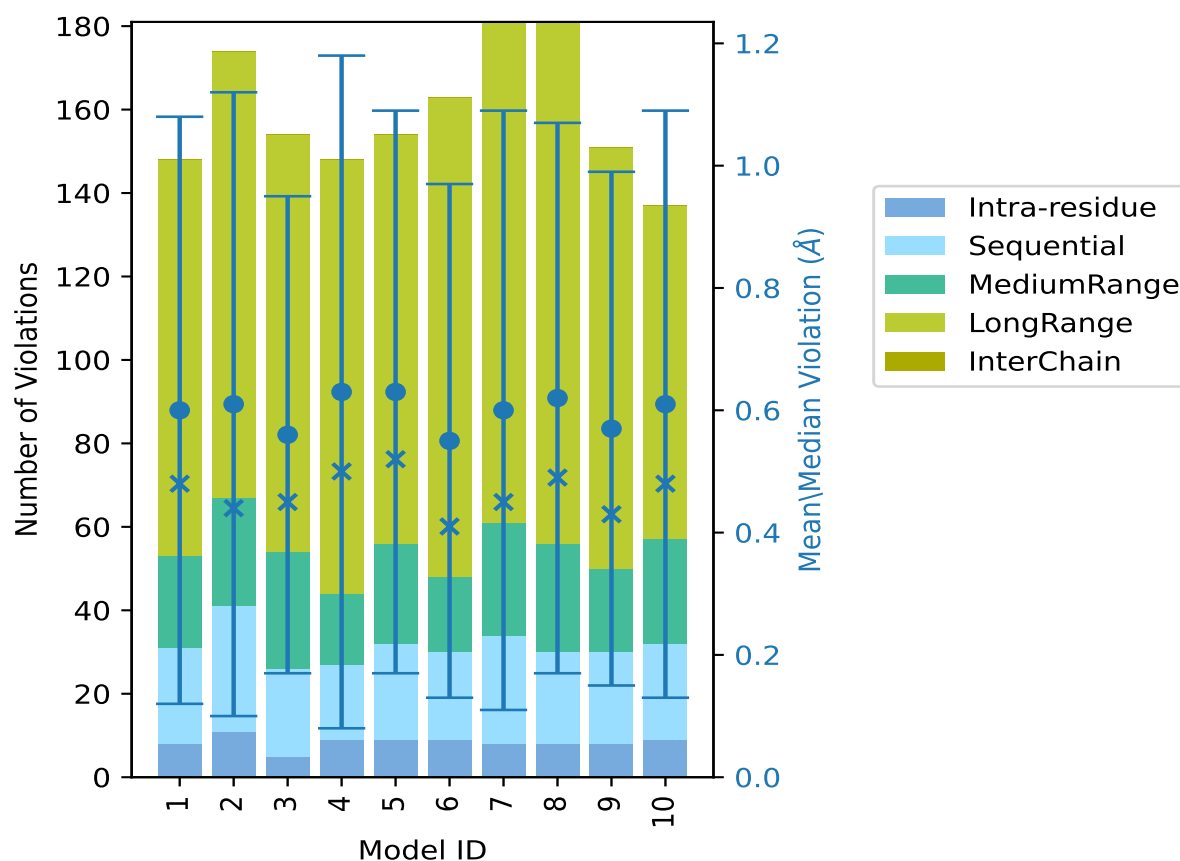
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	8	23	22	95	0	148	0.6	2.77	0.48	0.48
2	11	30	26	107	0	174	0.61	3.01	0.51	0.44
3	5	21	28	100	0	154	0.56	1.82	0.39	0.45
4	9	18	17	104	0	148	0.63	3.24	0.55	0.5
5	9	23	24	98	0	154	0.63	2.62	0.46	0.52
6	9	21	18	115	0	163	0.55	2.93	0.42	0.41
7	8	26	27	120	0	181	0.6	2.7	0.49	0.45
8	8	22	26	125	0	181	0.62	2.53	0.45	0.49
9	8	22	20	101	0	151	0.57	2.96	0.42	0.43
10	9	23	25	80	0	137	0.61	2.61	0.48	0.48

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

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 875(IR:279, SQ:295, MR:76, LR:225, 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	%
16	30	20	75	0	141	1	10.0
2	7	11	39	0	59	2	20.0
5	9	15	31	0	60	3	30.0

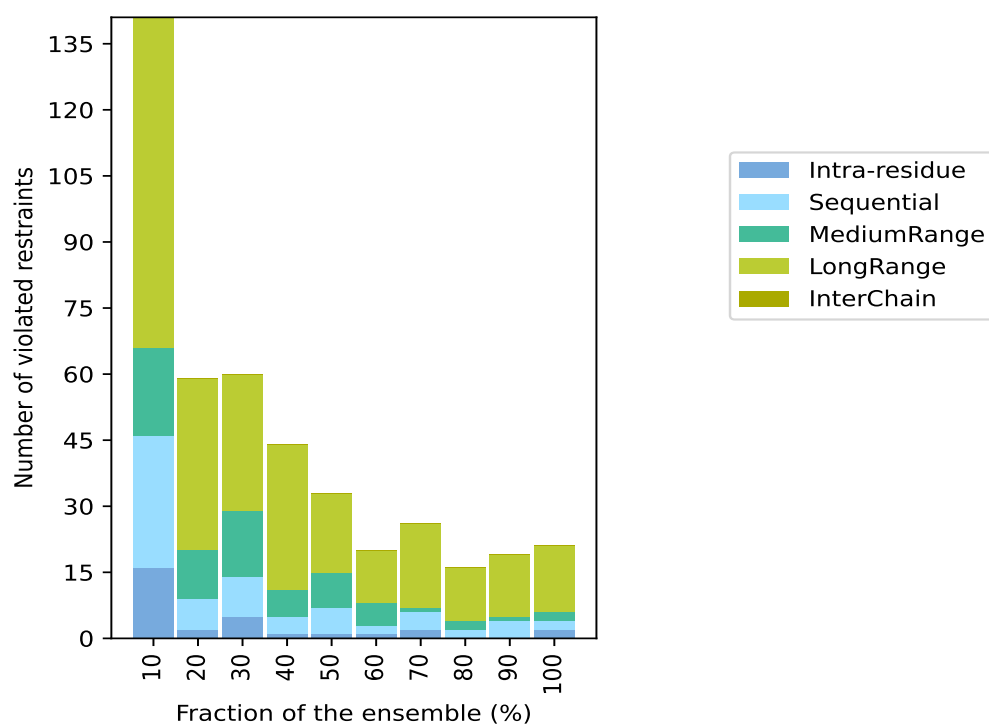
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	4	6	33	0	44	4	40.0
1	6	8	18	0	33	5	50.0
1	2	5	12	0	20	6	60.0
2	4	1	19	0	26	7	70.0
0	2	2	12	0	16	8	80.0
0	4	1	14	0	19	9	90.0
2	2	2	15	0	21	10	100.0

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

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

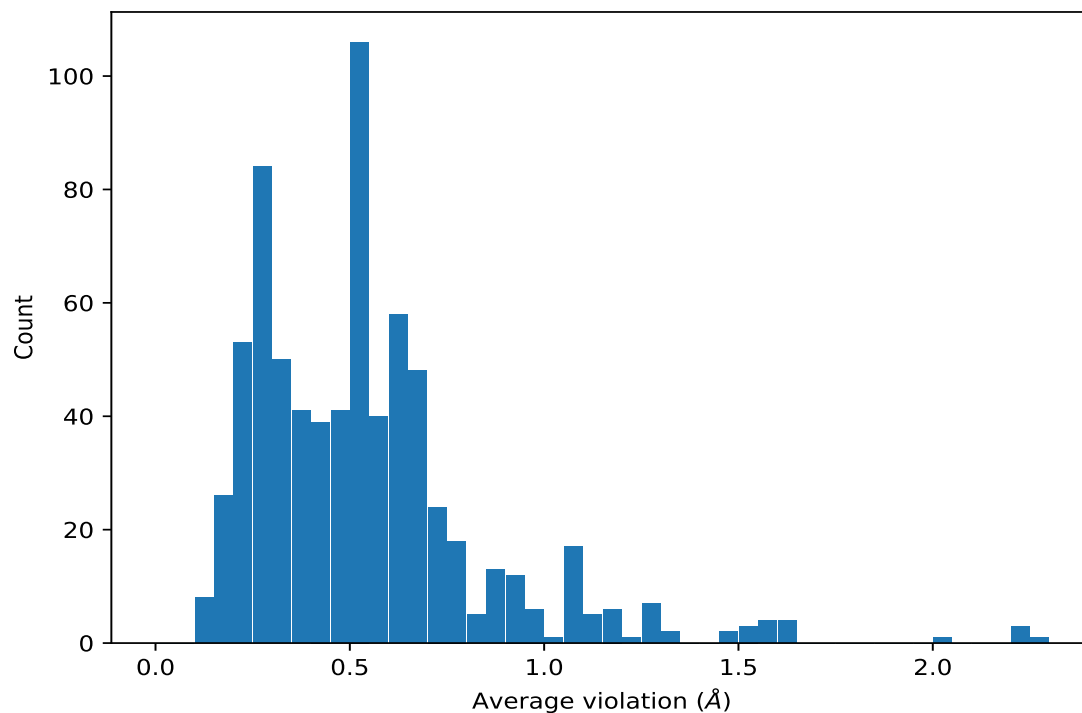


9.4 Most violated distance restraints in the ensemble ⓘ

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD21	10	2.22	0.87	2.6
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD22	10	2.22	0.87	2.6
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD23	10	2.22	0.87	2.6
(1,803)	1:523:A:GLY:H	1:525:A:TYR:HD1	10	2.03	1.05	2.62
(1,819)	1:523:A:GLY:H	1:538:A:LEU:HG	10	1.12	0.36	1.21
(1,628)	1:462:A:ASP:H	1:537:A:GLU:H	10	1.02	0.08	1.04
(1,824)	1:456:A:ILE:HD11	1:533:A:GLN:H	10	0.93	0.44	0.97
(1,824)	1:456:A:ILE:HD12	1:533:A:GLN:H	10	0.93	0.44	0.97
(1,824)	1:456:A:ILE:HD13	1:533:A:GLN:H	10	0.93	0.44	0.97
(1,802)	1:523:A:GLY:H	1:539:A:ILE:HA	10	0.84	0.37	0.85
(1,818)	1:523:A:GLY:H	1:538:A:LEU:HB3	10	0.83	0.44	0.7
(1,388)	1:486:A:TRP:HE1	1:510:A:HIS:HA	10	0.81	0.17	0.86
(1,386)	1:486:A:TRP:HE1	1:510:A:HIS:HB2	10	0.79	0.36	0.82
(1,1042)	1:459:A:PRO:HB2	1:535:A:LEU:H	10	0.75	0.38	0.8
(1,1042)	1:459:A:PRO:HB3	1:535:A:LEU:H	10	0.75	0.38	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,911)	1:458:A:ARG:H	1:478:A:SER:H	10	0.75	0.21	0.74
(1,970)	1:470:A:ARG:HA	1:514:A:ILE:H	10	0.68	0.19	0.7
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD21	10	0.66	0.2	0.62
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD22	10	0.66	0.2	0.62
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD23	10	0.66	0.2	0.62
(1,1012)	1:522:A:ALA:H	1:538:A:LEU:HG	10	0.63	0.33	0.5
(1,626)	1:462:A:ASP:HA	1:537:A:GLU:H	10	0.62	0.17	0.57
(1,930)	1:487:A:LEU:HB3	1:488:A:LYS:H	10	0.58	0.16	0.66
(1,561)	1:487:A:LEU:HA	1:491:A:VAL:H	10	0.57	0.22	0.55
(1,352)	1:464:A:LEU:HB2	1:539:A:ILE:H	10	0.56	0.41	0.4
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD21	10	0.52	0.09	0.49
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD22	10	0.52	0.09	0.49
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD23	10	0.52	0.09	0.49
(1,754)	1:463:A:GLN:HA	1:463:A:GLN:HE21	10	0.46	0.05	0.47
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD11	10	0.37	0.19	0.32
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD12	10	0.37	0.19	0.32
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD13	10	0.37	0.19	0.32
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD21	10	0.37	0.19	0.32
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD22	10	0.37	0.19	0.32
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD23	10	0.37	0.19	0.32
(1,1019)	1:524:A:HIS:H	1:525:A:TYR:HD1	9	1.64	0.81	1.93
(1,258)	1:501:A:TYR:HD1	1:502:A:TRP:HA	9	1.31	0.02	1.31
(1,319)	1:486:A:TRP:HD1	1:503:A:PHE:HD2	9	1.31	0.45	1.21
(1,318)	1:486:A:TRP:HD1	1:503:A:PHE:HE2	9	1.25	0.6	1.17
(1,1046)	1:524:A:HIS:H	1:538:A:LEU:H	9	1.06	0.2	1.16
(1,918)	1:486:A:TRP:HE1	1:504:A:LYS:H	9	0.82	0.22	0.88
(1,383)	1:486:A:TRP:HE1	1:511:A:HIS:H	9	0.79	0.25	0.81
(1,1021)	1:488:A:LYS:HG3	1:524:A:HIS:H	9	0.74	0.3	0.85
(1,897)	1:459:A:PRO:HA	1:476:A:GLU:H	9	0.73	0.26	0.67
(1,449)	1:463:A:GLN:HE22	1:472:A:GLU:H	9	0.73	0.28	0.75
(1,28)	1:456:A:ILE:HD11	1:534:A:ALA:HA	9	0.67	0.22	0.69
(1,28)	1:456:A:ILE:HD12	1:534:A:ALA:HA	9	0.67	0.22	0.69
(1,28)	1:456:A:ILE:HD13	1:534:A:ALA:HA	9	0.67	0.22	0.69
(1,514)	1:523:A:GLY:HA2	1:538:A:LEU:H	9	0.67	0.3	0.65
(1,434)	1:456:A:ILE:HD11	1:534:A:ALA:H	9	0.63	0.43	0.48
(1,434)	1:456:A:ILE:HD12	1:534:A:ALA:H	9	0.63	0.43	0.48
(1,434)	1:456:A:ILE:HD13	1:534:A:ALA:H	9	0.63	0.43	0.48
(1,719)	1:500:A:LYS:HD2	1:501:A:TYR:H	9	0.57	0.28	0.57
(1,719)	1:500:A:LYS:HD3	1:501:A:TYR:H	9	0.57	0.28	0.57
(1,43)	1:465:A:VAL:HG21	1:471:A:VAL:HA	9	0.55	0.22	0.55
(1,43)	1:465:A:VAL:HG22	1:471:A:VAL:HA	9	0.55	0.22	0.55
(1,43)	1:465:A:VAL:HG23	1:471:A:VAL:HA	9	0.55	0.22	0.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,663)	1:474:A:GLU:H	1:486:A:TRP:HH2	9	0.53	0.2	0.54
(1,384)	1:486:A:TRP:HE1	1:510:A:HIS:HB3	9	0.45	0.19	0.48
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB2	9	0.41	0.17	0.34
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB3	9	0.41	0.17	0.34
(1,996)	1:516:A:GLU:HG2	1:517:A:ALA:H	9	0.29	0.1	0.25
(1,996)	1:516:A:GLU:HG3	1:517:A:ALA:H	9	0.29	0.1	0.25
(1,448)	1:472:A:GLU:H	1:473:A:PHE:HD1	8	1.12	0.3	1.23
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG2	8	0.97	0.43	1.08
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG3	8	0.97	0.43	1.08
(1,784)	1:476:A:GLU:HG3	1:508:A:GLN:HE22	8	0.88	0.3	1.04
(1,101)	1:457:A:THR:HG21	1:478:A:SER:HA	8	0.76	0.45	0.76
(1,101)	1:457:A:THR:HG22	1:478:A:SER:HA	8	0.76	0.45	0.76
(1,101)	1:457:A:THR:HG23	1:478:A:SER:HA	8	0.76	0.45	0.76
(1,1024)	1:460:A:LEU:HB2	1:525:A:TYR:H	8	0.75	0.22	0.69
(1,1024)	1:460:A:LEU:HB3	1:525:A:TYR:H	8	0.75	0.22	0.69
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD11	8	0.74	0.2	0.76
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD12	8	0.74	0.2	0.76
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD13	8	0.74	0.2	0.76
(1,760)	1:465:A:VAL:HA	1:469:A:GLN:HE21	8	0.72	0.39	0.6
(1,624)	1:462:A:ASP:HB3	1:537:A:GLU:H	8	0.55	0.37	0.51
(1,624)	1:462:A:ASP:HB2	1:537:A:GLU:H	8	0.55	0.37	0.51
(1,387)	1:486:A:TRP:HE1	1:503:A:PHE:HA	8	0.53	0.23	0.5
(1,544)	1:486:A:TRP:H	1:492:A:GLU:HA	8	0.53	0.21	0.48
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA2	8	0.51	0.27	0.55
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA3	8	0.51	0.27	0.55
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB2	8	0.49	0.35	0.43
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB3	8	0.49	0.35	0.43
(1,316)	1:501:A:TYR:HB2	1:502:A:TRP:HD1	8	0.46	0.17	0.44
(1,316)	1:501:A:TYR:HB3	1:502:A:TRP:HD1	8	0.46	0.17	0.44
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG21	8	0.42	0.25	0.36
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG22	8	0.42	0.25	0.36
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG23	8	0.42	0.25	0.36
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB1	8	0.39	0.18	0.36
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB2	8	0.39	0.18	0.36
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB3	8	0.39	0.18	0.36
(1,843)	1:456:A:ILE:H	1:458:A:ARG:H	8	0.36	0.09	0.36
(1,515)	1:525:A:TYR:HD1	1:538:A:LEU:H	7	2.25	0.57	2.22
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD11	7	1.63	0.09	1.65
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD12	7	1.63	0.09	1.65
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD13	7	1.63	0.09	1.65
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD21	7	1.56	0.43	1.45
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD22	7	1.56	0.43	1.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD23	7	1.56	0.43	1.45
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD21	7	1.51	0.2	1.4
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD22	7	1.51	0.2	1.4
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD23	7	1.51	0.2	1.4
(1,427)	1:525:A:TYR:H	1:525:A:TYR:HD1	7	1.46	0.15	1.5
(1,771)	1:457:A:THR:HG21	1:478:A:SER:H	7	1.26	0.42	1.23
(1,771)	1:457:A:THR:HG22	1:478:A:SER:H	7	1.26	0.42	1.23
(1,771)	1:457:A:THR:HG23	1:478:A:SER:H	7	1.26	0.42	1.23
(1,1032)	1:529:A:THR:H	1:532:A:GLY:H	7	1.06	0.6	1.02
(1,313)	1:502:A:TRP:HD1	1:503:A:PHE:HA	7	0.99	0.06	1.02
(1,294)	1:474:A:GLU:HA	1:486:A:TRP:HZ2	7	0.76	0.31	0.75
(1,59)	1:468:A:GLY:HA3	1:516:A:GLU:HG2	7	0.73	0.34	0.87
(1,59)	1:468:A:GLY:HA3	1:516:A:GLU:HG3	7	0.73	0.34	0.87
(1,742)	1:468:A:GLY:H	1:516:A:GLU:HG2	7	0.64	0.25	0.61
(1,742)	1:468:A:GLY:H	1:516:A:GLU:HG3	7	0.64	0.25	0.61
(1,29)	1:456:A:ILE:HD11	1:533:A:GLN:HA	7	0.63	0.29	0.57
(1,29)	1:456:A:ILE:HD12	1:533:A:GLN:HA	7	0.63	0.29	0.57
(1,29)	1:456:A:ILE:HD13	1:533:A:GLN:HA	7	0.63	0.29	0.57
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG21	7	0.6	0.21	0.6
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG22	7	0.6	0.21	0.6
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG23	7	0.6	0.21	0.6
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD21	7	0.59	0.16	0.56
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD22	7	0.59	0.16	0.56
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD23	7	0.59	0.16	0.56
(1,472)	1:472:A:GLU:HG2	1:512:A:LEU:H	7	0.59	0.3	0.44
(1,472)	1:472:A:GLU:HG3	1:512:A:LEU:H	7	0.59	0.3	0.44
(1,301)	1:503:A:PHE:HB2	1:503:A:PHE:HE1	7	0.59	0.01	0.59
(1,463)	1:473:A:PHE:H	1:511:A:HIS:HA	7	0.52	0.3	0.48
(1,985)	1:470:A:ARG:HB2	1:516:A:GLU:H	7	0.51	0.22	0.44
(1,747)	1:460:A:LEU:H	1:534:A:ALA:HA	7	0.5	0.27	0.55
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG21	7	0.48	0.38	0.42
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG22	7	0.48	0.38	0.42
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG23	7	0.48	0.38	0.42
(1,492)	1:464:A:LEU:HA	1:540:A:VAL:H	7	0.42	0.13	0.38
(1,311)	1:502:A:TRP:HD1	1:503:A:PHE:H	7	0.42	0.1	0.48
(1,610)	1:458:A:ARG:H	1:459:A:PRO:HB2	7	0.37	0.09	0.36
(1,610)	1:458:A:ARG:H	1:459:A:PRO:HB3	7	0.37	0.09	0.36
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB1	7	0.29	0.06	0.27
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB2	7	0.29	0.06	0.27
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB3	7	0.29	0.06	0.27
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB1	7	0.29	0.06	0.27
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB2	7	0.29	0.06	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB3	7	0.29	0.06	0.27
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB1	7	0.29	0.06	0.27
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB2	7	0.29	0.06	0.27
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB3	7	0.29	0.06	0.27
(1,857)	1:462:A:ASP:H	1:463:A:GLN:HE21	7	0.27	0.15	0.22
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB1	7	0.25	0.14	0.22
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB2	7	0.25	0.14	0.22
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB3	7	0.25	0.14	0.22
(1,308)	1:505:A:LYS:HE2	1:510:A:HIS:HE1	6	0.88	0.36	0.95
(1,308)	1:505:A:LYS:HE3	1:510:A:HIS:HE1	6	0.88	0.36	0.95
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB1	6	0.66	0.18	0.66
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB2	6	0.66	0.18	0.66
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB3	6	0.66	0.18	0.66
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB1	6	0.66	0.18	0.66
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB2	6	0.66	0.18	0.66
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB3	6	0.66	0.18	0.66
(1,1146)	1:471:A:VAL:HG11	1:473:A:PHE:HD1	6	0.61	0.34	0.63
(1,1146)	1:471:A:VAL:HG12	1:473:A:PHE:HD1	6	0.61	0.34	0.63
(1,1146)	1:471:A:VAL:HG13	1:473:A:PHE:HD1	6	0.61	0.34	0.63
(1,1146)	1:471:A:VAL:HG21	1:473:A:PHE:HD1	6	0.61	0.34	0.63
(1,1146)	1:471:A:VAL:HG22	1:473:A:PHE:HD1	6	0.61	0.34	0.63
(1,1146)	1:471:A:VAL:HG23	1:473:A:PHE:HD1	6	0.61	0.34	0.63
(1,128)	1:453:A:PRO:HB2	1:531:A:GLY:HA2	6	0.58	0.38	0.55
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG21	6	0.57	0.34	0.54
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG22	6	0.57	0.34	0.54
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG23	6	0.57	0.34	0.54
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD11	6	0.54	0.2	0.56
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD12	6	0.54	0.2	0.56
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD13	6	0.54	0.2	0.56
(1,817)	1:523:A:GLY:H	1:540:A:VAL:HB	6	0.53	0.33	0.53
(1,726)	1:492:A:GLU:HG2	1:494:A:THR:H	6	0.53	0.43	0.34
(1,726)	1:492:A:GLU:HG3	1:494:A:THR:H	6	0.53	0.43	0.34
(1,780)	1:476:A:GLU:HG3	1:508:A:GLN:HE21	6	0.46	0.24	0.46
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD11	6	0.45	0.3	0.36
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD12	6	0.45	0.3	0.36
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD13	6	0.45	0.3	0.36
(1,330)	1:456:A:ILE:HG21	1:459:A:PRO:HB2	6	0.44	0.15	0.48
(1,330)	1:456:A:ILE:HG21	1:459:A:PRO:HB3	6	0.44	0.15	0.48
(1,330)	1:456:A:ILE:HG22	1:459:A:PRO:HB2	6	0.44	0.15	0.48
(1,330)	1:456:A:ILE:HG22	1:459:A:PRO:HB3	6	0.44	0.15	0.48
(1,330)	1:456:A:ILE:HG23	1:459:A:PRO:HB2	6	0.44	0.15	0.48
(1,330)	1:456:A:ILE:HG23	1:459:A:PRO:HB3	6	0.44	0.15	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,794)	1:529:A:THR:HG21	1:532:A:GLY:H	6	0.41	0.19	0.51
(1,794)	1:529:A:THR:HG22	1:532:A:GLY:H	6	0.41	0.19	0.51
(1,794)	1:529:A:THR:HG23	1:532:A:GLY:H	6	0.41	0.19	0.51
(1,921)	1:487:A:LEU:H	1:493:A:LEU:H	6	0.4	0.11	0.36
(1,652)	1:457:A:THR:H	1:457:A:THR:HG21	6	0.36	0.02	0.36
(1,652)	1:457:A:THR:H	1:457:A:THR:HG22	6	0.36	0.02	0.36
(1,652)	1:457:A:THR:H	1:457:A:THR:HG23	6	0.36	0.02	0.36
(1,636)	1:487:A:LEU:HB2	1:526:A:ALA:H	6	0.34	0.16	0.29
(1,1295)	1:532:A:GLY:H	1:533:A:GLN:HB2	6	0.33	0.05	0.34
(1,1295)	1:532:A:GLY:H	1:533:A:GLN:HB3	6	0.33	0.05	0.34
(1,479)	1:486:A:TRP:HZ2	1:512:A:LEU:H	6	0.33	0.23	0.2
(1,562)	1:488:A:LYS:H	1:491:A:VAL:H	6	0.32	0.09	0.34
(1,374)	1:490:A:GLY:H	1:525:A:TYR:HA	6	0.28	0.14	0.28
(1,755)	1:463:A:GLN:HE21	1:464:A:LEU:H	6	0.25	0.15	0.21
(1,312)	1:502:A:TRP:HD1	1:515:A:ASN:HD21	5	1.24	0.59	1.64
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD11	5	1.05	0.53	0.94
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD12	5	1.05	0.53	0.94
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD13	5	1.05	0.53	0.94
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD21	5	1.05	0.53	0.94
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD22	5	1.05	0.53	0.94
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD23	5	1.05	0.53	0.94
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD11	5	1.05	0.53	0.94
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD12	5	1.05	0.53	0.94
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD13	5	1.05	0.53	0.94
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD21	5	1.05	0.53	0.94
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD22	5	1.05	0.53	0.94
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD23	5	1.05	0.53	0.94
(1,307)	1:505:A:LYS:HD2	1:510:A:HIS:HE1	5	0.99	0.56	0.76
(1,307)	1:505:A:LYS:HD3	1:510:A:HIS:HE1	5	0.99	0.56	0.76
(1,302)	1:505:A:LYS:HB3	1:510:A:HIS:HE1	5	0.89	0.53	0.65
(1,1156)	1:473:A:PHE:HB2	1:486:A:TRP:HZ2	5	0.72	0.44	0.78
(1,1156)	1:473:A:PHE:HB3	1:486:A:TRP:HZ2	5	0.72	0.44	0.78
(1,455)	1:505:A:LYS:HD2	1:506:A:ASP:H	5	0.71	0.41	0.63
(1,455)	1:505:A:LYS:HD3	1:506:A:ASP:H	5	0.71	0.41	0.63
(1,1248)	1:509:A:ARG:HB2	1:511:A:HIS:HE1	5	0.66	0.37	0.74
(1,1248)	1:509:A:ARG:HB3	1:511:A:HIS:HE1	5	0.66	0.37	0.74
(1,303)	1:509:A:ARG:HD2	1:511:A:HIS:HE1	5	0.65	0.23	0.66
(1,303)	1:509:A:ARG:HD3	1:511:A:HIS:HE1	5	0.65	0.23	0.66
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD21	5	0.58	0.67	0.25
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD22	5	0.58	0.67	0.25
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD23	5	0.58	0.67	0.25
(1,115)	1:484:A:VAL:HG11	1:510:A:HIS:H	5	0.53	0.39	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,115)	1:484:A:VAL:HG12	1:510:A:HIS:H	5	0.53	0.39	0.26
(1,115)	1:484:A:VAL:HG13	1:510:A:HIS:H	5	0.53	0.39	0.26
(1,548)	1:486:A:TRP:H	1:493:A:LEU:H	5	0.52	0.14	0.52
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD11	5	0.5	0.2	0.35
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD12	5	0.5	0.2	0.35
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD13	5	0.5	0.2	0.35
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD21	5	0.5	0.2	0.35
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD22	5	0.5	0.2	0.35
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD23	5	0.5	0.2	0.35
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD11	5	0.5	0.2	0.35
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD12	5	0.5	0.2	0.35
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD13	5	0.5	0.2	0.35
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD21	5	0.5	0.2	0.35
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD22	5	0.5	0.2	0.35
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD23	5	0.5	0.2	0.35
(1,249)	1:460:A:LEU:HG	1:526:A:ALA:HA	5	0.45	0.33	0.33
(1,1037)	1:456:A:ILE:HD11	1:529:A:THR:H	5	0.43	0.15	0.38
(1,1037)	1:456:A:ILE:HD12	1:529:A:THR:H	5	0.43	0.15	0.38
(1,1037)	1:456:A:ILE:HD13	1:529:A:THR:H	5	0.43	0.15	0.38
(1,85)	1:457:A:THR:HG21	1:477:A:VAL:HA	5	0.41	0.16	0.44
(1,85)	1:457:A:THR:HG22	1:477:A:VAL:HA	5	0.41	0.16	0.44
(1,85)	1:457:A:THR:HG23	1:477:A:VAL:HA	5	0.41	0.16	0.44
(1,220)	1:468:A:GLY:HA2	1:516:A:GLU:HG2	5	0.39	0.04	0.37
(1,220)	1:468:A:GLY:HA2	1:516:A:GLU:HG3	5	0.39	0.04	0.37
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG11	5	0.38	0.04	0.4
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG12	5	0.38	0.04	0.4
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG13	5	0.38	0.04	0.4
(1,601)	1:458:A:ARG:H	1:459:A:PRO:HD2	5	0.37	0.06	0.37
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG11	5	0.37	0.18	0.34
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG12	5	0.37	0.18	0.34
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG13	5	0.37	0.18	0.34
(1,376)	1:487:A:LEU:HB3	1:490:A:GLY:H	5	0.34	0.19	0.26
(1,752)	1:459:A:PRO:HG2	1:460:A:LEU:H	5	0.29	0.05	0.29
(1,752)	1:459:A:PRO:HG3	1:460:A:LEU:H	5	0.29	0.05	0.29
(1,1097)	1:460:A:LEU:HD11	1:476:A:GLU:H	5	0.28	0.14	0.2
(1,1097)	1:460:A:LEU:HD12	1:476:A:GLU:H	5	0.28	0.14	0.2
(1,1097)	1:460:A:LEU:HD13	1:476:A:GLU:H	5	0.28	0.14	0.2
(1,1097)	1:460:A:LEU:HD21	1:476:A:GLU:H	5	0.28	0.14	0.2
(1,1097)	1:460:A:LEU:HD22	1:476:A:GLU:H	5	0.28	0.14	0.2
(1,1097)	1:460:A:LEU:HD23	1:476:A:GLU:H	5	0.28	0.14	0.2
(1,481)	1:472:A:GLU:HA	1:512:A:LEU:H	5	0.27	0.06	0.25
(1,1083)	1:456:A:ILE:HD11	1:527:A:LEU:HB2	5	0.27	0.12	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1083)	1:456:A:ILE:HD11	1:527:A:LEU:HB3	5	0.27	0.12	0.28
(1,1083)	1:456:A:ILE:HD12	1:527:A:LEU:HB2	5	0.27	0.12	0.28
(1,1083)	1:456:A:ILE:HD12	1:527:A:LEU:HB3	5	0.27	0.12	0.28
(1,1083)	1:456:A:ILE:HD13	1:527:A:LEU:HB2	5	0.27	0.12	0.28
(1,1083)	1:456:A:ILE:HD13	1:527:A:LEU:HB3	5	0.27	0.12	0.28
(1,851)	1:461:A:GLU:HG2	1:462:A:ASP:H	5	0.26	0.04	0.25
(1,851)	1:461:A:GLU:HG3	1:462:A:ASP:H	5	0.26	0.04	0.25
(1,1014)	1:524:A:HIS:H	1:537:A:GLU:HA	5	0.26	0.1	0.22
(1,1300)	1:533:A:GLN:HB2	1:535:A:LEU:H	5	0.26	0.09	0.21
(1,1300)	1:533:A:GLN:HB3	1:535:A:LEU:H	5	0.26	0.09	0.21
(1,1249)	1:509:A:ARG:HG2	1:510:A:HIS:H	5	0.25	0.13	0.19
(1,1249)	1:509:A:ARG:HG3	1:510:A:HIS:H	5	0.25	0.13	0.19
(1,1090)	1:460:A:LEU:H	1:475:A:CYS:HB2	5	0.24	0.06	0.23
(1,1090)	1:460:A:LEU:H	1:475:A:CYS:HB3	5	0.24	0.06	0.23
(1,880)	1:470:A:ARG:H	1:470:A:ARG:HD2	5	0.23	0.06	0.22
(1,880)	1:470:A:ARG:H	1:470:A:ARG:HD3	5	0.23	0.06	0.22
(1,404)	1:487:A:LEU:HA	1:492:A:GLU:H	5	0.22	0.08	0.18
(1,517)	1:535:A:LEU:HD11	1:536:A:ALA:H	5	0.2	0.06	0.18
(1,517)	1:535:A:LEU:HD12	1:536:A:ALA:H	5	0.2	0.06	0.18
(1,517)	1:535:A:LEU:HD13	1:536:A:ALA:H	5	0.2	0.06	0.18
(1,1011)	1:519:A:LEU:HB3	1:522:A:ALA:H	5	0.19	0.08	0.15
(1,1269)	1:519:A:LEU:HD11	1:540:A:VAL:HB	4	1.17	0.58	1.33
(1,1269)	1:519:A:LEU:HD12	1:540:A:VAL:HB	4	1.17	0.58	1.33
(1,1269)	1:519:A:LEU:HD13	1:540:A:VAL:HB	4	1.17	0.58	1.33
(1,1269)	1:519:A:LEU:HD21	1:540:A:VAL:HB	4	1.17	0.58	1.33
(1,1269)	1:519:A:LEU:HD22	1:540:A:VAL:HB	4	1.17	0.58	1.33
(1,1269)	1:519:A:LEU:HD23	1:540:A:VAL:HB	4	1.17	0.58	1.33
(1,763)	1:502:A:TRP:HD1	1:515:A:ASN:HD22	4	0.96	0.35	0.8
(1,19)	1:457:A:THR:HG21	1:478:A:SER:HB2	4	0.68	0.18	0.68
(1,19)	1:457:A:THR:HG21	1:478:A:SER:HB3	4	0.68	0.18	0.68
(1,19)	1:457:A:THR:HG22	1:478:A:SER:HB2	4	0.68	0.18	0.68
(1,19)	1:457:A:THR:HG22	1:478:A:SER:HB3	4	0.68	0.18	0.68
(1,19)	1:457:A:THR:HG23	1:478:A:SER:HB2	4	0.68	0.18	0.68
(1,19)	1:457:A:THR:HG23	1:478:A:SER:HB3	4	0.68	0.18	0.68
(1,1225)	1:500:A:LYS:HE2	1:514:A:ILE:HG21	4	0.68	0.27	0.67
(1,1225)	1:500:A:LYS:HE2	1:514:A:ILE:HG22	4	0.68	0.27	0.67
(1,1225)	1:500:A:LYS:HE2	1:514:A:ILE:HG23	4	0.68	0.27	0.67
(1,1225)	1:500:A:LYS:HE3	1:514:A:ILE:HG21	4	0.68	0.27	0.67
(1,1225)	1:500:A:LYS:HE3	1:514:A:ILE:HG22	4	0.68	0.27	0.67
(1,1225)	1:500:A:LYS:HE3	1:514:A:ILE:HG23	4	0.68	0.27	0.67
(1,765)	1:502:A:TRP:HZ2	1:515:A:ASN:HD22	4	0.65	0.32	0.62
(1,1227)	1:500:A:LYS:HE2	1:518:A:MET:HG2	4	0.63	0.42	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1227)	1:500:A:LYS:HE2	1:518:A:MET:HG3	4	0.63	0.42	0.52
(1,1227)	1:500:A:LYS:HE3	1:518:A:MET:HG2	4	0.63	0.42	0.52
(1,1227)	1:500:A:LYS:HE3	1:518:A:MET:HG3	4	0.63	0.42	0.52
(1,306)	1:505:A:LYS:HG2	1:510:A:HIS:HE1	4	0.62	0.34	0.56
(1,306)	1:505:A:LYS:HG3	1:510:A:HIS:HE1	4	0.62	0.34	0.56
(1,1262)	1:518:A:MET:HB2	1:520:A:GLU:HB2	4	0.59	0.37	0.59
(1,1262)	1:518:A:MET:HB2	1:520:A:GLU:HB3	4	0.59	0.37	0.59
(1,1262)	1:518:A:MET:HB3	1:520:A:GLU:HB2	4	0.59	0.37	0.59
(1,1262)	1:518:A:MET:HB3	1:520:A:GLU:HB3	4	0.59	0.37	0.59
(1,200)	1:514:A:ILE:HD11	1:521:A:ASP:HB2	4	0.58	0.58	0.26
(1,200)	1:514:A:ILE:HD12	1:521:A:ASP:HB2	4	0.58	0.58	0.26
(1,200)	1:514:A:ILE:HD13	1:521:A:ASP:HB2	4	0.58	0.58	0.26
(1,1098)	1:460:A:LEU:HD11	1:486:A:TRP:HZ2	4	0.58	0.4	0.46
(1,1098)	1:460:A:LEU:HD12	1:486:A:TRP:HZ2	4	0.58	0.4	0.46
(1,1098)	1:460:A:LEU:HD13	1:486:A:TRP:HZ2	4	0.58	0.4	0.46
(1,1098)	1:460:A:LEU:HD21	1:486:A:TRP:HZ2	4	0.58	0.4	0.46
(1,1098)	1:460:A:LEU:HD22	1:486:A:TRP:HZ2	4	0.58	0.4	0.46
(1,1098)	1:460:A:LEU:HD23	1:486:A:TRP:HZ2	4	0.58	0.4	0.46
(1,906)	1:476:A:GLU:HG3	1:477:A:VAL:H	4	0.57	0.36	0.57
(1,906)	1:476:A:GLU:HG2	1:477:A:VAL:H	4	0.57	0.36	0.57
(1,150)	1:486:A:TRP:HZ2	1:503:A:PHE:HB3	4	0.56	0.11	0.6
(1,1242)	1:506:A:ASP:H	1:509:A:ARG:HB2	4	0.53	0.09	0.52
(1,1242)	1:506:A:ASP:H	1:509:A:ARG:HB3	4	0.53	0.09	0.52
(1,224)	1:519:A:LEU:HA	1:540:A:VAL:HB	4	0.52	0.5	0.3
(1,552)	1:486:A:TRP:H	1:492:A:GLU:HG2	4	0.51	0.32	0.46
(1,552)	1:486:A:TRP:H	1:492:A:GLU:HG3	4	0.51	0.32	0.46
(1,650)	1:497:A:GLU:HB2	1:500:A:LYS:H	4	0.51	0.09	0.51
(1,650)	1:497:A:GLU:HB3	1:500:A:LYS:H	4	0.51	0.09	0.51
(1,656)	1:457:A:THR:H	1:476:A:GLU:HG2	4	0.51	0.15	0.5
(1,828)	1:479:A:GLU:H	1:508:A:GLN:HE21	4	0.48	0.28	0.44
(1,181)	1:470:A:ARG:HB3	1:513:A:ILE:HG21	4	0.48	0.33	0.32
(1,181)	1:470:A:ARG:HB3	1:513:A:ILE:HG22	4	0.48	0.33	0.32
(1,181)	1:470:A:ARG:HB3	1:513:A:ILE:HG23	4	0.48	0.33	0.32
(1,477)	1:486:A:TRP:HH2	1:512:A:LEU:H	4	0.45	0.2	0.44
(1,1189)	1:487:A:LEU:HD11	1:493:A:LEU:H	4	0.45	0.43	0.25
(1,1189)	1:487:A:LEU:HD12	1:493:A:LEU:H	4	0.45	0.43	0.25
(1,1189)	1:487:A:LEU:HD13	1:493:A:LEU:H	4	0.45	0.43	0.25
(1,1189)	1:487:A:LEU:HD21	1:493:A:LEU:H	4	0.45	0.43	0.25
(1,1189)	1:487:A:LEU:HD22	1:493:A:LEU:H	4	0.45	0.43	0.25
(1,1189)	1:487:A:LEU:HD23	1:493:A:LEU:H	4	0.45	0.43	0.25
(1,1287)	1:527:A:LEU:H	1:533:A:GLN:HB2	4	0.44	0.31	0.38
(1,1287)	1:527:A:LEU:H	1:533:A:GLN:HB3	4	0.44	0.31	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,361)	1:488:A:LYS:HD2	1:489:A:ASP:H	4	0.43	0.18	0.48
(1,248)	1:460:A:LEU:HB2	1:526:A:ALA:HA	4	0.38	0.08	0.38
(1,248)	1:460:A:LEU:HB3	1:526:A:ALA:HA	4	0.38	0.08	0.38
(1,816)	1:478:A:SER:H	1:508:A:GLN:HE22	4	0.36	0.21	0.3
(1,890)	1:475:A:CYS:H	1:486:A:TRP:HZ2	4	0.36	0.12	0.35
(1,1023)	1:488:A:LYS:HG2	1:524:A:HIS:H	4	0.36	0.12	0.34
(1,699)	1:495:A:ARG:HD2	1:496:A:GLU:H	4	0.36	0.35	0.19
(1,699)	1:495:A:ARG:HD3	1:496:A:GLU:H	4	0.36	0.35	0.19
(1,811)	1:465:A:VAL:HA	1:469:A:GLN:HE22	4	0.31	0.16	0.25
(1,41)	1:463:A:GLN:HG2	1:465:A:VAL:HG21	4	0.31	0.14	0.26
(1,41)	1:463:A:GLN:HG2	1:465:A:VAL:HG22	4	0.31	0.14	0.26
(1,41)	1:463:A:GLN:HG2	1:465:A:VAL:HG23	4	0.31	0.14	0.26
(1,41)	1:463:A:GLN:HG3	1:465:A:VAL:HG21	4	0.31	0.14	0.26
(1,41)	1:463:A:GLN:HG3	1:465:A:VAL:HG22	4	0.31	0.14	0.26
(1,41)	1:463:A:GLN:HG3	1:465:A:VAL:HG23	4	0.31	0.14	0.26
(1,1022)	1:524:A:HIS:H	1:537:A:GLU:HB2	4	0.31	0.2	0.21
(1,1022)	1:524:A:HIS:H	1:537:A:GLU:HB3	4	0.31	0.2	0.21
(1,333)	1:456:A:ILE:HG21	1:460:A:LEU:H	4	0.31	0.12	0.28
(1,333)	1:456:A:ILE:HG22	1:460:A:LEU:H	4	0.31	0.12	0.28
(1,333)	1:456:A:ILE:HG23	1:460:A:LEU:H	4	0.31	0.12	0.28
(1,1238)	1:505:A:LYS:HB2	1:505:A:LYS:HE2	4	0.31	0.07	0.31
(1,1238)	1:505:A:LYS:HB2	1:505:A:LYS:HE3	4	0.31	0.07	0.31
(1,1238)	1:505:A:LYS:HB3	1:505:A:LYS:HE2	4	0.31	0.07	0.31
(1,1238)	1:505:A:LYS:HB3	1:505:A:LYS:HE3	4	0.31	0.07	0.31
(1,879)	1:470:A:ARG:H	1:516:A:GLU:HA	4	0.3	0.1	0.28
(1,960)	1:486:A:TRP:HZ2	1:511:A:HIS:H	4	0.3	0.2	0.2
(1,439)	1:526:A:ALA:HA	1:534:A:ALA:H	4	0.26	0.19	0.16
(1,1085)	1:456:A:ILE:HD11	1:532:A:GLY:HA2	4	0.25	0.14	0.18
(1,1085)	1:456:A:ILE:HD11	1:532:A:GLY:HA3	4	0.25	0.14	0.18
(1,1085)	1:456:A:ILE:HD12	1:532:A:GLY:HA2	4	0.25	0.14	0.18
(1,1085)	1:456:A:ILE:HD12	1:532:A:GLY:HA3	4	0.25	0.14	0.18
(1,1085)	1:456:A:ILE:HD13	1:532:A:GLY:HA2	4	0.25	0.14	0.18
(1,1085)	1:456:A:ILE:HD13	1:532:A:GLY:HA3	4	0.25	0.14	0.18
(1,1052)	1:465:A:VAL:H	1:539:A:ILE:H	4	0.23	0.09	0.2
(1,134)	1:487:A:LEU:HG	1:492:A:GLU:HA	4	0.23	0.04	0.22
(1,672)	1:469:A:GLN:H	1:517:A:ALA:HA	4	0.22	0.06	0.23
(1,151)	1:502:A:TRP:H	1:503:A:PHE:HB3	4	0.22	0.05	0.24
(1,991)	1:469:A:GLN:HA	1:517:A:ALA:H	4	0.19	0.06	0.19
(1,282)	1:464:A:LEU:HA	1:540:A:VAL:HG21	4	0.18	0.07	0.18
(1,282)	1:464:A:LEU:HA	1:540:A:VAL:HG22	4	0.18	0.07	0.18
(1,282)	1:464:A:LEU:HA	1:540:A:VAL:HG23	4	0.18	0.07	0.18
(1,708)	1:467:A:VAL:H	1:541:A:GLN:H	4	0.16	0.03	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,556)	1:488:A:LYS:HD3	1:491:A:VAL:H	3	1.56	0.09	1.58
(1,359)	1:488:A:LYS:HD3	1:489:A:ASP:H	3	1.45	0.08	1.49
(1,323)	1:498:A:THR:HG21	1:501:A:TYR:HD1	3	1.05	0.66	1.25
(1,323)	1:498:A:THR:HG22	1:501:A:TYR:HD1	3	1.05	0.66	1.25
(1,323)	1:498:A:THR:HG23	1:501:A:TYR:HD1	3	1.05	0.66	1.25
(1,966)	1:511:A:HIS:H	1:513:A:ILE:HD11	3	0.94	0.18	0.97
(1,966)	1:511:A:HIS:H	1:513:A:ILE:HD12	3	0.94	0.18	0.97
(1,966)	1:511:A:HIS:H	1:513:A:ILE:HD13	3	0.94	0.18	0.97
(1,325)	1:472:A:GLU:HG2	1:513:A:ILE:HD11	3	0.89	0.26	0.77
(1,325)	1:472:A:GLU:HG2	1:513:A:ILE:HD12	3	0.89	0.26	0.77
(1,325)	1:472:A:GLU:HG2	1:513:A:ILE:HD13	3	0.89	0.26	0.77
(1,325)	1:472:A:GLU:HG3	1:513:A:ILE:HD11	3	0.89	0.26	0.77
(1,325)	1:472:A:GLU:HG3	1:513:A:ILE:HD12	3	0.89	0.26	0.77
(1,325)	1:472:A:GLU:HG3	1:513:A:ILE:HD13	3	0.89	0.26	0.77
(1,1220)	1:497:A:GLU:HG2	1:500:A:LYS:H	3	0.89	0.44	1.19
(1,1220)	1:497:A:GLU:HG3	1:500:A:LYS:H	3	0.89	0.44	1.19
(1,421)	1:525:A:TYR:H	1:536:A:ALA:H	3	0.89	0.61	0.91
(1,891)	1:475:A:CYS:H	1:510:A:HIS:H	3	0.8	0.15	0.85
(1,886)	1:475:A:CYS:H	1:509:A:ARG:HA	3	0.78	0.21	0.86
(1,470)	1:512:A:LEU:H	1:513:A:ILE:HD11	3	0.67	0.2	0.54
(1,470)	1:512:A:LEU:H	1:513:A:ILE:HD12	3	0.67	0.2	0.54
(1,470)	1:512:A:LEU:H	1:513:A:ILE:HD13	3	0.67	0.2	0.54
(1,1240)	1:505:A:LYS:HB2	1:510:A:HIS:HE1	3	0.66	0.43	0.67
(1,1240)	1:505:A:LYS:HB3	1:510:A:HIS:HE1	3	0.66	0.43	0.67
(1,642)	1:482:A:ALA:H	1:508:A:GLN:HB3	3	0.64	0.26	0.66
(1,642)	1:482:A:ALA:H	1:508:A:GLN:HB2	3	0.64	0.26	0.66
(1,238)	1:522:A:ALA:HB1	1:540:A:VAL:HG21	3	0.62	0.34	0.53
(1,238)	1:522:A:ALA:HB1	1:540:A:VAL:HG22	3	0.62	0.34	0.53
(1,238)	1:522:A:ALA:HB1	1:540:A:VAL:HG23	3	0.62	0.34	0.53
(1,238)	1:522:A:ALA:HB2	1:540:A:VAL:HG21	3	0.62	0.34	0.53
(1,238)	1:522:A:ALA:HB2	1:540:A:VAL:HG22	3	0.62	0.34	0.53
(1,238)	1:522:A:ALA:HB2	1:540:A:VAL:HG23	3	0.62	0.34	0.53
(1,238)	1:522:A:ALA:HB3	1:540:A:VAL:HG21	3	0.62	0.34	0.53
(1,238)	1:522:A:ALA:HB3	1:540:A:VAL:HG22	3	0.62	0.34	0.53
(1,238)	1:522:A:ALA:HB3	1:540:A:VAL:HG23	3	0.62	0.34	0.53
(1,974)	1:513:A:ILE:HG13	1:514:A:ILE:H	3	0.62	0.06	0.59
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD11	3	0.6	0.22	0.54
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD12	3	0.6	0.22	0.54
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD13	3	0.6	0.22	0.54
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD21	3	0.6	0.22	0.54
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD22	3	0.6	0.22	0.54
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD23	3	0.6	0.22	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD11	3	0.6	0.22	0.54
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD12	3	0.6	0.22	0.54
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD13	3	0.6	0.22	0.54
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD21	3	0.6	0.22	0.54
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD22	3	0.6	0.22	0.54
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD23	3	0.6	0.22	0.54
(1,1121)	1:466:A:MET:HB2	1:469:A:GLN:HG2	3	0.54	0.38	0.34
(1,1121)	1:466:A:MET:HB2	1:469:A:GLN:HG3	3	0.54	0.38	0.34
(1,1121)	1:466:A:MET:HB3	1:469:A:GLN:HG2	3	0.54	0.38	0.34
(1,1121)	1:466:A:MET:HB3	1:469:A:GLN:HG3	3	0.54	0.38	0.34
(1,973)	1:471:A:VAL:HB	1:514:A:ILE:H	3	0.53	0.18	0.6
(1,1261)	1:518:A:MET:HB2	1:518:A:MET:HE1	3	0.51	0.0	0.51
(1,1261)	1:518:A:MET:HB2	1:518:A:MET:HE2	3	0.51	0.0	0.51
(1,1261)	1:518:A:MET:HB2	1:518:A:MET:HE3	3	0.51	0.0	0.51
(1,1261)	1:518:A:MET:HB3	1:518:A:MET:HE1	3	0.51	0.0	0.51
(1,1261)	1:518:A:MET:HB3	1:518:A:MET:HE2	3	0.51	0.0	0.51
(1,1261)	1:518:A:MET:HB3	1:518:A:MET:HE3	3	0.51	0.0	0.51
(1,627)	1:524:A:HIS:HA	1:537:A:GLU:H	3	0.51	0.25	0.68
(1,1001)	1:518:A:MET:H	1:520:A:GLU:H	3	0.51	0.18	0.51
(1,602)	1:458:A:ARG:H	1:477:A:VAL:HA	3	0.5	0.17	0.44
(1,982)	1:502:A:TRP:HD1	1:515:A:ASN:H	3	0.5	0.25	0.62
(1,1243)	1:506:A:ASP:H	1:509:A:ARG:HG2	3	0.46	0.14	0.43
(1,1243)	1:506:A:ASP:H	1:509:A:ARG:HG3	3	0.46	0.14	0.43
(1,1265)	1:518:A:MET:HG2	1:520:A:GLU:H	3	0.46	0.24	0.32
(1,1265)	1:518:A:MET:HG3	1:520:A:GLU:H	3	0.46	0.24	0.32
(1,512)	1:522:A:ALA:HA	1:538:A:LEU:H	3	0.45	0.14	0.49
(1,592)	1:519:A:LEU:H	1:540:A:VAL:HG11	3	0.44	0.16	0.54
(1,592)	1:519:A:LEU:H	1:540:A:VAL:HG12	3	0.44	0.16	0.54
(1,592)	1:519:A:LEU:H	1:540:A:VAL:HG13	3	0.44	0.16	0.54
(1,1009)	1:517:A:ALA:HB1	1:521:A:ASP:H	3	0.41	0.21	0.53
(1,1009)	1:517:A:ALA:HB2	1:521:A:ASP:H	3	0.41	0.21	0.53
(1,1009)	1:517:A:ALA:HB3	1:521:A:ASP:H	3	0.41	0.21	0.53
(1,426)	1:525:A:TYR:H	1:537:A:GLU:HA	3	0.4	0.09	0.37
(1,657)	1:457:A:THR:H	1:477:A:VAL:HB	3	0.36	0.21	0.29
(1,782)	1:457:A:THR:HG21	1:508:A:GLN:HE21	3	0.36	0.2	0.23
(1,782)	1:457:A:THR:HG22	1:508:A:GLN:HE21	3	0.36	0.2	0.23
(1,782)	1:457:A:THR:HG23	1:508:A:GLN:HE21	3	0.36	0.2	0.23
(1,583)	1:528:A:CYS:H	1:533:A:GLN:HA	3	0.35	0.12	0.39
(1,61)	1:488:A:LYS:HA	1:488:A:LYS:HD3	3	0.34	0.04	0.36
(1,331)	1:456:A:ILE:HG21	1:459:A:PRO:HA	3	0.33	0.09	0.32
(1,331)	1:456:A:ILE:HG22	1:459:A:PRO:HA	3	0.33	0.09	0.32
(1,331)	1:456:A:ILE:HG23	1:459:A:PRO:HA	3	0.33	0.09	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1063)	1:453:A:PRO:HB2	1:531:A:GLY:H	3	0.33	0.11	0.28
(1,1063)	1:453:A:PRO:HB3	1:531:A:GLY:H	3	0.33	0.11	0.28
(1,958)	1:474:A:GLU:HA	1:511:A:HIS:H	3	0.33	0.03	0.33
(1,1123)	1:466:A:MET:HG2	1:469:A:GLN:HG2	3	0.32	0.08	0.28
(1,1123)	1:466:A:MET:HG2	1:469:A:GLN:HG3	3	0.32	0.08	0.28
(1,1123)	1:466:A:MET:HG3	1:469:A:GLN:HG2	3	0.32	0.08	0.28
(1,1123)	1:466:A:MET:HG3	1:469:A:GLN:HG3	3	0.32	0.08	0.28
(1,382)	1:455:A:LEU:H	1:479:A:GLU:H	3	0.31	0.06	0.27
(1,309)	1:524:A:HIS:HE1	1:537:A:GLU:HB2	3	0.31	0.08	0.28
(1,309)	1:524:A:HIS:HE1	1:537:A:GLU:HB3	3	0.31	0.08	0.28
(1,503)	1:473:A:PHE:H	1:513:A:ILE:HG13	3	0.3	0.09	0.35
(1,1226)	1:500:A:LYS:HE2	1:518:A:MET:H	3	0.29	0.19	0.2
(1,1226)	1:500:A:LYS:HE3	1:518:A:MET:H	3	0.29	0.19	0.2
(1,142)	1:460:A:LEU:HD11	1:475:A:CYS:HB3	3	0.27	0.07	0.23
(1,142)	1:460:A:LEU:HD12	1:475:A:CYS:HB3	3	0.27	0.07	0.23
(1,142)	1:460:A:LEU:HD13	1:475:A:CYS:HB3	3	0.27	0.07	0.23
(1,158)	1:508:A:GLN:HA	1:510:A:HIS:HD2	3	0.27	0.15	0.2
(1,473)	1:512:A:LEU:H	1:513:A:ILE:HG13	3	0.27	0.06	0.23
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD11	3	0.26	0.11	0.22
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD12	3	0.26	0.11	0.22
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD13	3	0.26	0.11	0.22
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD21	3	0.26	0.11	0.22
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD22	3	0.26	0.11	0.22
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD23	3	0.26	0.11	0.22
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD11	3	0.26	0.11	0.22
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD12	3	0.26	0.11	0.22
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD13	3	0.26	0.11	0.22
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD21	3	0.26	0.11	0.22
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD22	3	0.26	0.11	0.22
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD23	3	0.26	0.11	0.22
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD11	3	0.26	0.11	0.22
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD12	3	0.26	0.11	0.22
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD13	3	0.26	0.11	0.22
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD21	3	0.26	0.11	0.22
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD22	3	0.26	0.11	0.22
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD23	3	0.26	0.11	0.22
(1,1217)	1:496:A:GLU:H	1:496:A:GLU:HB2	3	0.26	0.12	0.18
(1,1217)	1:496:A:GLU:H	1:496:A:GLU:HB3	3	0.26	0.12	0.18
(1,444)	1:472:A:GLU:H	1:514:A:ILE:HB	3	0.25	0.11	0.27
(1,716)	1:466:A:MET:H	1:466:A:MET:HE1	3	0.25	0.07	0.21
(1,716)	1:466:A:MET:H	1:466:A:MET:HE2	3	0.25	0.07	0.21
(1,716)	1:466:A:MET:H	1:466:A:MET:HE3	3	0.25	0.07	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1314)	1:542:A:GLU:HG2	1:543:A:LYS:H	3	0.25	0.1	0.3
(1,1314)	1:542:A:GLU:HG3	1:543:A:LYS:H	3	0.25	0.1	0.3
(1,1185)	1:487:A:LEU:HD11	1:492:A:GLU:H	3	0.23	0.13	0.16
(1,1185)	1:487:A:LEU:HD12	1:492:A:GLU:H	3	0.23	0.13	0.16
(1,1185)	1:487:A:LEU:HD13	1:492:A:GLU:H	3	0.23	0.13	0.16
(1,1185)	1:487:A:LEU:HD21	1:492:A:GLU:H	3	0.23	0.13	0.16
(1,1185)	1:487:A:LEU:HD22	1:492:A:GLU:H	3	0.23	0.13	0.16
(1,1185)	1:487:A:LEU:HD23	1:492:A:GLU:H	3	0.23	0.13	0.16
(1,901)	1:476:A:GLU:H	1:477:A:VAL:HG21	3	0.22	0.08	0.24
(1,901)	1:476:A:GLU:H	1:477:A:VAL:HG22	3	0.22	0.08	0.24
(1,901)	1:476:A:GLU:H	1:477:A:VAL:HG23	3	0.22	0.08	0.24
(1,569)	1:522:A:ALA:H	1:540:A:VAL:HB	3	0.22	0.05	0.25
(1,721)	1:500:A:LYS:HG2	1:501:A:TYR:H	3	0.21	0.0	0.21
(1,721)	1:500:A:LYS:HG3	1:501:A:TYR:H	3	0.21	0.0	0.21
(1,1095)	1:460:A:LEU:HD11	1:475:A:CYS:H	3	0.2	0.05	0.18
(1,1095)	1:460:A:LEU:HD12	1:475:A:CYS:H	3	0.2	0.05	0.18
(1,1095)	1:460:A:LEU:HD13	1:475:A:CYS:H	3	0.2	0.05	0.18
(1,1095)	1:460:A:LEU:HD21	1:475:A:CYS:H	3	0.2	0.05	0.18
(1,1095)	1:460:A:LEU:HD22	1:475:A:CYS:H	3	0.2	0.05	0.18
(1,1095)	1:460:A:LEU:HD23	1:475:A:CYS:H	3	0.2	0.05	0.18
(1,595)	1:518:A:MET:HE1	1:519:A:LEU:H	3	0.19	0.05	0.17
(1,595)	1:518:A:MET:HE2	1:519:A:LEU:H	3	0.19	0.05	0.17
(1,595)	1:518:A:MET:HE3	1:519:A:LEU:H	3	0.19	0.05	0.17
(1,731)	1:498:A:THR:H	1:501:A:TYR:H	3	0.17	0.03	0.18
(1,34)	1:460:A:LEU:HA	1:536:A:ALA:HB1	3	0.16	0.03	0.17
(1,34)	1:460:A:LEU:HA	1:536:A:ALA:HB2	3	0.16	0.03	0.17
(1,34)	1:460:A:LEU:HA	1:536:A:ALA:HB3	3	0.16	0.03	0.17
(1,1160)	1:475:A:CYS:HB2	1:476:A:GLU:H	3	0.16	0.0	0.16
(1,1160)	1:475:A:CYS:HB3	1:476:A:GLU:H	3	0.16	0.0	0.16
(1,887)	1:475:A:CYS:H	1:510:A:HIS:HB3	3	0.15	0.05	0.14
(1,912)	1:479:A:GLU:H	1:482:A:ALA:H	3	0.13	0.02	0.11
(1,859)	1:463:A:GLN:H	1:463:A:GLN:HE21	3	0.12	0.01	0.12
(1,344)	1:526:A:ALA:HB1	1:535:A:LEU:HG	2	1.27	0.11	1.27
(1,344)	1:526:A:ALA:HB2	1:535:A:LEU:HG	2	1.27	0.11	1.27
(1,344)	1:526:A:ALA:HB3	1:535:A:LEU:HG	2	1.27	0.11	1.27
(1,328)	1:503:A:PHE:HB2	1:513:A:ILE:HD11	2	1.14	0.01	1.14
(1,328)	1:503:A:PHE:HB2	1:513:A:ILE:HD12	2	1.14	0.01	1.14
(1,328)	1:503:A:PHE:HB2	1:513:A:ILE:HD13	2	1.14	0.01	1.14
(1,76)	1:472:A:GLU:HG2	1:513:A:ILE:HG13	2	0.94	0.18	0.94
(1,76)	1:472:A:GLU:HG3	1:513:A:ILE:HG13	2	0.94	0.18	0.94
(1,156)	1:505:A:LYS:HE2	1:506:A:ASP:HA	2	0.93	0.16	0.93
(1,156)	1:505:A:LYS:HE3	1:506:A:ASP:HA	2	0.93	0.16	0.93

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1196)	1:488:A:LYS:HE2	1:524:A:HIS:H	2	0.9	0.04	0.9
(1,1196)	1:488:A:LYS:HE3	1:524:A:HIS:H	2	0.9	0.04	0.9
(1,946)	1:503:A:PHE:H	1:513:A:ILE:HD11	2	0.79	0.1	0.79
(1,946)	1:503:A:PHE:H	1:513:A:ILE:HD12	2	0.79	0.1	0.79
(1,946)	1:503:A:PHE:H	1:513:A:ILE:HD13	2	0.79	0.1	0.79
(1,525)	1:525:A:TYR:HA	1:536:A:ALA:H	2	0.76	0.22	0.76
(1,77)	1:471:A:VAL:HA	1:472:A:GLU:HG2	2	0.76	0.54	0.76
(1,77)	1:471:A:VAL:HA	1:472:A:GLU:HG3	2	0.76	0.54	0.76
(1,641)	1:479:A:GLU:HG2	1:482:A:ALA:H	2	0.74	0.42	0.74
(1,641)	1:479:A:GLU:HG3	1:482:A:ALA:H	2	0.74	0.42	0.74
(1,1219)	1:497:A:GLU:HG2	1:498:A:THR:HG21	2	0.72	0.1	0.72
(1,1219)	1:497:A:GLU:HG2	1:498:A:THR:HG22	2	0.72	0.1	0.72
(1,1219)	1:497:A:GLU:HG2	1:498:A:THR:HG23	2	0.72	0.1	0.72
(1,1219)	1:497:A:GLU:HG3	1:498:A:THR:HG21	2	0.72	0.1	0.72
(1,1219)	1:497:A:GLU:HG3	1:498:A:THR:HG22	2	0.72	0.1	0.72
(1,1219)	1:497:A:GLU:HG3	1:498:A:THR:HG23	2	0.72	0.1	0.72
(1,50)	1:465:A:VAL:HG11	1:471:A:VAL:HB	2	0.7	0.32	0.7
(1,50)	1:465:A:VAL:HG12	1:471:A:VAL:HB	2	0.7	0.32	0.7
(1,50)	1:465:A:VAL:HG13	1:471:A:VAL:HB	2	0.7	0.32	0.7
(1,1270)	1:519:A:LEU:HD11	1:541:A:GLN:HA	2	0.66	0.25	0.66
(1,1270)	1:519:A:LEU:HD12	1:541:A:GLN:HA	2	0.66	0.25	0.66
(1,1270)	1:519:A:LEU:HD13	1:541:A:GLN:HA	2	0.66	0.25	0.66
(1,1270)	1:519:A:LEU:HD21	1:541:A:GLN:HA	2	0.66	0.25	0.66
(1,1270)	1:519:A:LEU:HD22	1:541:A:GLN:HA	2	0.66	0.25	0.66
(1,1270)	1:519:A:LEU:HD23	1:541:A:GLN:HA	2	0.66	0.25	0.66
(1,272)	1:539:A:ILE:HG21	1:541:A:GLN:HG2	2	0.65	0.27	0.65
(1,272)	1:539:A:ILE:HG21	1:541:A:GLN:HG3	2	0.65	0.27	0.65
(1,272)	1:539:A:ILE:HG22	1:541:A:GLN:HG2	2	0.65	0.27	0.65
(1,272)	1:539:A:ILE:HG22	1:541:A:GLN:HG3	2	0.65	0.27	0.65
(1,272)	1:539:A:ILE:HG23	1:541:A:GLN:HG2	2	0.65	0.27	0.65
(1,272)	1:539:A:ILE:HG23	1:541:A:GLN:HG3	2	0.65	0.27	0.65
(1,286)	1:521:A:ASP:HB2	1:540:A:VAL:HG21	2	0.64	0.34	0.64
(1,286)	1:521:A:ASP:HB2	1:540:A:VAL:HG22	2	0.64	0.34	0.64
(1,286)	1:521:A:ASP:HB2	1:540:A:VAL:HG23	2	0.64	0.34	0.64
(1,120)	1:525:A:TYR:HB2	1:536:A:ALA:HB1	2	0.64	0.36	0.64
(1,120)	1:525:A:TYR:HB2	1:536:A:ALA:HB2	2	0.64	0.36	0.64
(1,120)	1:525:A:TYR:HB2	1:536:A:ALA:HB3	2	0.64	0.36	0.64
(1,684)	1:504:A:LYS:H	1:513:A:ILE:HD11	2	0.62	0.14	0.62
(1,684)	1:504:A:LYS:H	1:513:A:ILE:HD12	2	0.62	0.14	0.62
(1,684)	1:504:A:LYS:H	1:513:A:ILE:HD13	2	0.62	0.14	0.62
(1,608)	1:458:A:ARG:H	1:476:A:GLU:HG2	2	0.59	0.37	0.59
(1,178)	1:470:A:ARG:HB2	1:513:A:ILE:HG21	2	0.54	0.25	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,178)	1:470:A:ARG:HB2	1:513:A:ILE:HG22	2	0.54	0.25	0.54
(1,178)	1:470:A:ARG:HB2	1:513:A:ILE:HG23	2	0.54	0.25	0.54
(1,1148)	1:471:A:VAL:HG11	1:514:A:ILE:HD11	2	0.54	0.28	0.54
(1,1148)	1:471:A:VAL:HG11	1:514:A:ILE:HD12	2	0.54	0.28	0.54
(1,1148)	1:471:A:VAL:HG11	1:514:A:ILE:HD13	2	0.54	0.28	0.54
(1,1148)	1:471:A:VAL:HG12	1:514:A:ILE:HD11	2	0.54	0.28	0.54
(1,1148)	1:471:A:VAL:HG12	1:514:A:ILE:HD12	2	0.54	0.28	0.54
(1,1148)	1:471:A:VAL:HG12	1:514:A:ILE:HD13	2	0.54	0.28	0.54
(1,1148)	1:471:A:VAL:HG13	1:514:A:ILE:HD11	2	0.54	0.28	0.54
(1,1148)	1:471:A:VAL:HG13	1:514:A:ILE:HD12	2	0.54	0.28	0.54
(1,1148)	1:471:A:VAL:HG13	1:514:A:ILE:HD13	2	0.54	0.28	0.54
(1,1148)	1:471:A:VAL:HG21	1:514:A:ILE:HD11	2	0.54	0.28	0.54
(1,1148)	1:471:A:VAL:HG21	1:514:A:ILE:HD12	2	0.54	0.28	0.54
(1,1148)	1:471:A:VAL:HG21	1:514:A:ILE:HD13	2	0.54	0.28	0.54
(1,1148)	1:471:A:VAL:HG22	1:514:A:ILE:HD11	2	0.54	0.28	0.54
(1,1148)	1:471:A:VAL:HG22	1:514:A:ILE:HD12	2	0.54	0.28	0.54
(1,1148)	1:471:A:VAL:HG22	1:514:A:ILE:HD13	2	0.54	0.28	0.54
(1,1148)	1:471:A:VAL:HG23	1:514:A:ILE:HD11	2	0.54	0.28	0.54
(1,1148)	1:471:A:VAL:HG23	1:514:A:ILE:HD12	2	0.54	0.28	0.54
(1,1148)	1:471:A:VAL:HG23	1:514:A:ILE:HD13	2	0.54	0.28	0.54
(1,304)	1:484:A:VAL:HG11	1:510:A:HIS:HE1	2	0.52	0.3	0.52
(1,304)	1:484:A:VAL:HG12	1:510:A:HIS:HE1	2	0.52	0.3	0.52
(1,304)	1:484:A:VAL:HG13	1:510:A:HIS:HE1	2	0.52	0.3	0.52
(1,304)	1:484:A:VAL:HG21	1:510:A:HIS:HE1	2	0.52	0.3	0.52
(1,304)	1:484:A:VAL:HG22	1:510:A:HIS:HE1	2	0.52	0.3	0.52
(1,304)	1:484:A:VAL:HG23	1:510:A:HIS:HE1	2	0.52	0.3	0.52
(1,193)	1:471:A:VAL:HB	1:514:A:ILE:HD11	2	0.52	0.4	0.52
(1,193)	1:471:A:VAL:HB	1:514:A:ILE:HD12	2	0.52	0.4	0.52
(1,193)	1:471:A:VAL:HB	1:514:A:ILE:HD13	2	0.52	0.4	0.52
(1,905)	1:477:A:VAL:H	1:508:A:GLN:HG2	2	0.5	0.36	0.5
(1,905)	1:477:A:VAL:H	1:508:A:GLN:HG3	2	0.5	0.36	0.5
(1,1212)	1:493:A:LEU:HD11	1:512:A:LEU:HD11	2	0.5	0.19	0.5
(1,1212)	1:493:A:LEU:HD11	1:512:A:LEU:HD12	2	0.5	0.19	0.5
(1,1212)	1:493:A:LEU:HD11	1:512:A:LEU:HD13	2	0.5	0.19	0.5
(1,1212)	1:493:A:LEU:HD12	1:512:A:LEU:HD11	2	0.5	0.19	0.5
(1,1212)	1:493:A:LEU:HD12	1:512:A:LEU:HD12	2	0.5	0.19	0.5
(1,1212)	1:493:A:LEU:HD12	1:512:A:LEU:HD13	2	0.5	0.19	0.5
(1,1212)	1:493:A:LEU:HD13	1:512:A:LEU:HD11	2	0.5	0.19	0.5
(1,1212)	1:493:A:LEU:HD13	1:512:A:LEU:HD12	2	0.5	0.19	0.5
(1,1212)	1:493:A:LEU:HD13	1:512:A:LEU:HD13	2	0.5	0.19	0.5
(1,1212)	1:493:A:LEU:HD21	1:512:A:LEU:HD11	2	0.5	0.19	0.5
(1,1212)	1:493:A:LEU:HD21	1:512:A:LEU:HD12	2	0.5	0.19	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1212)	1:493:A:LEU:HD21	1:512:A:LEU:HD13	2	0.5	0.19	0.5
(1,1212)	1:493:A:LEU:HD22	1:512:A:LEU:HD11	2	0.5	0.19	0.5
(1,1212)	1:493:A:LEU:HD22	1:512:A:LEU:HD12	2	0.5	0.19	0.5
(1,1212)	1:493:A:LEU:HD22	1:512:A:LEU:HD13	2	0.5	0.19	0.5
(1,1212)	1:493:A:LEU:HD23	1:512:A:LEU:HD11	2	0.5	0.19	0.5
(1,1212)	1:493:A:LEU:HD23	1:512:A:LEU:HD12	2	0.5	0.19	0.5
(1,1212)	1:493:A:LEU:HD23	1:512:A:LEU:HD13	2	0.5	0.19	0.5
(1,1101)	1:460:A:LEU:HD11	1:527:A:LEU:H	2	0.49	0.15	0.49
(1,1101)	1:460:A:LEU:HD12	1:527:A:LEU:H	2	0.49	0.15	0.49
(1,1101)	1:460:A:LEU:HD13	1:527:A:LEU:H	2	0.49	0.15	0.49
(1,1101)	1:460:A:LEU:HD21	1:527:A:LEU:H	2	0.49	0.15	0.49
(1,1101)	1:460:A:LEU:HD22	1:527:A:LEU:H	2	0.49	0.15	0.49
(1,1101)	1:460:A:LEU:HD23	1:527:A:LEU:H	2	0.49	0.15	0.49
(1,1082)	1:456:A:ILE:HG12	1:533:A:GLN:H	2	0.48	0.31	0.48
(1,1082)	1:456:A:ILE:HG13	1:533:A:GLN:H	2	0.48	0.31	0.48
(1,195)	1:514:A:ILE:HD11	1:521:A:ASP:HB3	2	0.46	0.32	0.46
(1,195)	1:514:A:ILE:HD12	1:521:A:ASP:HB3	2	0.46	0.32	0.46
(1,195)	1:514:A:ILE:HD13	1:521:A:ASP:HB3	2	0.46	0.32	0.46
(1,502)	1:473:A:PHE:H	1:513:A:ILE:HD11	2	0.44	0.01	0.44
(1,502)	1:473:A:PHE:H	1:513:A:ILE:HD12	2	0.44	0.01	0.44
(1,502)	1:473:A:PHE:H	1:513:A:ILE:HD13	2	0.44	0.01	0.44
(1,791)	1:529:A:THR:HB	1:532:A:GLY:H	2	0.44	0.02	0.44
(1,1313)	1:542:A:GLU:HB2	1:543:A:LYS:H	2	0.44	0.03	0.44
(1,1313)	1:542:A:GLU:HB3	1:543:A:LYS:H	2	0.44	0.03	0.44
(1,1158)	1:473:A:PHE:HB2	1:512:A:LEU:H	2	0.36	0.1	0.36
(1,1158)	1:473:A:PHE:HB3	1:512:A:LEU:H	2	0.36	0.1	0.36
(1,390)	1:484:A:VAL:HB	1:486:A:TRP:HE1	2	0.36	0.16	0.36
(1,428)	1:525:A:TYR:H	1:537:A:GLU:HB2	2	0.36	0.07	0.36
(1,428)	1:525:A:TYR:H	1:537:A:GLU:HB3	2	0.36	0.07	0.36
(1,1271)	1:519:A:LEU:HD11	1:542:A:GLU:H	2	0.34	0.2	0.34
(1,1271)	1:519:A:LEU:HD12	1:542:A:GLU:H	2	0.34	0.2	0.34
(1,1271)	1:519:A:LEU:HD13	1:542:A:GLU:H	2	0.34	0.2	0.34
(1,1271)	1:519:A:LEU:HD21	1:542:A:GLU:H	2	0.34	0.2	0.34
(1,1271)	1:519:A:LEU:HD22	1:542:A:GLU:H	2	0.34	0.2	0.34
(1,1271)	1:519:A:LEU:HD23	1:542:A:GLU:H	2	0.34	0.2	0.34
(1,143)	1:495:A:ARG:HA	1:495:A:ARG:HD2	2	0.34	0.14	0.34
(1,143)	1:495:A:ARG:HA	1:495:A:ARG:HD3	2	0.34	0.14	0.34
(1,447)	1:472:A:GLU:H	1:513:A:ILE:HA	2	0.32	0.17	0.32
(1,504)	1:473:A:PHE:H	1:512:A:LEU:HB2	2	0.3	0.07	0.3
(1,774)	1:456:A:ILE:HA	1:478:A:SER:H	2	0.3	0.02	0.3
(1,16)	1:459:A:PRO:HA	1:534:A:ALA:HB1	2	0.29	0.09	0.29
(1,16)	1:459:A:PRO:HA	1:534:A:ALA:HB2	2	0.29	0.09	0.29

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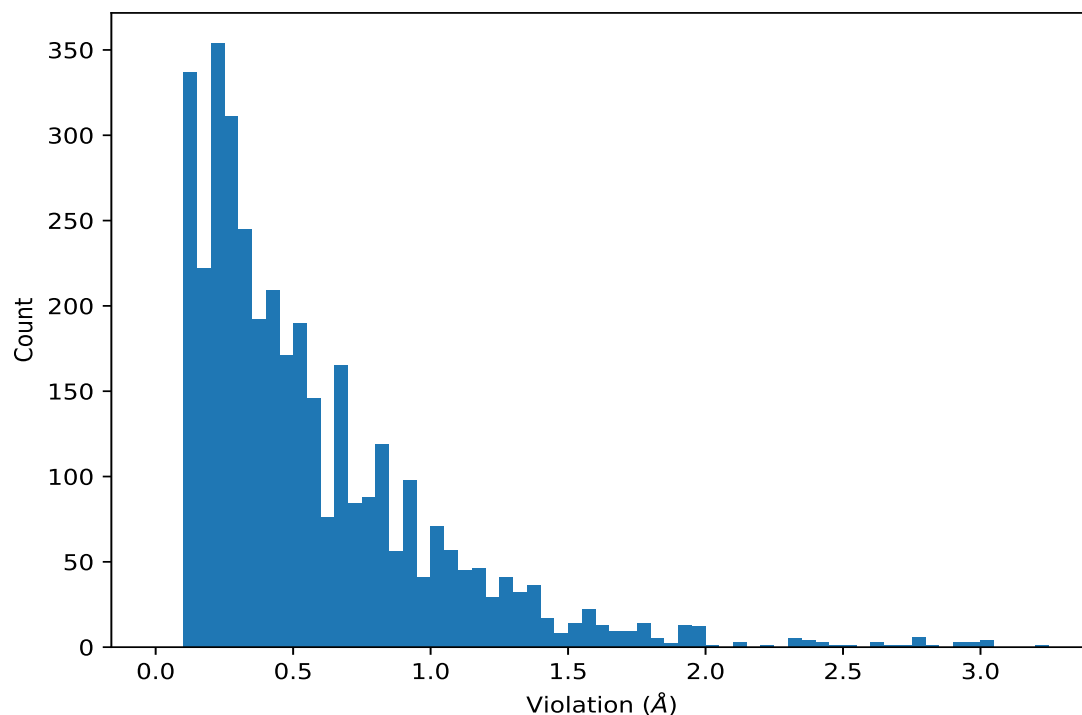
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,16)	1:459:A:PRO:HA	1:534:A:ALA:HB3	2	0.29	0.09	0.29
(1,889)	1:475:A:CYS:H	1:486:A:TRP:HH2	2	0.28	0.06	0.28
(1,926)	1:487:A:LEU:H	1:492:A:GLU:HA	2	0.28	0.06	0.28
(1,1041)	1:526:A:ALA:HA	1:535:A:LEU:H	2	0.24	0.04	0.24
(1,989)	1:469:A:GLN:H	1:517:A:ALA:H	2	0.23	0.0	0.23
(1,801)	1:529:A:THR:H	1:531:A:GLY:H	2	0.23	0.06	0.23
(1,1298)	1:533:A:GLN:HB2	1:533:A:GLN:HE21	2	0.22	0.01	0.22
(1,1298)	1:533:A:GLN:HB2	1:533:A:GLN:HE22	2	0.22	0.01	0.22
(1,1298)	1:533:A:GLN:HB3	1:533:A:GLN:HE21	2	0.22	0.01	0.22
(1,1298)	1:533:A:GLN:HB3	1:533:A:GLN:HE22	2	0.22	0.01	0.22
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG11	2	0.22	0.02	0.22
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG12	2	0.22	0.02	0.22
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG13	2	0.22	0.02	0.22
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG21	2	0.22	0.02	0.22
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG22	2	0.22	0.02	0.22
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG23	2	0.22	0.02	0.22
(1,566)	1:518:A:MET:H	1:522:A:ALA:H	2	0.22	0.07	0.22
(1,866)	1:463:A:GLN:HG2	1:465:A:VAL:H	2	0.2	0.04	0.2
(1,866)	1:463:A:GLN:HG3	1:465:A:VAL:H	2	0.2	0.04	0.2
(1,215)	1:470:A:ARG:HB2	1:515:A:ASN:HA	2	0.2	0.09	0.2
(1,1068)	1:454:A:VAL:HG11	1:478:A:SER:H	2	0.2	0.06	0.2
(1,1068)	1:454:A:VAL:HG12	1:478:A:SER:H	2	0.2	0.06	0.2
(1,1068)	1:454:A:VAL:HG13	1:478:A:SER:H	2	0.2	0.06	0.2
(1,1068)	1:454:A:VAL:HG21	1:478:A:SER:H	2	0.2	0.06	0.2
(1,1068)	1:454:A:VAL:HG22	1:478:A:SER:H	2	0.2	0.06	0.2
(1,1068)	1:454:A:VAL:HG23	1:478:A:SER:H	2	0.2	0.06	0.2
(1,570)	1:520:A:GLU:HB2	1:522:A:ALA:H	2	0.18	0.02	0.18
(1,570)	1:520:A:GLU:HB3	1:522:A:ALA:H	2	0.18	0.02	0.18
(1,606)	1:457:A:THR:HG21	1:458:A:ARG:H	2	0.16	0.02	0.16
(1,606)	1:457:A:THR:HG22	1:458:A:ARG:H	2	0.16	0.02	0.16
(1,606)	1:457:A:THR:HG23	1:458:A:ARG:H	2	0.16	0.02	0.16
(1,709)	1:467:A:VAL:H	1:542:A:GLU:H	2	0.15	0.02	0.15
(1,1049)	1:541:A:GLN:H	1:542:A:GLU:HA	2	0.15	0.01	0.15
(1,35)	1:522:A:ALA:HA	1:538:A:LEU:HD11	2	0.15	0.02	0.15
(1,35)	1:522:A:ALA:HA	1:538:A:LEU:HD12	2	0.15	0.02	0.15
(1,35)	1:522:A:ALA:HA	1:538:A:LEU:HD13	2	0.15	0.02	0.15
(1,758)	1:461:A:GLU:H	1:463:A:GLN:HE22	2	0.14	0.01	0.14
(1,218)	1:468:A:GLY:HA2	1:516:A:GLU:HA	2	0.14	0.01	0.14
(1,604)	1:456:A:ILE:HA	1:458:A:ARG:H	2	0.12	0.02	0.12
(1,979)	1:470:A:ARG:H	1:517:A:ALA:H	2	0.11	0.01	0.11
(1,1299)	1:533:A:GLN:HB2	1:534:A:ALA:H	2	0.11	0.0	0.11
(1,1299)	1:533:A:GLN:HB3	1:534:A:ALA:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,515)	1:525:A:TYR:HD1	1:538:A:LEU:H	4	3.24
(1,803)	1:523:A:GLY:H	1:525:A:TYR:HD1	4	3.05
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD21	2	3.01
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD22	2	3.01
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD23	2	3.01
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD21	9	2.96
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD22	9	2.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD23	9	2.96
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD21	6	2.93
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD22	6	2.93
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD23	6	2.93
(1,803)	1:523:A:GLY:H	1:525:A:TYR:HD1	2	2.83
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD21	1	2.77
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD22	1	2.77
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD23	1	2.77
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD21	4	2.75
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD22	4	2.75
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD23	4	2.75
(1,515)	1:525:A:TYR:HD1	1:538:A:LEU:H	7	2.7
(1,803)	1:523:A:GLY:H	1:525:A:TYR:HD1	1	2.68
(1,803)	1:523:A:GLY:H	1:525:A:TYR:HD1	5	2.62
(1,803)	1:523:A:GLY:H	1:525:A:TYR:HD1	7	2.62
(1,803)	1:523:A:GLY:H	1:525:A:TYR:HD1	10	2.61
(1,803)	1:523:A:GLY:H	1:525:A:TYR:HD1	8	2.53
(1,515)	1:525:A:TYR:HD1	1:538:A:LEU:H	8	2.48
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD21	5	2.44
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD22	5	2.44
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD23	5	2.44
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD21	4	2.37
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD22	4	2.37
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD23	4	2.37
(1,1019)	1:524:A:HIS:H	1:525:A:TYR:HD1	10	2.35
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD21	8	2.33
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD22	8	2.33
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD23	8	2.33
(1,1019)	1:524:A:HIS:H	1:525:A:TYR:HD1	2	2.31
(1,318)	1:486:A:TRP:HD1	1:503:A:PHE:HE2	2	2.31
(1,515)	1:525:A:TYR:HD1	1:538:A:LEU:H	1	2.22
(1,1032)	1:529:A:THR:H	1:532:A:GLY:H	7	2.14
(1,319)	1:486:A:TRP:HD1	1:503:A:PHE:HD2	2	2.13
(1,1019)	1:524:A:HIS:H	1:525:A:TYR:HD1	5	2.1
(1,1019)	1:524:A:HIS:H	1:525:A:TYR:HD1	4	2.01
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD11	7	1.96
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD12	7	1.96
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD13	7	1.96
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD21	7	1.96
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD22	7	1.96
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD23	7	1.96
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD11	7	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD12	7	1.96
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD13	7	1.96
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD21	7	1.96
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD22	7	1.96
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD23	7	1.96
(1,319)	1:486:A:TRP:HD1	1:503:A:PHE:HD2	9	1.95
(1,1019)	1:524:A:HIS:H	1:525:A:TYR:HD1	7	1.93
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD21	7	1.93
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD22	7	1.93
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD23	7	1.93
(1,1019)	1:524:A:HIS:H	1:525:A:TYR:HD1	1	1.92
(1,515)	1:525:A:TYR:HD1	1:538:A:LEU:H	2	1.92
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD21	4	1.91
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD22	4	1.91
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD23	4	1.91
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD21	10	1.91
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD22	10	1.91
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD23	10	1.91
(1,307)	1:505:A:LYS:HD2	1:510:A:HIS:HE1	6	1.87
(1,307)	1:505:A:LYS:HD3	1:510:A:HIS:HE1	6	1.87
(1,1019)	1:524:A:HIS:H	1:525:A:TYR:HD1	8	1.83
(1,771)	1:457:A:THR:HG21	1:478:A:SER:H	7	1.83
(1,771)	1:457:A:THR:HG22	1:478:A:SER:H	7	1.83
(1,771)	1:457:A:THR:HG23	1:478:A:SER:H	7	1.83
(1,302)	1:505:A:LYS:HB3	1:510:A:HIS:HE1	3	1.82
(1,318)	1:486:A:TRP:HD1	1:503:A:PHE:HE2	3	1.79
(1,318)	1:486:A:TRP:HD1	1:503:A:PHE:HE2	10	1.79
(1,1269)	1:519:A:LEU:HD11	1:540:A:VAL:HB	4	1.78
(1,1269)	1:519:A:LEU:HD12	1:540:A:VAL:HB	4	1.78
(1,1269)	1:519:A:LEU:HD13	1:540:A:VAL:HB	4	1.78
(1,1269)	1:519:A:LEU:HD21	1:540:A:VAL:HB	4	1.78
(1,1269)	1:519:A:LEU:HD22	1:540:A:VAL:HB	4	1.78
(1,1269)	1:519:A:LEU:HD23	1:540:A:VAL:HB	4	1.78
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD11	2	1.77
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD12	2	1.77
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD13	2	1.77
(1,323)	1:498:A:THR:HG21	1:501:A:TYR:HD1	10	1.75
(1,323)	1:498:A:THR:HG22	1:501:A:TYR:HD1	10	1.75
(1,323)	1:498:A:THR:HG23	1:501:A:TYR:HD1	10	1.75
(1,824)	1:456:A:ILE:HD11	1:533:A:GLN:H	5	1.74
(1,824)	1:456:A:ILE:HD12	1:533:A:GLN:H	5	1.74
(1,824)	1:456:A:ILE:HD13	1:533:A:GLN:H	5	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,427)	1:525:A:TYR:H	1:525:A:TYR:HD1	1	1.73
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD11	1	1.72
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD12	1	1.72
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD13	1	1.72
(1,84)	1:458:A:ARG:HB2	1:476:A:GLU:HG2	6	1.71
(1,84)	1:458:A:ARG:HB3	1:476:A:GLU:HG2	6	1.71
(1,312)	1:502:A:TRP:HD1	1:515:A:ASN:HD21	8	1.69
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD11	6	1.69
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD12	6	1.69
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD13	6	1.69
(1,312)	1:502:A:TRP:HD1	1:515:A:ASN:HD21	4	1.68
(1,556)	1:488:A:LYS:HD3	1:491:A:VAL:H	2	1.67
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD21	5	1.67
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD22	5	1.67
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD23	5	1.67
(1,818)	1:523:A:GLY:H	1:538:A:LEU:HB3	7	1.65
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD11	9	1.65
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD12	9	1.65
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD13	9	1.65
(1,312)	1:502:A:TRP:HD1	1:515:A:ASN:HD21	6	1.64
(1,515)	1:525:A:TYR:HD1	1:538:A:LEU:H	5	1.63
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD21	1	1.63
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD22	1	1.63
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD23	1	1.63
(1,421)	1:525:A:TYR:H	1:536:A:ALA:H	7	1.62
(1,101)	1:457:A:THR:HG21	1:478:A:SER:HA	7	1.62
(1,101)	1:457:A:THR:HG22	1:478:A:SER:HA	7	1.62
(1,101)	1:457:A:THR:HG23	1:478:A:SER:HA	7	1.62
(1,1032)	1:529:A:THR:H	1:532:A:GLY:H	1	1.59
(1,200)	1:514:A:ILE:HD11	1:521:A:ASP:HB2	5	1.59
(1,200)	1:514:A:ILE:HD12	1:521:A:ASP:HB2	5	1.59
(1,200)	1:514:A:ILE:HD13	1:521:A:ASP:HB2	5	1.59
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD11	4	1.59
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD12	4	1.59
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD13	4	1.59
(1,556)	1:488:A:LYS:HD3	1:491:A:VAL:H	4	1.58
(1,1269)	1:519:A:LEU:HD11	1:540:A:VAL:HB	7	1.57
(1,1269)	1:519:A:LEU:HD12	1:540:A:VAL:HB	7	1.57
(1,1269)	1:519:A:LEU:HD13	1:540:A:VAL:HB	7	1.57
(1,1269)	1:519:A:LEU:HD21	1:540:A:VAL:HB	7	1.57
(1,1269)	1:519:A:LEU:HD22	1:540:A:VAL:HB	7	1.57
(1,1269)	1:519:A:LEU:HD23	1:540:A:VAL:HB	7	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,818)	1:523:A:GLY:H	1:538:A:LEU:HB3	4	1.57
(1,771)	1:457:A:THR:HG21	1:478:A:SER:H	2	1.56
(1,771)	1:457:A:THR:HG22	1:478:A:SER:H	2	1.56
(1,771)	1:457:A:THR:HG23	1:478:A:SER:H	2	1.56
(1,771)	1:457:A:THR:HG21	1:478:A:SER:H	10	1.56
(1,771)	1:457:A:THR:HG22	1:478:A:SER:H	10	1.56
(1,771)	1:457:A:THR:HG23	1:478:A:SER:H	10	1.56
(1,763)	1:502:A:TRP:HD1	1:515:A:ASN:HD22	3	1.56
(1,427)	1:525:A:TYR:H	1:525:A:TYR:HD1	10	1.54
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD21	1	1.54
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD22	1	1.54
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD23	1	1.54
(1,515)	1:525:A:TYR:HD1	1:538:A:LEU:H	10	1.53
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD11	8	1.52
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD12	8	1.52
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD13	8	1.52
(1,427)	1:525:A:TYR:H	1:525:A:TYR:HD1	2	1.51
(1,359)	1:488:A:LYS:HD3	1:489:A:ASP:H	4	1.51
(1,427)	1:525:A:TYR:H	1:525:A:TYR:HD1	8	1.5
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD11	5	1.5
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD12	5	1.5
(1,166)	1:503:A:PHE:HD2	1:512:A:LEU:HD13	5	1.5
(1,359)	1:488:A:LYS:HD3	1:489:A:ASP:H	2	1.49
(1,165)	1:501:A:TYR:HE2	1:512:A:LEU:HD11	10	1.48
(1,165)	1:501:A:TYR:HE2	1:512:A:LEU:HD12	10	1.48
(1,165)	1:501:A:TYR:HE2	1:512:A:LEU:HD13	10	1.48
(1,726)	1:492:A:GLU:HG2	1:494:A:THR:H	3	1.46
(1,726)	1:492:A:GLU:HG3	1:494:A:THR:H	3	1.46
(1,455)	1:505:A:LYS:HD2	1:506:A:ASP:H	7	1.46
(1,455)	1:505:A:LYS:HD3	1:506:A:ASP:H	7	1.46
(1,819)	1:523:A:GLY:H	1:538:A:LEU:HG	10	1.45
(1,352)	1:464:A:LEU:HB2	1:539:A:ILE:H	5	1.45
(1,318)	1:486:A:TRP:HD1	1:503:A:PHE:HE2	9	1.45
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD21	8	1.45
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD22	8	1.45
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD23	8	1.45
(1,1042)	1:459:A:PRO:HB2	1:535:A:LEU:H	6	1.44
(1,1042)	1:459:A:PRO:HB3	1:535:A:LEU:H	6	1.44
(1,556)	1:488:A:LYS:HD3	1:491:A:VAL:H	9	1.44
(1,819)	1:523:A:GLY:H	1:538:A:LEU:HG	4	1.43
(1,645)	1:500:A:LYS:H	1:501:A:TYR:HD1	10	1.43
(1,386)	1:486:A:TRP:HE1	1:510:A:HIS:HB2	8	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,434)	1:456:A:ILE:HD11	1:534:A:ALA:H	8	1.41
(1,434)	1:456:A:ILE:HD12	1:534:A:ALA:H	8	1.41
(1,434)	1:456:A:ILE:HD13	1:534:A:ALA:H	8	1.41
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG2	2	1.41
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG3	2	1.41
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD21	10	1.4
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD22	10	1.4
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD23	10	1.4
(1,427)	1:525:A:TYR:H	1:525:A:TYR:HD1	4	1.39
(1,819)	1:523:A:GLY:H	1:538:A:LEU:HG	3	1.38
(1,819)	1:523:A:GLY:H	1:538:A:LEU:HG	5	1.38
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG2	6	1.38
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG3	6	1.38
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD21	7	1.38
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD22	7	1.38
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD23	7	1.38
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD21	8	1.38
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD22	8	1.38
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD23	8	1.38
(1,224)	1:519:A:LEU:HA	1:540:A:VAL:HB	6	1.38
(1,427)	1:525:A:TYR:H	1:525:A:TYR:HD1	5	1.37
(1,344)	1:526:A:ALA:HB1	1:535:A:LEU:HG	2	1.37
(1,344)	1:526:A:ALA:HB2	1:535:A:LEU:HG	2	1.37
(1,344)	1:526:A:ALA:HB3	1:535:A:LEU:HG	2	1.37
(1,319)	1:486:A:TRP:HD1	1:503:A:PHE:HD2	5	1.37
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD21	10	1.37
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD22	10	1.37
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD23	10	1.37
(1,821)	1:523:A:GLY:H	1:540:A:VAL:HG21	6	1.36
(1,821)	1:523:A:GLY:H	1:540:A:VAL:HG22	6	1.36
(1,821)	1:523:A:GLY:H	1:540:A:VAL:HG23	6	1.36
(1,760)	1:465:A:VAL:HA	1:469:A:GLN:HE21	5	1.36
(1,1046)	1:524:A:HIS:H	1:538:A:LEU:H	10	1.35
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG21	6	1.35
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG22	6	1.35
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG23	6	1.35
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG2	3	1.35
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG3	3	1.35
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG2	8	1.35
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG3	8	1.35
(1,257)	1:454:A:VAL:HB	1:529:A:THR:HB	7	1.35
(1,1156)	1:473:A:PHE:HB2	1:486:A:TRP:HZ2	1	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1156)	1:473:A:PHE:HB3	1:486:A:TRP:HZ2	1	1.34
(1,802)	1:523:A:GLY:H	1:539:A:ILE:HA	9	1.34
(1,359)	1:488:A:LYS:HD3	1:489:A:ASP:H	9	1.34
(1,624)	1:462:A:ASP:HB3	1:537:A:GLU:H	9	1.33
(1,624)	1:462:A:ASP:HB2	1:537:A:GLU:H	9	1.33
(1,307)	1:505:A:LYS:HD2	1:510:A:HIS:HE1	10	1.33
(1,307)	1:505:A:LYS:HD3	1:510:A:HIS:HE1	10	1.33
(1,258)	1:501:A:TYR:HD1	1:502:A:TRP:HA	2	1.33
(1,258)	1:501:A:TYR:HD1	1:502:A:TRP:HA	9	1.33
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD21	3	1.33
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD22	3	1.33
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD23	3	1.33
(1,258)	1:501:A:TYR:HD1	1:502:A:TRP:HA	7	1.32
(1,258)	1:501:A:TYR:HD1	1:502:A:TRP:HA	8	1.32
(1,824)	1:456:A:ILE:HD11	1:533:A:GLN:H	3	1.31
(1,824)	1:456:A:ILE:HD12	1:533:A:GLN:H	3	1.31
(1,824)	1:456:A:ILE:HD13	1:533:A:GLN:H	3	1.31
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB2	4	1.31
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB3	4	1.31
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD21	2	1.31
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD22	2	1.31
(1,299)	1:525:A:TYR:HD1	1:538:A:LEU:HD23	2	1.31
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD21	2	1.31
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD22	2	1.31
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD23	2	1.31
(1,258)	1:501:A:TYR:HD1	1:502:A:TRP:HA	6	1.31
(1,1227)	1:500:A:LYS:HE2	1:518:A:MET:HG2	1	1.3
(1,1227)	1:500:A:LYS:HE2	1:518:A:MET:HG3	1	1.3
(1,1227)	1:500:A:LYS:HE3	1:518:A:MET:HG2	1	1.3
(1,1227)	1:500:A:LYS:HE3	1:518:A:MET:HG3	1	1.3
(1,514)	1:523:A:GLY:HA2	1:538:A:LEU:H	7	1.3
(1,802)	1:523:A:GLY:H	1:539:A:ILE:HA	5	1.29
(1,319)	1:486:A:TRP:HD1	1:503:A:PHE:HD2	3	1.29
(1,258)	1:501:A:TYR:HD1	1:502:A:TRP:HA	3	1.29
(1,258)	1:501:A:TYR:HD1	1:502:A:TRP:HA	4	1.29
(1,258)	1:501:A:TYR:HD1	1:502:A:TRP:HA	5	1.29
(1,77)	1:471:A:VAL:HA	1:472:A:GLU:HG2	2	1.29
(1,77)	1:471:A:VAL:HA	1:472:A:GLU:HG3	2	1.29
(1,258)	1:501:A:TYR:HD1	1:502:A:TRP:HA	1	1.28
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD11	10	1.27
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD12	10	1.27
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD13	10	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD21	10	1.27
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD22	10	1.27
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD23	10	1.27
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD11	10	1.27
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD12	10	1.27
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD13	10	1.27
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD21	10	1.27
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD22	10	1.27
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD23	10	1.27
(1,434)	1:456:A:ILE:HD11	1:534:A:ALA:H	2	1.27
(1,434)	1:456:A:ILE:HD12	1:534:A:ALA:H	2	1.27
(1,434)	1:456:A:ILE:HD13	1:534:A:ALA:H	2	1.27
(1,284)	1:522:A:ALA:HA	1:540:A:VAL:HG21	6	1.27
(1,284)	1:522:A:ALA:HA	1:540:A:VAL:HG22	6	1.27
(1,284)	1:522:A:ALA:HA	1:540:A:VAL:HG23	6	1.27
(1,308)	1:505:A:LYS:HE2	1:510:A:HIS:HE1	8	1.26
(1,308)	1:505:A:LYS:HE3	1:510:A:HIS:HE1	8	1.26
(1,128)	1:453:A:PRO:HB2	1:531:A:GLY:HA2	8	1.26
(1,448)	1:472:A:GLU:H	1:473:A:PHE:HD1	6	1.25
(1,325)	1:472:A:GLU:HG2	1:513:A:ILE:HD11	8	1.25
(1,325)	1:472:A:GLU:HG2	1:513:A:ILE:HD12	8	1.25
(1,325)	1:472:A:GLU:HG2	1:513:A:ILE:HD13	8	1.25
(1,325)	1:472:A:GLU:HG3	1:513:A:ILE:HD11	8	1.25
(1,325)	1:472:A:GLU:HG3	1:513:A:ILE:HD12	8	1.25
(1,325)	1:472:A:GLU:HG3	1:513:A:ILE:HD13	8	1.25
(1,323)	1:498:A:THR:HG21	1:501:A:TYR:HD1	8	1.25
(1,323)	1:498:A:THR:HG22	1:501:A:TYR:HD1	8	1.25
(1,323)	1:498:A:THR:HG23	1:501:A:TYR:HD1	8	1.25
(1,308)	1:505:A:LYS:HE2	1:510:A:HIS:HE1	9	1.25
(1,308)	1:505:A:LYS:HE3	1:510:A:HIS:HE1	9	1.25
(1,819)	1:523:A:GLY:H	1:538:A:LEU:HG	6	1.24
(1,448)	1:472:A:GLU:H	1:473:A:PHE:HD1	2	1.24
(1,448)	1:472:A:GLU:H	1:473:A:PHE:HD1	5	1.24
(1,352)	1:464:A:LEU:HB2	1:539:A:ILE:H	9	1.24
(1,1146)	1:471:A:VAL:HG11	1:473:A:PHE:HD1	8	1.23
(1,1146)	1:471:A:VAL:HG12	1:473:A:PHE:HD1	8	1.23
(1,1146)	1:471:A:VAL:HG13	1:473:A:PHE:HD1	8	1.23
(1,1146)	1:471:A:VAL:HG21	1:473:A:PHE:HD1	8	1.23
(1,1146)	1:471:A:VAL:HG22	1:473:A:PHE:HD1	8	1.23
(1,1146)	1:471:A:VAL:HG23	1:473:A:PHE:HD1	8	1.23
(1,1032)	1:529:A:THR:H	1:532:A:GLY:H	5	1.23
(1,1012)	1:522:A:ALA:H	1:538:A:LEU:HG	3	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,824)	1:456:A:ILE:HD11	1:533:A:GLN:H	7	1.23
(1,824)	1:456:A:ILE:HD12	1:533:A:GLN:H	7	1.23
(1,824)	1:456:A:ILE:HD13	1:533:A:GLN:H	7	1.23
(1,771)	1:457:A:THR:HG21	1:478:A:SER:H	1	1.23
(1,771)	1:457:A:THR:HG22	1:478:A:SER:H	1	1.23
(1,771)	1:457:A:THR:HG23	1:478:A:SER:H	1	1.23
(1,448)	1:472:A:GLU:H	1:473:A:PHE:HD1	1	1.23
(1,1220)	1:497:A:GLU:HG2	1:500:A:LYS:H	1	1.22
(1,1220)	1:497:A:GLU:HG3	1:500:A:LYS:H	1	1.22
(1,824)	1:456:A:ILE:HD11	1:533:A:GLN:H	9	1.22
(1,824)	1:456:A:ILE:HD12	1:533:A:GLN:H	9	1.22
(1,824)	1:456:A:ILE:HD13	1:533:A:GLN:H	9	1.22
(1,448)	1:472:A:GLU:H	1:473:A:PHE:HD1	3	1.22
(1,448)	1:472:A:GLU:H	1:473:A:PHE:HD1	7	1.22
(1,448)	1:472:A:GLU:H	1:473:A:PHE:HD1	10	1.22
(1,1046)	1:524:A:HIS:H	1:538:A:LEU:H	6	1.21
(1,319)	1:486:A:TRP:HD1	1:503:A:PHE:HD2	1	1.21
(1,1235)	1:504:A:LYS:HG2	1:513:A:ILE:HD11	1	1.2
(1,1235)	1:504:A:LYS:HG2	1:513:A:ILE:HD12	1	1.2
(1,1235)	1:504:A:LYS:HG2	1:513:A:ILE:HD13	1	1.2
(1,1235)	1:504:A:LYS:HG3	1:513:A:ILE:HD11	1	1.2
(1,1235)	1:504:A:LYS:HG3	1:513:A:ILE:HD12	1	1.2
(1,1235)	1:504:A:LYS:HG3	1:513:A:ILE:HD13	1	1.2
(1,771)	1:457:A:THR:HG21	1:478:A:SER:H	6	1.2
(1,771)	1:457:A:THR:HG22	1:478:A:SER:H	6	1.2
(1,771)	1:457:A:THR:HG23	1:478:A:SER:H	6	1.2
(1,767)	1:501:A:TYR:HA	1:515:A:ASN:HD22	3	1.2
(1,427)	1:525:A:TYR:H	1:525:A:TYR:HD1	7	1.2
(1,1220)	1:497:A:GLU:HG2	1:500:A:LYS:H	2	1.19
(1,1220)	1:497:A:GLU:HG3	1:500:A:LYS:H	2	1.19
(1,1046)	1:524:A:HIS:H	1:538:A:LEU:H	5	1.19
(1,819)	1:523:A:GLY:H	1:538:A:LEU:HG	7	1.19
(1,802)	1:523:A:GLY:H	1:539:A:ILE:HA	1	1.19
(1,1248)	1:509:A:ARG:HB2	1:511:A:HIS:HE1	7	1.18
(1,1248)	1:509:A:ARG:HB3	1:511:A:HIS:HE1	7	1.18
(1,1240)	1:505:A:LYS:HB2	1:510:A:HIS:HE1	3	1.18
(1,1240)	1:505:A:LYS:HB3	1:510:A:HIS:HE1	3	1.18
(1,1189)	1:487:A:LEU:HD11	1:493:A:LEU:H	2	1.18
(1,1189)	1:487:A:LEU:HD12	1:493:A:LEU:H	2	1.18
(1,1189)	1:487:A:LEU:HD13	1:493:A:LEU:H	2	1.18
(1,1189)	1:487:A:LEU:HD21	1:493:A:LEU:H	2	1.18
(1,1189)	1:487:A:LEU:HD22	1:493:A:LEU:H	2	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1189)	1:487:A:LEU:HD23	1:493:A:LEU:H	2	1.18
(1,1098)	1:460:A:LEU:HD11	1:486:A:TRP:HZ2	9	1.18
(1,1098)	1:460:A:LEU:HD12	1:486:A:TRP:HZ2	9	1.18
(1,1098)	1:460:A:LEU:HD13	1:486:A:TRP:HZ2	9	1.18
(1,1098)	1:460:A:LEU:HD21	1:486:A:TRP:HZ2	9	1.18
(1,1098)	1:460:A:LEU:HD22	1:486:A:TRP:HZ2	9	1.18
(1,1098)	1:460:A:LEU:HD23	1:486:A:TRP:HZ2	9	1.18
(1,1046)	1:524:A:HIS:H	1:538:A:LEU:H	3	1.17
(1,318)	1:486:A:TRP:HD1	1:503:A:PHE:HE2	5	1.17
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD21	5	1.17
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD22	5	1.17
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD23	5	1.17
(1,1046)	1:524:A:HIS:H	1:538:A:LEU:H	2	1.16
(1,760)	1:465:A:VAL:HA	1:469:A:GLN:HE21	7	1.16
(1,641)	1:479:A:GLU:HG2	1:482:A:ALA:H	2	1.16
(1,641)	1:479:A:GLU:HG3	1:482:A:ALA:H	2	1.16
(1,344)	1:526:A:ALA:HB1	1:535:A:LEU:HG	4	1.16
(1,344)	1:526:A:ALA:HB2	1:535:A:LEU:HG	4	1.16
(1,344)	1:526:A:ALA:HB3	1:535:A:LEU:HG	4	1.16
(1,306)	1:505:A:LYS:HG2	1:510:A:HIS:HE1	7	1.16
(1,306)	1:505:A:LYS:HG3	1:510:A:HIS:HE1	7	1.16
(1,328)	1:503:A:PHE:HB2	1:513:A:ILE:HD11	2	1.15
(1,328)	1:503:A:PHE:HB2	1:513:A:ILE:HD12	2	1.15
(1,328)	1:503:A:PHE:HB2	1:513:A:ILE:HD13	2	1.15
(1,1024)	1:460:A:LEU:HB2	1:525:A:TYR:H	8	1.14
(1,1024)	1:460:A:LEU:HB3	1:525:A:TYR:H	8	1.14
(1,966)	1:511:A:HIS:H	1:513:A:ILE:HD11	8	1.14
(1,966)	1:511:A:HIS:H	1:513:A:ILE:HD12	8	1.14
(1,966)	1:511:A:HIS:H	1:513:A:ILE:HD13	8	1.14
(1,628)	1:462:A:ASP:H	1:537:A:GLU:H	1	1.14
(1,319)	1:486:A:TRP:HD1	1:503:A:PHE:HD2	8	1.14
(1,1046)	1:524:A:HIS:H	1:538:A:LEU:H	8	1.13
(1,824)	1:456:A:ILE:HD11	1:533:A:GLN:H	6	1.13
(1,824)	1:456:A:ILE:HD12	1:533:A:GLN:H	6	1.13
(1,824)	1:456:A:ILE:HD13	1:533:A:GLN:H	6	1.13
(1,319)	1:486:A:TRP:HD1	1:503:A:PHE:HD2	10	1.13
(1,1283)	1:526:A:ALA:HB1	1:533:A:GLN:HE21	8	1.12
(1,1283)	1:526:A:ALA:HB1	1:533:A:GLN:HE22	8	1.12
(1,1283)	1:526:A:ALA:HB2	1:533:A:GLN:HE21	8	1.12
(1,1283)	1:526:A:ALA:HB2	1:533:A:GLN:HE22	8	1.12
(1,1283)	1:526:A:ALA:HB3	1:533:A:GLN:HE21	8	1.12
(1,1283)	1:526:A:ALA:HB3	1:533:A:GLN:HE22	8	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,819)	1:523:A:GLY:H	1:538:A:LEU:HG	1	1.12
(1,647)	1:498:A:THR:HB	1:500:A:LYS:H	8	1.12
(1,328)	1:503:A:PHE:HB2	1:513:A:ILE:HD11	8	1.12
(1,328)	1:503:A:PHE:HB2	1:513:A:ILE:HD12	8	1.12
(1,328)	1:503:A:PHE:HB2	1:513:A:ILE:HD13	8	1.12
(1,76)	1:472:A:GLU:HG2	1:513:A:ILE:HG13	8	1.12
(1,76)	1:472:A:GLU:HG3	1:513:A:ILE:HG13	8	1.12
(1,302)	1:505:A:LYS:HB3	1:510:A:HIS:HE1	2	1.11
(1,1012)	1:522:A:ALA:H	1:538:A:LEU:HG	1	1.1
(1,897)	1:459:A:PRO:HA	1:476:A:GLU:H	9	1.1
(1,784)	1:476:A:GLU:HG3	1:508:A:GLN:HE22	2	1.1
(1,463)	1:473:A:PHE:H	1:511:A:HIS:HA	9	1.1
(1,386)	1:486:A:TRP:HE1	1:510:A:HIS:HB2	4	1.1
(1,287)	1:538:A:LEU:HB3	1:540:A:VAL:HG21	6	1.1
(1,287)	1:538:A:LEU:HB3	1:540:A:VAL:HG22	6	1.1
(1,287)	1:538:A:LEU:HB3	1:540:A:VAL:HG23	6	1.1
(1,101)	1:457:A:THR:HG21	1:478:A:SER:HA	2	1.1
(1,101)	1:457:A:THR:HG22	1:478:A:SER:HA	2	1.1
(1,101)	1:457:A:THR:HG23	1:478:A:SER:HA	2	1.1
(1,59)	1:468:A:GLY:HA3	1:516:A:GLU:HG2	8	1.1
(1,59)	1:468:A:GLY:HA3	1:516:A:GLU:HG3	8	1.1
(1,29)	1:456:A:ILE:HD11	1:533:A:GLN:HA	2	1.1
(1,29)	1:456:A:ILE:HD12	1:533:A:GLN:HA	2	1.1
(1,29)	1:456:A:ILE:HD13	1:533:A:GLN:HA	2	1.1
(1,156)	1:505:A:LYS:HE2	1:506:A:ASP:HA	7	1.09
(1,156)	1:505:A:LYS:HE3	1:506:A:ASP:HA	7	1.09
(1,59)	1:468:A:GLY:HA3	1:516:A:GLU:HG2	4	1.09
(1,59)	1:468:A:GLY:HA3	1:516:A:GLU:HG3	4	1.09
(1,1269)	1:519:A:LEU:HD11	1:540:A:VAL:HB	6	1.08
(1,1269)	1:519:A:LEU:HD12	1:540:A:VAL:HB	6	1.08
(1,1269)	1:519:A:LEU:HD13	1:540:A:VAL:HB	6	1.08
(1,1269)	1:519:A:LEU:HD21	1:540:A:VAL:HB	6	1.08
(1,1269)	1:519:A:LEU:HD22	1:540:A:VAL:HB	6	1.08
(1,1269)	1:519:A:LEU:HD23	1:540:A:VAL:HB	6	1.08
(1,970)	1:470:A:ARG:HA	1:514:A:ILE:H	7	1.08
(1,765)	1:502:A:TRP:HZ2	1:515:A:ASN:HD22	3	1.08
(1,238)	1:522:A:ALA:HB1	1:540:A:VAL:HG21	6	1.08
(1,238)	1:522:A:ALA:HB1	1:540:A:VAL:HG22	6	1.08
(1,238)	1:522:A:ALA:HB1	1:540:A:VAL:HG23	6	1.08
(1,238)	1:522:A:ALA:HB2	1:540:A:VAL:HG21	6	1.08
(1,238)	1:522:A:ALA:HB2	1:540:A:VAL:HG22	6	1.08
(1,238)	1:522:A:ALA:HB2	1:540:A:VAL:HG23	6	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,238)	1:522:A:ALA:HB3	1:540:A:VAL:HG21	6	1.08
(1,238)	1:522:A:ALA:HB3	1:540:A:VAL:HG22	6	1.08
(1,238)	1:522:A:ALA:HB3	1:540:A:VAL:HG23	6	1.08
(1,1225)	1:500:A:LYS:HE2	1:514:A:ILE:HG21	8	1.07
(1,1225)	1:500:A:LYS:HE2	1:514:A:ILE:HG22	8	1.07
(1,1225)	1:500:A:LYS:HE2	1:514:A:ILE:HG23	8	1.07
(1,1225)	1:500:A:LYS:HE3	1:514:A:ILE:HG21	8	1.07
(1,1225)	1:500:A:LYS:HE3	1:514:A:ILE:HG22	8	1.07
(1,1225)	1:500:A:LYS:HE3	1:514:A:ILE:HG23	8	1.07
(1,1121)	1:466:A:MET:HB2	1:469:A:GLN:HG2	5	1.07
(1,1121)	1:466:A:MET:HB2	1:469:A:GLN:HG3	5	1.07
(1,1121)	1:466:A:MET:HB3	1:469:A:GLN:HG2	5	1.07
(1,1121)	1:466:A:MET:HB3	1:469:A:GLN:HG3	5	1.07
(1,897)	1:459:A:PRO:HA	1:476:A:GLU:H	7	1.07
(1,784)	1:476:A:GLU:HG3	1:508:A:GLN:HE22	3	1.07
(1,308)	1:505:A:LYS:HE2	1:510:A:HIS:HE1	5	1.07
(1,308)	1:505:A:LYS:HE3	1:510:A:HIS:HE1	5	1.07
(1,294)	1:474:A:GLU:HA	1:486:A:TRP:HZ2	4	1.07
(1,294)	1:474:A:GLU:HA	1:486:A:TRP:HZ2	6	1.07
(1,1254)	1:514:A:ILE:HD11	1:521:A:ASP:HB2	5	1.06
(1,1254)	1:514:A:ILE:HD11	1:521:A:ASP:HB3	5	1.06
(1,1254)	1:514:A:ILE:HD12	1:521:A:ASP:HB2	5	1.06
(1,1254)	1:514:A:ILE:HD12	1:521:A:ASP:HB3	5	1.06
(1,1254)	1:514:A:ILE:HD13	1:521:A:ASP:HB2	5	1.06
(1,1254)	1:514:A:ILE:HD13	1:521:A:ASP:HB3	5	1.06
(1,1042)	1:459:A:PRO:HB2	1:535:A:LEU:H	5	1.06
(1,1042)	1:459:A:PRO:HB3	1:535:A:LEU:H	5	1.06
(1,819)	1:523:A:GLY:H	1:538:A:LEU:HG	2	1.06
(1,628)	1:462:A:ASP:H	1:537:A:GLU:H	6	1.06
(1,628)	1:462:A:ASP:H	1:537:A:GLU:H	8	1.06
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD21	10	1.06
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD22	10	1.06
(1,296)	1:525:A:TYR:HE1	1:538:A:LEU:HD23	10	1.06
(1,802)	1:523:A:GLY:H	1:539:A:ILE:HA	3	1.05
(1,784)	1:476:A:GLU:HG3	1:508:A:GLN:HE22	5	1.05
(1,784)	1:476:A:GLU:HG3	1:508:A:GLN:HE22	8	1.05
(1,628)	1:462:A:ASP:H	1:537:A:GLU:H	2	1.05
(1,628)	1:462:A:ASP:H	1:537:A:GLU:H	5	1.05
(1,313)	1:502:A:TRP:HD1	1:503:A:PHE:HA	3	1.05
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD21	3	1.04
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD22	3	1.04
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD23	3	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,784)	1:476:A:GLU:HG3	1:508:A:GLN:HE22	9	1.04
(1,628)	1:462:A:ASP:H	1:537:A:GLU:H	7	1.04
(1,514)	1:523:A:GLY:HA2	1:538:A:LEU:H	4	1.04
(1,472)	1:472:A:GLU:HG2	1:512:A:LEU:H	8	1.04
(1,472)	1:472:A:GLU:HG3	1:512:A:LEU:H	8	1.04
(1,449)	1:463:A:GLN:HE22	1:472:A:GLU:H	7	1.04
(1,386)	1:486:A:TRP:HE1	1:510:A:HIS:HB2	5	1.04
(1,383)	1:486:A:TRP:HE1	1:511:A:HIS:H	7	1.04
(1,294)	1:474:A:GLU:HA	1:486:A:TRP:HZ2	2	1.04
(1,181)	1:470:A:ARG:HB3	1:513:A:ILE:HG21	7	1.04
(1,181)	1:470:A:ARG:HB3	1:513:A:ILE:HG22	7	1.04
(1,181)	1:470:A:ARG:HB3	1:513:A:ILE:HG23	7	1.04
(1,1021)	1:488:A:LYS:HG3	1:524:A:HIS:H	3	1.03
(1,918)	1:486:A:TRP:HE1	1:504:A:LYS:H	2	1.03
(1,918)	1:486:A:TRP:HE1	1:504:A:LYS:H	3	1.03
(1,911)	1:458:A:ARG:H	1:478:A:SER:H	7	1.03
(1,818)	1:523:A:GLY:H	1:538:A:LEU:HB3	3	1.03
(1,817)	1:523:A:GLY:H	1:540:A:VAL:HB	5	1.03
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG21	8	1.03
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG22	8	1.03
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG23	8	1.03
(1,249)	1:460:A:LEU:HG	1:526:A:ALA:HA	8	1.03
(1,1032)	1:529:A:THR:H	1:532:A:GLY:H	10	1.02
(1,918)	1:486:A:TRP:HE1	1:504:A:LYS:H	9	1.02
(1,760)	1:465:A:VAL:HA	1:469:A:GLN:HE21	3	1.02
(1,747)	1:460:A:LEU:H	1:534:A:ALA:HA	6	1.02
(1,628)	1:462:A:ASP:H	1:537:A:GLU:H	4	1.02
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD11	10	1.02
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD12	10	1.02
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD13	10	1.02
(1,388)	1:486:A:TRP:HE1	1:510:A:HIS:HA	7	1.02
(1,313)	1:502:A:TRP:HD1	1:503:A:PHE:HA	5	1.02
(1,313)	1:502:A:TRP:HD1	1:503:A:PHE:HA	7	1.02
(1,313)	1:502:A:TRP:HD1	1:503:A:PHE:HA	9	1.02
(1,313)	1:502:A:TRP:HD1	1:503:A:PHE:HA	10	1.02
(1,50)	1:465:A:VAL:HG11	1:471:A:VAL:HB	7	1.02
(1,50)	1:465:A:VAL:HG12	1:471:A:VAL:HB	7	1.02
(1,50)	1:465:A:VAL:HG13	1:471:A:VAL:HB	7	1.02
(1,1156)	1:473:A:PHE:HB2	1:486:A:TRP:HZ2	9	1.01
(1,1156)	1:473:A:PHE:HB3	1:486:A:TRP:HZ2	9	1.01
(1,911)	1:458:A:ARG:H	1:478:A:SER:H	3	1.01
(1,897)	1:459:A:PRO:HA	1:476:A:GLU:H	10	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,784)	1:476:A:GLU:HG3	1:508:A:GLN:HE22	7	1.01
(1,628)	1:462:A:ASP:H	1:537:A:GLU:H	10	1.01
(1,449)	1:463:A:GLN:HE22	1:472:A:GLU:H	9	1.01
(1,383)	1:486:A:TRP:HE1	1:511:A:HIS:H	8	1.01
(1,1042)	1:459:A:PRO:HB2	1:535:A:LEU:H	10	1.0
(1,1042)	1:459:A:PRO:HB3	1:535:A:LEU:H	10	1.0
(1,764)	1:515:A:ASN:H	1:515:A:ASN:HD22	3	1.0
(1,742)	1:468:A:GLY:H	1:516:A:GLU:HG2	6	1.0
(1,742)	1:468:A:GLY:H	1:516:A:GLU:HG3	6	1.0
(1,449)	1:463:A:GLN:HE22	1:472:A:GLU:H	5	1.0
(1,388)	1:486:A:TRP:HE1	1:510:A:HIS:HA	4	1.0
(1,383)	1:486:A:TRP:HE1	1:511:A:HIS:H	1	1.0
(1,383)	1:486:A:TRP:HE1	1:511:A:HIS:H	4	1.0
(1,319)	1:486:A:TRP:HD1	1:503:A:PHE:HD2	4	1.0
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG21	7	1.0
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG22	7	1.0
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG23	7	1.0
(1,120)	1:525:A:TYR:HB2	1:536:A:ALA:HB1	7	1.0
(1,120)	1:525:A:TYR:HB2	1:536:A:ALA:HB2	7	1.0
(1,120)	1:525:A:TYR:HB2	1:536:A:ALA:HB3	7	1.0
(1,115)	1:484:A:VAL:HG11	1:510:A:HIS:H	1	1.0
(1,115)	1:484:A:VAL:HG12	1:510:A:HIS:H	1	1.0
(1,115)	1:484:A:VAL:HG13	1:510:A:HIS:H	1	1.0
(1,115)	1:484:A:VAL:HG11	1:510:A:HIS:H	8	1.0
(1,115)	1:484:A:VAL:HG12	1:510:A:HIS:H	8	1.0
(1,115)	1:484:A:VAL:HG13	1:510:A:HIS:H	8	1.0
(1,1021)	1:488:A:LYS:HG3	1:524:A:HIS:H	10	0.99
(1,911)	1:458:A:ARG:H	1:478:A:SER:H	5	0.99
(1,388)	1:486:A:TRP:HE1	1:510:A:HIS:HA	1	0.99
(1,312)	1:502:A:TRP:HD1	1:515:A:ASN:HD21	3	0.99
(1,101)	1:457:A:THR:HG21	1:478:A:SER:HA	10	0.99
(1,101)	1:457:A:THR:HG22	1:478:A:SER:HA	10	0.99
(1,101)	1:457:A:THR:HG23	1:478:A:SER:HA	10	0.99
(1,886)	1:475:A:CYS:H	1:509:A:ARG:HA	9	0.98
(1,525)	1:525:A:TYR:HA	1:536:A:ALA:H	7	0.98
(1,313)	1:502:A:TRP:HD1	1:503:A:PHE:HA	1	0.98
(1,286)	1:521:A:ASP:HB2	1:540:A:VAL:HG21	9	0.98
(1,286)	1:521:A:ASP:HB2	1:540:A:VAL:HG22	9	0.98
(1,286)	1:521:A:ASP:HB2	1:540:A:VAL:HG23	9	0.98
(1,1262)	1:518:A:MET:HB2	1:520:A:GLU:HB2	3	0.97
(1,1262)	1:518:A:MET:HB2	1:520:A:GLU:HB3	3	0.97
(1,1262)	1:518:A:MET:HB3	1:520:A:GLU:HB2	3	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1262)	1:518:A:MET:HB3	1:520:A:GLU:HB3	3	0.97
(1,1042)	1:459:A:PRO:HB2	1:535:A:LEU:H	9	0.97
(1,1042)	1:459:A:PRO:HB3	1:535:A:LEU:H	9	0.97
(1,1021)	1:488:A:LYS:HG3	1:524:A:HIS:H	8	0.97
(1,966)	1:511:A:HIS:H	1:513:A:ILE:HD11	2	0.97
(1,966)	1:511:A:HIS:H	1:513:A:ILE:HD12	2	0.97
(1,966)	1:511:A:HIS:H	1:513:A:ILE:HD13	2	0.97
(1,628)	1:462:A:ASP:H	1:537:A:GLU:H	9	0.97
(1,1024)	1:460:A:LEU:HB2	1:525:A:TYR:H	5	0.96
(1,1024)	1:460:A:LEU:HB3	1:525:A:TYR:H	5	0.96
(1,985)	1:470:A:ARG:HB2	1:516:A:GLU:H	10	0.96
(1,771)	1:457:A:THR:HG21	1:478:A:SER:H	8	0.96
(1,771)	1:457:A:THR:HG22	1:478:A:SER:H	8	0.96
(1,771)	1:457:A:THR:HG23	1:478:A:SER:H	8	0.96
(1,735)	1:454:A:VAL:HB	1:530:A:SER:H	7	0.96
(1,608)	1:458:A:ARG:H	1:476:A:GLU:HG2	6	0.96
(1,552)	1:486:A:TRP:H	1:492:A:GLU:HG2	9	0.96
(1,552)	1:486:A:TRP:H	1:492:A:GLU:HG3	9	0.96
(1,386)	1:486:A:TRP:HE1	1:510:A:HIS:HB2	1	0.96
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD11	3	0.96
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD12	3	0.96
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD13	3	0.96
(1,29)	1:456:A:ILE:HD11	1:533:A:GLN:HA	8	0.96
(1,29)	1:456:A:ILE:HD12	1:533:A:GLN:HA	8	0.96
(1,29)	1:456:A:ILE:HD13	1:533:A:GLN:HA	8	0.96
(1,1301)	1:533:A:GLN:HE21	1:535:A:LEU:HB2	10	0.95
(1,1301)	1:533:A:GLN:HE21	1:535:A:LEU:HB3	10	0.95
(1,1301)	1:533:A:GLN:HE22	1:535:A:LEU:HB2	10	0.95
(1,1301)	1:533:A:GLN:HE22	1:535:A:LEU:HB3	10	0.95
(1,906)	1:476:A:GLU:HG3	1:477:A:VAL:H	2	0.95
(1,906)	1:476:A:GLU:HG2	1:477:A:VAL:H	2	0.95
(1,891)	1:475:A:CYS:H	1:510:A:HIS:H	9	0.95
(1,719)	1:500:A:LYS:HD2	1:501:A:TYR:H	4	0.95
(1,719)	1:500:A:LYS:HD3	1:501:A:TYR:H	4	0.95
(1,699)	1:495:A:ARG:HD2	1:496:A:GLU:H	1	0.95
(1,699)	1:495:A:ARG:HD3	1:496:A:GLU:H	1	0.95
(1,642)	1:482:A:ALA:H	1:508:A:GLN:HB3	2	0.95
(1,642)	1:482:A:ALA:H	1:508:A:GLN:HB2	2	0.95
(1,470)	1:512:A:LEU:H	1:513:A:ILE:HD11	3	0.95
(1,470)	1:512:A:LEU:H	1:513:A:ILE:HD12	3	0.95
(1,470)	1:512:A:LEU:H	1:513:A:ILE:HD13	3	0.95
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG21	4	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG22	4	0.95
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG23	4	0.95
(1,28)	1:456:A:ILE:HD11	1:534:A:ALA:HA	8	0.95
(1,28)	1:456:A:ILE:HD12	1:534:A:ALA:HA	8	0.95
(1,28)	1:456:A:ILE:HD13	1:534:A:ALA:HA	8	0.95
(1,1262)	1:518:A:MET:HB2	1:520:A:GLU:HB2	9	0.94
(1,1262)	1:518:A:MET:HB2	1:520:A:GLU:HB3	9	0.94
(1,1262)	1:518:A:MET:HB3	1:520:A:GLU:HB2	9	0.94
(1,1262)	1:518:A:MET:HB3	1:520:A:GLU:HB3	9	0.94
(1,1196)	1:488:A:LYS:HE2	1:524:A:HIS:H	9	0.94
(1,1196)	1:488:A:LYS:HE3	1:524:A:HIS:H	9	0.94
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD11	8	0.94
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD12	8	0.94
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD13	8	0.94
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD21	8	0.94
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD22	8	0.94
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD23	8	0.94
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD11	8	0.94
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD12	8	0.94
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD13	8	0.94
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD21	8	0.94
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD22	8	0.94
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD23	8	0.94
(1,1012)	1:522:A:ALA:H	1:538:A:LEU:HG	10	0.94
(1,303)	1:509:A:ARG:HD2	1:511:A:HIS:HE1	3	0.94
(1,303)	1:509:A:ARG:HD3	1:511:A:HIS:HE1	3	0.94
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD21	10	0.93
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD22	10	0.93
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD23	10	0.93
(1,918)	1:486:A:TRP:HE1	1:504:A:LYS:H	1	0.93
(1,472)	1:472:A:GLU:HG2	1:512:A:LEU:H	1	0.93
(1,472)	1:472:A:GLU:HG3	1:512:A:LEU:H	1	0.93
(1,449)	1:463:A:GLN:HE22	1:472:A:GLU:H	4	0.93
(1,386)	1:486:A:TRP:HE1	1:510:A:HIS:HB2	9	0.93
(1,318)	1:486:A:TRP:HD1	1:503:A:PHE:HE2	4	0.93
(1,906)	1:476:A:GLU:HG3	1:477:A:VAL:H	5	0.92
(1,906)	1:476:A:GLU:HG2	1:477:A:VAL:H	5	0.92
(1,534)	1:470:A:ARG:HG2	1:515:A:ASN:H	8	0.92
(1,534)	1:470:A:ARG:HG3	1:515:A:ASN:H	8	0.92
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD11	3	0.92
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD12	3	0.92
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD13	3	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	1:486:A:TRP:HE1	1:510:A:HIS:HA	10	0.92
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB1	2	0.92
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB2	2	0.92
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB3	2	0.92
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB1	2	0.92
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB2	2	0.92
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB3	2	0.92
(1,272)	1:539:A:ILE:HG21	1:541:A:GLN:HG2	6	0.92
(1,272)	1:539:A:ILE:HG21	1:541:A:GLN:HG3	6	0.92
(1,272)	1:539:A:ILE:HG22	1:541:A:GLN:HG2	6	0.92
(1,272)	1:539:A:ILE:HG22	1:541:A:GLN:HG3	6	0.92
(1,272)	1:539:A:ILE:HG23	1:541:A:GLN:HG2	6	0.92
(1,272)	1:539:A:ILE:HG23	1:541:A:GLN:HG3	6	0.92
(1,193)	1:471:A:VAL:HB	1:514:A:ILE:HD11	5	0.92
(1,193)	1:471:A:VAL:HB	1:514:A:ILE:HD12	5	0.92
(1,193)	1:471:A:VAL:HB	1:514:A:ILE:HD13	5	0.92
(1,19)	1:457:A:THR:HG21	1:478:A:SER:HB2	7	0.92
(1,19)	1:457:A:THR:HG21	1:478:A:SER:HB3	7	0.92
(1,19)	1:457:A:THR:HG22	1:478:A:SER:HB2	7	0.92
(1,19)	1:457:A:THR:HG22	1:478:A:SER:HB3	7	0.92
(1,19)	1:457:A:THR:HG23	1:478:A:SER:HB2	7	0.92
(1,19)	1:457:A:THR:HG23	1:478:A:SER:HB3	7	0.92
(1,1270)	1:519:A:LEU:HD11	1:541:A:GLN:HA	4	0.91
(1,1270)	1:519:A:LEU:HD12	1:541:A:GLN:HA	4	0.91
(1,1270)	1:519:A:LEU:HD13	1:541:A:GLN:HA	4	0.91
(1,1270)	1:519:A:LEU:HD21	1:541:A:GLN:HA	4	0.91
(1,1270)	1:519:A:LEU:HD22	1:541:A:GLN:HA	4	0.91
(1,1270)	1:519:A:LEU:HD23	1:541:A:GLN:HA	4	0.91
(1,561)	1:487:A:LEU:HA	1:491:A:VAL:H	7	0.91
(1,421)	1:525:A:TYR:H	1:536:A:ALA:H	4	0.91
(1,1307)	1:539:A:ILE:HG21	1:541:A:GLN:HB2	5	0.9
(1,1307)	1:539:A:ILE:HG21	1:541:A:GLN:HB3	5	0.9
(1,1307)	1:539:A:ILE:HG22	1:541:A:GLN:HB2	5	0.9
(1,1307)	1:539:A:ILE:HG22	1:541:A:GLN:HB3	5	0.9
(1,1307)	1:539:A:ILE:HG23	1:541:A:GLN:HB2	5	0.9
(1,1307)	1:539:A:ILE:HG23	1:541:A:GLN:HB3	5	0.9
(1,802)	1:523:A:GLY:H	1:539:A:ILE:HA	6	0.9
(1,742)	1:468:A:GLY:H	1:516:A:GLU:HG2	9	0.9
(1,742)	1:468:A:GLY:H	1:516:A:GLU:HG3	9	0.9
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD11	10	0.89
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD12	10	0.89
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD13	10	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD21	10	0.89
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD22	10	0.89
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD23	10	0.89
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD11	10	0.89
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD12	10	0.89
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD13	10	0.89
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD21	10	0.89
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD22	10	0.89
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD23	10	0.89
(1,946)	1:503:A:PHE:H	1:513:A:ILE:HD11	8	0.89
(1,946)	1:503:A:PHE:H	1:513:A:ILE:HD12	8	0.89
(1,946)	1:503:A:PHE:H	1:513:A:ILE:HD13	8	0.89
(1,663)	1:474:A:GLU:H	1:486:A:TRP:HH2	4	0.89
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD11	1	0.89
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD12	1	0.89
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD13	1	0.89
(1,59)	1:468:A:GLY:HA3	1:516:A:GLU:HG2	9	0.89
(1,59)	1:468:A:GLY:HA3	1:516:A:GLU:HG3	9	0.89
(1,1287)	1:527:A:LEU:H	1:533:A:GLN:HB2	4	0.88
(1,1287)	1:527:A:LEU:H	1:533:A:GLN:HB3	4	0.88
(1,918)	1:486:A:TRP:HE1	1:504:A:LYS:H	5	0.88
(1,388)	1:486:A:TRP:HE1	1:510:A:HIS:HA	8	0.88
(1,1248)	1:509:A:ARG:HB2	1:511:A:HIS:HE1	3	0.87
(1,1248)	1:509:A:ARG:HB3	1:511:A:HIS:HE1	3	0.87
(1,1021)	1:488:A:LYS:HG3	1:524:A:HIS:H	1	0.87
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD21	10	0.87
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD22	10	0.87
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD23	10	0.87
(1,745)	1:468:A:GLY:H	1:540:A:VAL:HG11	6	0.87
(1,745)	1:468:A:GLY:H	1:540:A:VAL:HG12	6	0.87
(1,745)	1:468:A:GLY:H	1:540:A:VAL:HG13	6	0.87
(1,719)	1:500:A:LYS:HD2	1:501:A:TYR:H	3	0.87
(1,719)	1:500:A:LYS:HD3	1:501:A:TYR:H	3	0.87
(1,626)	1:462:A:ASP:HA	1:537:A:GLU:H	5	0.87
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD11	5	0.87
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD12	5	0.87
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD13	5	0.87
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG21	9	0.87
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG22	9	0.87
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG23	9	0.87
(1,59)	1:468:A:GLY:HA3	1:516:A:GLU:HG2	7	0.87
(1,59)	1:468:A:GLY:HA3	1:516:A:GLU:HG3	7	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:456:A:ILE:HD11	1:534:A:ALA:HA	5	0.87
(1,28)	1:456:A:ILE:HD12	1:534:A:ALA:HA	5	0.87
(1,28)	1:456:A:ILE:HD13	1:534:A:ALA:HA	5	0.87
(1,1196)	1:488:A:LYS:HE2	1:524:A:HIS:H	2	0.86
(1,1196)	1:488:A:LYS:HE3	1:524:A:HIS:H	2	0.86
(1,886)	1:475:A:CYS:H	1:509:A:ARG:HA	8	0.86
(1,763)	1:502:A:TRP:HD1	1:515:A:ASN:HD22	6	0.86
(1,544)	1:486:A:TRP:H	1:492:A:GLU:HA	9	0.86
(1,43)	1:465:A:VAL:HG21	1:471:A:VAL:HA	5	0.86
(1,43)	1:465:A:VAL:HG22	1:471:A:VAL:HA	5	0.86
(1,43)	1:465:A:VAL:HG23	1:471:A:VAL:HA	5	0.86
(1,1024)	1:460:A:LEU:HB2	1:525:A:TYR:H	6	0.85
(1,1024)	1:460:A:LEU:HB3	1:525:A:TYR:H	6	0.85
(1,1021)	1:488:A:LYS:HG3	1:524:A:HIS:H	5	0.85
(1,905)	1:477:A:VAL:H	1:508:A:GLN:HG2	1	0.85
(1,905)	1:477:A:VAL:H	1:508:A:GLN:HG3	1	0.85
(1,891)	1:475:A:CYS:H	1:510:A:HIS:H	8	0.85
(1,828)	1:479:A:GLU:H	1:508:A:GLN:HE21	1	0.85
(1,626)	1:462:A:ASP:HA	1:537:A:GLU:H	9	0.85
(1,429)	1:525:A:TYR:H	1:536:A:ALA:HB1	7	0.85
(1,429)	1:525:A:TYR:H	1:536:A:ALA:HB2	7	0.85
(1,429)	1:525:A:TYR:H	1:536:A:ALA:HB3	7	0.85
(1,387)	1:486:A:TRP:HE1	1:503:A:PHE:HA	3	0.85
(1,313)	1:502:A:TRP:HD1	1:503:A:PHE:HA	2	0.85
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA2	3	0.84
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA3	3	0.84
(1,719)	1:500:A:LYS:HD2	1:501:A:TYR:H	9	0.84
(1,719)	1:500:A:LYS:HD3	1:501:A:TYR:H	9	0.84
(1,560)	1:487:A:LEU:HG	1:491:A:VAL:H	7	0.84
(1,388)	1:486:A:TRP:HE1	1:510:A:HIS:HA	5	0.84
(1,1219)	1:497:A:GLU:HG2	1:498:A:THR:HG21	8	0.83
(1,1219)	1:497:A:GLU:HG2	1:498:A:THR:HG22	8	0.83
(1,1219)	1:497:A:GLU:HG2	1:498:A:THR:HG23	8	0.83
(1,1219)	1:497:A:GLU:HG3	1:498:A:THR:HG21	8	0.83
(1,1219)	1:497:A:GLU:HG3	1:498:A:THR:HG22	8	0.83
(1,1219)	1:497:A:GLU:HG3	1:498:A:THR:HG23	8	0.83
(1,1046)	1:524:A:HIS:H	1:538:A:LEU:H	7	0.83
(1,904)	1:477:A:VAL:H	1:508:A:GLN:HA	3	0.83
(1,387)	1:486:A:TRP:HE1	1:503:A:PHE:HA	9	0.83
(1,308)	1:505:A:LYS:HE2	1:510:A:HIS:HE1	2	0.83
(1,308)	1:505:A:LYS:HE3	1:510:A:HIS:HE1	2	0.83
(1,304)	1:484:A:VAL:HG11	1:510:A:HIS:HE1	1	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,304)	1:484:A:VAL:HG12	1:510:A:HIS:HE1	1	0.83
(1,304)	1:484:A:VAL:HG13	1:510:A:HIS:HE1	1	0.83
(1,304)	1:484:A:VAL:HG21	1:510:A:HIS:HE1	1	0.83
(1,304)	1:484:A:VAL:HG22	1:510:A:HIS:HE1	1	0.83
(1,304)	1:484:A:VAL:HG23	1:510:A:HIS:HE1	1	0.83
(1,824)	1:456:A:ILE:HD11	1:533:A:GLN:H	2	0.82
(1,824)	1:456:A:ILE:HD12	1:533:A:GLN:H	2	0.82
(1,824)	1:456:A:ILE:HD13	1:533:A:GLN:H	2	0.82
(1,818)	1:523:A:GLY:H	1:538:A:LEU:HB3	1	0.82
(1,765)	1:502:A:TRP:HZ2	1:515:A:ASN:HD22	1	0.82
(1,561)	1:487:A:LEU:HA	1:491:A:VAL:H	8	0.82
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG21	10	0.82
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG22	10	0.82
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG23	10	0.82
(1,241)	1:522:A:ALA:HB1	1:540:A:VAL:HB	6	0.82
(1,241)	1:522:A:ALA:HB2	1:540:A:VAL:HB	6	0.82
(1,241)	1:522:A:ALA:HB3	1:540:A:VAL:HB	6	0.82
(1,97)	1:477:A:VAL:HG21	1:508:A:GLN:HA	3	0.82
(1,97)	1:477:A:VAL:HG22	1:508:A:GLN:HA	3	0.82
(1,97)	1:477:A:VAL:HG23	1:508:A:GLN:HA	3	0.82
(1,43)	1:465:A:VAL:HG21	1:471:A:VAL:HA	9	0.82
(1,43)	1:465:A:VAL:HG22	1:471:A:VAL:HA	9	0.82
(1,43)	1:465:A:VAL:HG23	1:471:A:VAL:HA	9	0.82
(1,1148)	1:471:A:VAL:HG11	1:514:A:ILE:HD11	5	0.81
(1,1148)	1:471:A:VAL:HG11	1:514:A:ILE:HD12	5	0.81
(1,1148)	1:471:A:VAL:HG11	1:514:A:ILE:HD13	5	0.81
(1,1148)	1:471:A:VAL:HG12	1:514:A:ILE:HD11	5	0.81
(1,1148)	1:471:A:VAL:HG12	1:514:A:ILE:HD12	5	0.81
(1,1148)	1:471:A:VAL:HG12	1:514:A:ILE:HD13	5	0.81
(1,1148)	1:471:A:VAL:HG13	1:514:A:ILE:HD11	5	0.81
(1,1148)	1:471:A:VAL:HG13	1:514:A:ILE:HD12	5	0.81
(1,1148)	1:471:A:VAL:HG13	1:514:A:ILE:HD13	5	0.81
(1,1148)	1:471:A:VAL:HG21	1:514:A:ILE:HD11	5	0.81
(1,1148)	1:471:A:VAL:HG21	1:514:A:ILE:HD12	5	0.81
(1,1148)	1:471:A:VAL:HG21	1:514:A:ILE:HD13	5	0.81
(1,1148)	1:471:A:VAL:HG22	1:514:A:ILE:HD11	5	0.81
(1,1148)	1:471:A:VAL:HG22	1:514:A:ILE:HD12	5	0.81
(1,1148)	1:471:A:VAL:HG22	1:514:A:ILE:HD13	5	0.81
(1,1148)	1:471:A:VAL:HG23	1:514:A:ILE:HD11	5	0.81
(1,1148)	1:471:A:VAL:HG23	1:514:A:ILE:HD12	5	0.81
(1,1148)	1:471:A:VAL:HG23	1:514:A:ILE:HD13	5	0.81
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA2	6	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA3	6	0.81
(1,1042)	1:459:A:PRO:HB2	1:535:A:LEU:H	8	0.81
(1,1042)	1:459:A:PRO:HB3	1:535:A:LEU:H	8	0.81
(1,911)	1:458:A:ARG:H	1:478:A:SER:H	2	0.81
(1,628)	1:462:A:ASP:H	1:537:A:GLU:H	3	0.81
(1,561)	1:487:A:LEU:HA	1:491:A:VAL:H	4	0.81
(1,434)	1:456:A:ILE:HD11	1:534:A:ALA:H	3	0.81
(1,434)	1:456:A:ILE:HD12	1:534:A:ALA:H	3	0.81
(1,434)	1:456:A:ILE:HD13	1:534:A:ALA:H	3	0.81
(1,383)	1:486:A:TRP:HE1	1:511:A:HIS:H	5	0.81
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD11	4	0.81
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD12	4	0.81
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD13	4	0.81
(1,128)	1:453:A:PRO:HB2	1:531:A:GLY:HA2	2	0.81
(1,28)	1:456:A:ILE:HD11	1:534:A:ALA:HA	3	0.81
(1,28)	1:456:A:ILE:HD12	1:534:A:ALA:HA	3	0.81
(1,28)	1:456:A:ILE:HD13	1:534:A:ALA:HA	3	0.81
(1,28)	1:456:A:ILE:HD11	1:534:A:ALA:HA	9	0.81
(1,28)	1:456:A:ILE:HD12	1:534:A:ALA:HA	9	0.81
(1,28)	1:456:A:ILE:HD13	1:534:A:ALA:HA	9	0.81
(1,1265)	1:518:A:MET:HG2	1:520:A:GLU:H	2	0.8
(1,1265)	1:518:A:MET:HG3	1:520:A:GLU:H	2	0.8
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD11	2	0.8
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD12	2	0.8
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD13	2	0.8
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD21	2	0.8
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD22	2	0.8
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD23	2	0.8
(1,1046)	1:524:A:HIS:H	1:538:A:LEU:H	1	0.8
(1,809)	1:519:A:LEU:HB2	1:520:A:GLU:H	6	0.8
(1,802)	1:523:A:GLY:H	1:539:A:ILE:HA	8	0.8
(1,472)	1:472:A:GLU:HG2	1:512:A:LEU:H	9	0.8
(1,472)	1:472:A:GLU:HG3	1:512:A:LEU:H	9	0.8
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB1	9	0.8
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB2	9	0.8
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB3	9	0.8
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB1	9	0.8
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB2	9	0.8
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB3	9	0.8
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG2	9	0.8
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG3	9	0.8
(1,303)	1:509:A:ARG:HD2	1:511:A:HIS:HE1	5	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:509:A:ARG:HD3	1:511:A:HIS:HE1	5	0.8
(1,101)	1:457:A:THR:HG21	1:478:A:SER:HA	6	0.8
(1,101)	1:457:A:THR:HG22	1:478:A:SER:HA	6	0.8
(1,101)	1:457:A:THR:HG23	1:478:A:SER:HA	6	0.8
(1,1082)	1:456:A:ILE:HG12	1:533:A:GLN:H	5	0.79
(1,1082)	1:456:A:ILE:HG13	1:533:A:GLN:H	5	0.79
(1,1042)	1:459:A:PRO:HB2	1:535:A:LEU:H	7	0.79
(1,1042)	1:459:A:PRO:HB3	1:535:A:LEU:H	7	0.79
(1,970)	1:470:A:ARG:HA	1:514:A:ILE:H	8	0.79
(1,802)	1:523:A:GLY:H	1:539:A:ILE:HA	4	0.79
(1,780)	1:476:A:GLU:HG3	1:508:A:GLN:HE21	2	0.79
(1,544)	1:486:A:TRP:H	1:492:A:GLU:HA	8	0.79
(1,1156)	1:473:A:PHE:HB2	1:486:A:TRP:HZ2	8	0.78
(1,1156)	1:473:A:PHE:HB3	1:486:A:TRP:HZ2	8	0.78
(1,1021)	1:488:A:LYS:HG3	1:524:A:HIS:H	9	0.78
(1,673)	1:469:A:GLN:H	1:469:A:GLN:HG2	5	0.78
(1,673)	1:469:A:GLN:H	1:469:A:GLN:HG3	5	0.78
(1,663)	1:474:A:GLU:H	1:486:A:TRP:HH2	8	0.78
(1,463)	1:473:A:PHE:H	1:511:A:HIS:HA	8	0.78
(1,195)	1:514:A:ILE:HD11	1:521:A:ASP:HB3	5	0.78
(1,195)	1:514:A:ILE:HD12	1:521:A:ASP:HB3	5	0.78
(1,195)	1:514:A:ILE:HD13	1:521:A:ASP:HB3	5	0.78
(1,178)	1:470:A:ARG:HB2	1:513:A:ILE:HG21	7	0.78
(1,178)	1:470:A:ARG:HB2	1:513:A:ILE:HG22	7	0.78
(1,178)	1:470:A:ARG:HB2	1:513:A:ILE:HG23	7	0.78
(1,19)	1:457:A:THR:HG21	1:478:A:SER:HB2	10	0.78
(1,19)	1:457:A:THR:HG21	1:478:A:SER:HB3	10	0.78
(1,19)	1:457:A:THR:HG22	1:478:A:SER:HB2	10	0.78
(1,19)	1:457:A:THR:HG22	1:478:A:SER:HB3	10	0.78
(1,19)	1:457:A:THR:HG23	1:478:A:SER:HB2	10	0.78
(1,19)	1:457:A:THR:HG23	1:478:A:SER:HB3	10	0.78
(1,970)	1:470:A:ARG:HA	1:514:A:ILE:H	6	0.77
(1,970)	1:470:A:ARG:HA	1:514:A:ILE:H	10	0.77
(1,897)	1:459:A:PRO:HA	1:476:A:GLU:H	2	0.77
(1,325)	1:472:A:GLU:HG2	1:513:A:ILE:HD11	2	0.77
(1,325)	1:472:A:GLU:HG2	1:513:A:ILE:HD12	2	0.77
(1,325)	1:472:A:GLU:HG2	1:513:A:ILE:HD13	2	0.77
(1,325)	1:472:A:GLU:HG3	1:513:A:ILE:HD11	2	0.77
(1,325)	1:472:A:GLU:HG3	1:513:A:ILE:HD12	2	0.77
(1,325)	1:472:A:GLU:HG3	1:513:A:ILE:HD13	2	0.77
(1,316)	1:501:A:TYR:HB2	1:502:A:TRP:HD1	4	0.77
(1,316)	1:501:A:TYR:HB3	1:502:A:TRP:HD1	4	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	1:505:A:LYS:HE2	1:506:A:ASP:HA	3	0.77
(1,156)	1:505:A:LYS:HE3	1:506:A:ASP:HA	3	0.77
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA2	2	0.76
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA3	2	0.76
(1,1021)	1:488:A:LYS:HG3	1:524:A:HIS:H	6	0.76
(1,918)	1:486:A:TRP:HE1	1:504:A:LYS:H	7	0.76
(1,878)	1:469:A:GLN:HB2	1:470:A:ARG:H	5	0.76
(1,817)	1:523:A:GLY:H	1:540:A:VAL:HB	10	0.76
(1,684)	1:504:A:LYS:H	1:513:A:ILE:HD11	8	0.76
(1,684)	1:504:A:LYS:H	1:513:A:ILE:HD12	8	0.76
(1,684)	1:504:A:LYS:H	1:513:A:ILE:HD13	8	0.76
(1,455)	1:505:A:LYS:HD2	1:506:A:ASP:H	4	0.76
(1,455)	1:505:A:LYS:HD3	1:506:A:ASP:H	4	0.76
(1,307)	1:505:A:LYS:HD2	1:510:A:HIS:HE1	7	0.76
(1,307)	1:505:A:LYS:HD3	1:510:A:HIS:HE1	7	0.76
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB2	10	0.76
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB3	10	0.76
(1,76)	1:472:A:GLU:HG2	1:513:A:ILE:HG13	2	0.76
(1,76)	1:472:A:GLU:HG3	1:513:A:ILE:HG13	2	0.76
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD11	10	0.75
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD12	10	0.75
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD13	10	0.75
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD21	10	0.75
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD22	10	0.75
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD23	10	0.75
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD11	10	0.75
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD12	10	0.75
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD13	10	0.75
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD21	10	0.75
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD22	10	0.75
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD23	10	0.75
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD21	9	0.75
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD22	9	0.75
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD23	9	0.75
(1,911)	1:458:A:ARG:H	1:478:A:SER:H	10	0.75
(1,817)	1:523:A:GLY:H	1:540:A:VAL:HB	9	0.75
(1,797)	1:454:A:VAL:HB	1:531:A:GLY:H	7	0.75
(1,624)	1:462:A:ASP:HB3	1:537:A:GLU:H	2	0.75
(1,624)	1:462:A:ASP:HB2	1:537:A:GLU:H	2	0.75
(1,449)	1:463:A:GLN:HE22	1:472:A:GLU:H	8	0.75
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB1	8	0.75
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB2	8	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB3	8	0.75
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB1	8	0.75
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB2	8	0.75
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB3	8	0.75
(1,294)	1:474:A:GLU:HA	1:486:A:TRP:HZ2	10	0.75
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG21	4	0.75
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG22	4	0.75
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG23	4	0.75
(1,1248)	1:509:A:ARG:HB2	1:511:A:HIS:HE1	2	0.74
(1,1248)	1:509:A:ARG:HB3	1:511:A:HIS:HE1	2	0.74
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD11	8	0.74
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD12	8	0.74
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD13	8	0.74
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD21	8	0.74
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD22	8	0.74
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD23	8	0.74
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD11	8	0.74
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD12	8	0.74
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD13	8	0.74
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD21	8	0.74
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD22	8	0.74
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD23	8	0.74
(1,1046)	1:524:A:HIS:H	1:538:A:LEU:H	4	0.74
(1,911)	1:458:A:ARG:H	1:478:A:SER:H	4	0.74
(1,911)	1:458:A:ARG:H	1:478:A:SER:H	8	0.74
(1,763)	1:502:A:TRP:HD1	1:515:A:ASN:HD22	8	0.74
(1,742)	1:468:A:GLY:H	1:516:A:GLU:HG2	7	0.74
(1,742)	1:468:A:GLY:H	1:516:A:GLU:HG3	7	0.74
(1,656)	1:457:A:THR:H	1:476:A:GLU:HG2	8	0.74
(1,602)	1:458:A:ARG:H	1:477:A:VAL:HA	5	0.74
(1,477)	1:486:A:TRP:HH2	1:512:A:LEU:H	7	0.74
(1,384)	1:486:A:TRP:HE1	1:510:A:HIS:HB3	8	0.74
(1,383)	1:486:A:TRP:HE1	1:511:A:HIS:H	2	0.74
(1,383)	1:486:A:TRP:HE1	1:511:A:HIS:H	9	0.74
(1,318)	1:486:A:TRP:HD1	1:503:A:PHE:HE2	1	0.74
(1,307)	1:505:A:LYS:HD2	1:510:A:HIS:HE1	3	0.74
(1,307)	1:505:A:LYS:HD3	1:510:A:HIS:HE1	3	0.74
(1,289)	1:538:A:LEU:HG	1:540:A:VAL:HG21	6	0.74
(1,289)	1:538:A:LEU:HG	1:540:A:VAL:HG22	6	0.74
(1,289)	1:538:A:LEU:HG	1:540:A:VAL:HG23	6	0.74
(1,43)	1:465:A:VAL:HG21	1:471:A:VAL:HA	10	0.74
(1,43)	1:465:A:VAL:HG22	1:471:A:VAL:HA	10	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:465:A:VAL:HG23	1:471:A:VAL:HA	10	0.74
(1,1001)	1:518:A:MET:H	1:520:A:GLU:H	3	0.73
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD21	2	0.73
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD22	2	0.73
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD23	2	0.73
(1,626)	1:462:A:ASP:HA	1:537:A:GLU:H	1	0.73
(1,626)	1:462:A:ASP:HA	1:537:A:GLU:H	6	0.73
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG21	3	0.73
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG22	3	0.73
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG23	3	0.73
(1,141)	1:466:A:MET:HA	1:540:A:VAL:HG11	6	0.73
(1,141)	1:466:A:MET:HA	1:540:A:VAL:HG12	6	0.73
(1,141)	1:466:A:MET:HA	1:540:A:VAL:HG13	6	0.73
(1,101)	1:457:A:THR:HG21	1:478:A:SER:HA	8	0.73
(1,101)	1:457:A:THR:HG22	1:478:A:SER:HA	8	0.73
(1,101)	1:457:A:THR:HG23	1:478:A:SER:HA	8	0.73
(1,982)	1:502:A:TRP:HD1	1:515:A:ASN:H	4	0.72
(1,970)	1:470:A:ARG:HA	1:514:A:ILE:H	5	0.72
(1,803)	1:523:A:GLY:H	1:525:A:TYR:HD1	9	0.72
(1,719)	1:500:A:LYS:HD2	1:501:A:TYR:H	6	0.72
(1,719)	1:500:A:LYS:HD3	1:501:A:TYR:H	6	0.72
(1,1098)	1:460:A:LEU:HD11	1:486:A:TRP:HZ2	1	0.71
(1,1098)	1:460:A:LEU:HD12	1:486:A:TRP:HZ2	1	0.71
(1,1098)	1:460:A:LEU:HD13	1:486:A:TRP:HZ2	1	0.71
(1,1098)	1:460:A:LEU:HD21	1:486:A:TRP:HZ2	1	0.71
(1,1098)	1:460:A:LEU:HD22	1:486:A:TRP:HZ2	1	0.71
(1,1098)	1:460:A:LEU:HD23	1:486:A:TRP:HZ2	1	0.71
(1,1037)	1:456:A:ILE:HD11	1:529:A:THR:H	5	0.71
(1,1037)	1:456:A:ILE:HD12	1:529:A:THR:H	5	0.71
(1,1037)	1:456:A:ILE:HD13	1:529:A:THR:H	5	0.71
(1,974)	1:513:A:ILE:HG13	1:514:A:ILE:H	3	0.71
(1,973)	1:471:A:VAL:HB	1:514:A:ILE:H	8	0.71
(1,930)	1:487:A:LEU:HB3	1:488:A:LYS:H	2	0.71
(1,918)	1:486:A:TRP:HE1	1:504:A:LYS:H	8	0.71
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB1	8	0.71
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB2	8	0.71
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB3	8	0.71
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD21	4	0.71
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD22	4	0.71
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD23	4	0.71
(1,818)	1:523:A:GLY:H	1:538:A:LEU:HB3	10	0.71
(1,816)	1:478:A:SER:H	1:508:A:GLN:HE22	1	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,548)	1:486:A:TRP:H	1:493:A:LEU:H	8	0.71
(1,386)	1:486:A:TRP:HE1	1:510:A:HIS:HB2	2	0.71
(1,138)	1:467:A:VAL:HA	1:540:A:VAL:HG11	6	0.71
(1,138)	1:467:A:VAL:HA	1:540:A:VAL:HG12	6	0.71
(1,138)	1:467:A:VAL:HA	1:540:A:VAL:HG13	6	0.71
(1,29)	1:456:A:ILE:HD11	1:533:A:GLN:HA	9	0.71
(1,29)	1:456:A:ILE:HD12	1:533:A:GLN:HA	9	0.71
(1,29)	1:456:A:ILE:HD13	1:533:A:GLN:HA	9	0.71
(1,1146)	1:471:A:VAL:HG11	1:473:A:PHE:HD1	10	0.7
(1,1146)	1:471:A:VAL:HG12	1:473:A:PHE:HD1	10	0.7
(1,1146)	1:471:A:VAL:HG13	1:473:A:PHE:HD1	10	0.7
(1,1146)	1:471:A:VAL:HG21	1:473:A:PHE:HD1	10	0.7
(1,1146)	1:471:A:VAL:HG22	1:473:A:PHE:HD1	10	0.7
(1,1146)	1:471:A:VAL:HG23	1:473:A:PHE:HD1	10	0.7
(1,1024)	1:460:A:LEU:HB2	1:525:A:TYR:H	4	0.7
(1,1024)	1:460:A:LEU:HB3	1:525:A:TYR:H	4	0.7
(1,966)	1:511:A:HIS:H	1:513:A:ILE:HD11	3	0.7
(1,966)	1:511:A:HIS:H	1:513:A:ILE:HD12	3	0.7
(1,966)	1:511:A:HIS:H	1:513:A:ILE:HD13	3	0.7
(1,930)	1:487:A:LEU:HB3	1:488:A:LYS:H	10	0.7
(1,918)	1:486:A:TRP:HE1	1:504:A:LYS:H	10	0.7
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD21	7	0.7
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD22	7	0.7
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD23	7	0.7
(1,818)	1:523:A:GLY:H	1:538:A:LEU:HB3	9	0.7
(1,627)	1:524:A:HIS:HA	1:537:A:GLU:H	4	0.7
(1,514)	1:523:A:GLY:HA2	1:538:A:LEU:H	3	0.7
(1,388)	1:486:A:TRP:HE1	1:510:A:HIS:HA	2	0.7
(1,376)	1:487:A:LEU:HB3	1:490:A:GLY:H	1	0.7
(1,212)	1:471:A:VAL:HB	1:514:A:ILE:HG21	8	0.7
(1,212)	1:471:A:VAL:HB	1:514:A:ILE:HG22	8	0.7
(1,212)	1:471:A:VAL:HB	1:514:A:ILE:HG23	8	0.7
(1,1225)	1:500:A:LYS:HE2	1:514:A:ILE:HG21	4	0.69
(1,1225)	1:500:A:LYS:HE2	1:514:A:ILE:HG22	4	0.69
(1,1225)	1:500:A:LYS:HE2	1:514:A:ILE:HG23	4	0.69
(1,1225)	1:500:A:LYS:HE3	1:514:A:ILE:HG21	4	0.69
(1,1225)	1:500:A:LYS:HE3	1:514:A:ILE:HG22	4	0.69
(1,1225)	1:500:A:LYS:HE3	1:514:A:ILE:HG23	4	0.69
(1,1100)	1:460:A:LEU:HD11	1:526:A:ALA:HA	5	0.69
(1,1100)	1:460:A:LEU:HD12	1:526:A:ALA:HA	5	0.69
(1,1100)	1:460:A:LEU:HD13	1:526:A:ALA:HA	5	0.69
(1,1100)	1:460:A:LEU:HD21	1:526:A:ALA:HA	5	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1100)	1:460:A:LEU:HD22	1:526:A:ALA:HA	5	0.69
(1,1100)	1:460:A:LEU:HD23	1:526:A:ALA:HA	5	0.69
(1,946)	1:503:A:PHE:H	1:513:A:ILE:HD11	2	0.69
(1,946)	1:503:A:PHE:H	1:513:A:ILE:HD12	2	0.69
(1,946)	1:503:A:PHE:H	1:513:A:ILE:HD13	2	0.69
(1,760)	1:465:A:VAL:HA	1:469:A:GLN:HE21	1	0.69
(1,624)	1:462:A:ASP:HB3	1:537:A:GLU:H	1	0.69
(1,624)	1:462:A:ASP:HB2	1:537:A:GLU:H	1	0.69
(1,449)	1:463:A:GLN:HE22	1:472:A:GLU:H	1	0.69
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG2	1	0.69
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG3	1	0.69
(1,152)	1:500:A:LYS:HG2	1:501:A:TYR:HD1	10	0.69
(1,152)	1:500:A:LYS:HG3	1:501:A:TYR:HD1	10	0.69
(1,28)	1:456:A:ILE:HD11	1:534:A:ALA:HA	7	0.69
(1,28)	1:456:A:ILE:HD12	1:534:A:ALA:HA	7	0.69
(1,28)	1:456:A:ILE:HD13	1:534:A:ALA:HA	7	0.69
(1,1212)	1:493:A:LEU:HD11	1:512:A:LEU:HD11	7	0.68
(1,1212)	1:493:A:LEU:HD11	1:512:A:LEU:HD12	7	0.68
(1,1212)	1:493:A:LEU:HD11	1:512:A:LEU:HD13	7	0.68
(1,1212)	1:493:A:LEU:HD12	1:512:A:LEU:HD11	7	0.68
(1,1212)	1:493:A:LEU:HD12	1:512:A:LEU:HD12	7	0.68
(1,1212)	1:493:A:LEU:HD12	1:512:A:LEU:HD13	7	0.68
(1,1212)	1:493:A:LEU:HD13	1:512:A:LEU:HD11	7	0.68
(1,1212)	1:493:A:LEU:HD13	1:512:A:LEU:HD12	7	0.68
(1,1212)	1:493:A:LEU:HD13	1:512:A:LEU:HD13	7	0.68
(1,1212)	1:493:A:LEU:HD21	1:512:A:LEU:HD11	7	0.68
(1,1212)	1:493:A:LEU:HD21	1:512:A:LEU:HD12	7	0.68
(1,1212)	1:493:A:LEU:HD21	1:512:A:LEU:HD13	7	0.68
(1,1212)	1:493:A:LEU:HD22	1:512:A:LEU:HD11	7	0.68
(1,1212)	1:493:A:LEU:HD22	1:512:A:LEU:HD12	7	0.68
(1,1212)	1:493:A:LEU:HD22	1:512:A:LEU:HD13	7	0.68
(1,1212)	1:493:A:LEU:HD23	1:512:A:LEU:HD11	7	0.68
(1,1212)	1:493:A:LEU:HD23	1:512:A:LEU:HD12	7	0.68
(1,1212)	1:493:A:LEU:HD23	1:512:A:LEU:HD13	7	0.68
(1,1024)	1:460:A:LEU:HB2	1:525:A:TYR:H	10	0.68
(1,1024)	1:460:A:LEU:HB3	1:525:A:TYR:H	10	0.68
(1,930)	1:487:A:LEU:HB3	1:488:A:LYS:H	1	0.68
(1,763)	1:502:A:TRP:HD1	1:515:A:ASN:HD22	4	0.68
(1,627)	1:524:A:HIS:HA	1:537:A:GLU:H	7	0.68
(1,552)	1:486:A:TRP:H	1:492:A:GLU:HG2	3	0.68
(1,552)	1:486:A:TRP:H	1:492:A:GLU:HG3	3	0.68
(1,434)	1:456:A:ILE:HD11	1:534:A:ALA:H	9	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,434)	1:456:A:ILE:HD12	1:534:A:ALA:H	9	0.68
(1,434)	1:456:A:ILE:HD13	1:534:A:ALA:H	9	0.68
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD11	6	0.68
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD12	6	0.68
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD13	6	0.68
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD11	10	0.68
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD12	10	0.68
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD13	10	0.68
(1,85)	1:457:A:THR:HG21	1:477:A:VAL:HA	2	0.68
(1,85)	1:457:A:THR:HG22	1:477:A:VAL:HA	2	0.68
(1,85)	1:457:A:THR:HG23	1:477:A:VAL:HA	2	0.68
(1,1240)	1:505:A:LYS:HB2	1:510:A:HIS:HE1	2	0.67
(1,1240)	1:505:A:LYS:HB3	1:510:A:HIS:HE1	2	0.67
(1,1146)	1:471:A:VAL:HG11	1:473:A:PHE:HD1	7	0.67
(1,1146)	1:471:A:VAL:HG12	1:473:A:PHE:HD1	7	0.67
(1,1146)	1:471:A:VAL:HG13	1:473:A:PHE:HD1	7	0.67
(1,1146)	1:471:A:VAL:HG21	1:473:A:PHE:HD1	7	0.67
(1,1146)	1:471:A:VAL:HG22	1:473:A:PHE:HD1	7	0.67
(1,1146)	1:471:A:VAL:HG23	1:473:A:PHE:HD1	7	0.67
(1,970)	1:470:A:ARG:HA	1:514:A:ILE:H	4	0.67
(1,930)	1:487:A:LEU:HB3	1:488:A:LYS:H	6	0.67
(1,897)	1:459:A:PRO:HA	1:476:A:GLU:H	8	0.67
(1,819)	1:523:A:GLY:H	1:538:A:LEU:HG	8	0.67
(1,561)	1:487:A:LEU:HA	1:491:A:VAL:H	5	0.67
(1,514)	1:523:A:GLY:HA2	1:538:A:LEU:H	8	0.67
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD21	5	0.67
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD22	5	0.67
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD23	5	0.67
(1,388)	1:486:A:TRP:HE1	1:510:A:HIS:HA	3	0.67
(1,387)	1:486:A:TRP:HE1	1:503:A:PHE:HA	2	0.67
(1,318)	1:486:A:TRP:HD1	1:503:A:PHE:HE2	6	0.67
(1,28)	1:456:A:ILE:HD11	1:534:A:ALA:HA	2	0.67
(1,28)	1:456:A:ILE:HD12	1:534:A:ALA:HA	2	0.67
(1,28)	1:456:A:ILE:HD13	1:534:A:ALA:HA	2	0.67
(1,1242)	1:506:A:ASP:H	1:509:A:ARG:HB2	7	0.66
(1,1242)	1:506:A:ASP:H	1:509:A:ARG:HB3	7	0.66
(1,1022)	1:524:A:HIS:H	1:537:A:GLU:HB2	8	0.66
(1,1022)	1:524:A:HIS:H	1:537:A:GLU:HB3	8	0.66
(1,1016)	1:489:A:ASP:HA	1:524:A:HIS:H	4	0.66
(1,985)	1:470:A:ARG:HB2	1:516:A:GLU:H	4	0.66
(1,930)	1:487:A:LEU:HB3	1:488:A:LYS:H	3	0.66
(1,828)	1:479:A:GLU:H	1:508:A:GLN:HE21	5	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,642)	1:482:A:ALA:H	1:508:A:GLN:HB3	5	0.66
(1,642)	1:482:A:ALA:H	1:508:A:GLN:HB2	5	0.66
(1,479)	1:486:A:TRP:HZ2	1:512:A:LEU:H	1	0.66
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD21	9	0.66
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD22	9	0.66
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD23	9	0.66
(1,325)	1:472:A:GLU:HG2	1:513:A:ILE:HD11	10	0.66
(1,325)	1:472:A:GLU:HG2	1:513:A:ILE:HD12	10	0.66
(1,325)	1:472:A:GLU:HG2	1:513:A:ILE:HD13	10	0.66
(1,325)	1:472:A:GLU:HG3	1:513:A:ILE:HD11	10	0.66
(1,325)	1:472:A:GLU:HG3	1:513:A:ILE:HD12	10	0.66
(1,325)	1:472:A:GLU:HG3	1:513:A:ILE:HD13	10	0.66
(1,303)	1:509:A:ARG:HD2	1:511:A:HIS:HE1	8	0.66
(1,303)	1:509:A:ARG:HD3	1:511:A:HIS:HE1	8	0.66
(1,150)	1:486:A:TRP:HZ2	1:503:A:PHE:HB3	10	0.66
(1,28)	1:456:A:ILE:HD11	1:534:A:ALA:HA	1	0.66
(1,28)	1:456:A:ILE:HD12	1:534:A:ALA:HA	1	0.66
(1,28)	1:456:A:ILE:HD13	1:534:A:ALA:HA	1	0.66
(1,1225)	1:500:A:LYS:HE2	1:514:A:ILE:HG21	3	0.65
(1,1225)	1:500:A:LYS:HE2	1:514:A:ILE:HG22	3	0.65
(1,1225)	1:500:A:LYS:HE2	1:514:A:ILE:HG23	3	0.65
(1,1225)	1:500:A:LYS:HE3	1:514:A:ILE:HG21	3	0.65
(1,1225)	1:500:A:LYS:HE3	1:514:A:ILE:HG22	3	0.65
(1,1225)	1:500:A:LYS:HE3	1:514:A:ILE:HG23	3	0.65
(1,1024)	1:460:A:LEU:HB2	1:525:A:TYR:H	7	0.65
(1,1024)	1:460:A:LEU:HB3	1:525:A:TYR:H	7	0.65
(1,930)	1:487:A:LEU:HB3	1:488:A:LYS:H	5	0.65
(1,780)	1:476:A:GLU:HG3	1:508:A:GLN:HE21	5	0.65
(1,514)	1:523:A:GLY:HA2	1:538:A:LEU:H	6	0.65
(1,479)	1:486:A:TRP:HZ2	1:512:A:LEU:H	8	0.65
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD11	2	0.65
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD12	2	0.65
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD13	2	0.65
(1,386)	1:486:A:TRP:HE1	1:510:A:HIS:HB2	6	0.65
(1,330)	1:456:A:ILE:HG21	1:459:A:PRO:HB2	9	0.65
(1,330)	1:456:A:ILE:HG21	1:459:A:PRO:HB3	9	0.65
(1,330)	1:456:A:ILE:HG22	1:459:A:PRO:HB2	9	0.65
(1,330)	1:456:A:ILE:HG22	1:459:A:PRO:HB3	9	0.65
(1,330)	1:456:A:ILE:HG23	1:459:A:PRO:HB2	9	0.65
(1,330)	1:456:A:ILE:HG23	1:459:A:PRO:HB3	9	0.65
(1,302)	1:505:A:LYS:HB3	1:510:A:HIS:HE1	1	0.65
(1,294)	1:474:A:GLU:HA	1:486:A:TRP:HZ2	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB2	2	0.65
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB3	2	0.65
(1,43)	1:465:A:VAL:HG21	1:471:A:VAL:HA	1	0.65
(1,43)	1:465:A:VAL:HG22	1:471:A:VAL:HA	1	0.65
(1,43)	1:465:A:VAL:HG23	1:471:A:VAL:HA	1	0.65
(1,1243)	1:506:A:ASP:H	1:509:A:ARG:HG2	4	0.64
(1,1243)	1:506:A:ASP:H	1:509:A:ARG:HG3	4	0.64
(1,1101)	1:460:A:LEU:HD11	1:527:A:LEU:H	5	0.64
(1,1101)	1:460:A:LEU:HD12	1:527:A:LEU:H	5	0.64
(1,1101)	1:460:A:LEU:HD13	1:527:A:LEU:H	5	0.64
(1,1101)	1:460:A:LEU:HD21	1:527:A:LEU:H	5	0.64
(1,1101)	1:460:A:LEU:HD22	1:527:A:LEU:H	5	0.64
(1,1101)	1:460:A:LEU:HD23	1:527:A:LEU:H	5	0.64
(1,960)	1:486:A:TRP:HZ2	1:511:A:HIS:H	7	0.64
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD21	1	0.64
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD22	1	0.64
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD23	1	0.64
(1,818)	1:523:A:GLY:H	1:538:A:LEU:HB3	6	0.64
(1,782)	1:457:A:THR:HG21	1:508:A:GLN:HE21	3	0.64
(1,782)	1:457:A:THR:HG22	1:508:A:GLN:HE21	3	0.64
(1,782)	1:457:A:THR:HG23	1:508:A:GLN:HE21	3	0.64
(1,780)	1:476:A:GLU:HG3	1:508:A:GLN:HE21	3	0.64
(1,657)	1:457:A:THR:H	1:477:A:VAL:HB	5	0.64
(1,636)	1:487:A:LEU:HB2	1:526:A:ALA:H	10	0.64
(1,544)	1:486:A:TRP:H	1:492:A:GLU:HA	3	0.64
(1,386)	1:486:A:TRP:HE1	1:510:A:HIS:HB2	7	0.64
(1,361)	1:488:A:LYS:HD2	1:489:A:ASP:H	9	0.64
(1,316)	1:501:A:TYR:HB2	1:502:A:TRP:HD1	8	0.64
(1,316)	1:501:A:TYR:HB3	1:502:A:TRP:HD1	8	0.64
(1,192)	1:517:A:ALA:HB1	1:540:A:VAL:HG11	6	0.64
(1,192)	1:517:A:ALA:HB1	1:540:A:VAL:HG12	6	0.64
(1,192)	1:517:A:ALA:HB1	1:540:A:VAL:HG13	6	0.64
(1,192)	1:517:A:ALA:HB2	1:540:A:VAL:HG11	6	0.64
(1,192)	1:517:A:ALA:HB2	1:540:A:VAL:HG12	6	0.64
(1,192)	1:517:A:ALA:HB2	1:540:A:VAL:HG13	6	0.64
(1,192)	1:517:A:ALA:HB3	1:540:A:VAL:HG11	6	0.64
(1,192)	1:517:A:ALA:HB3	1:540:A:VAL:HG12	6	0.64
(1,192)	1:517:A:ALA:HB3	1:540:A:VAL:HG13	6	0.64
(1,150)	1:486:A:TRP:HZ2	1:503:A:PHE:HB3	3	0.64
(1,1232)	1:504:A:LYS:HB2	1:511:A:HIS:H	3	0.63
(1,1232)	1:504:A:LYS:HB3	1:511:A:HIS:H	3	0.63
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA2	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA3	5	0.63
(1,1012)	1:522:A:ALA:H	1:538:A:LEU:HG	2	0.63
(1,650)	1:497:A:GLU:HB2	1:500:A:LYS:H	9	0.63
(1,650)	1:497:A:GLU:HB3	1:500:A:LYS:H	9	0.63
(1,455)	1:505:A:LYS:HD2	1:506:A:ASP:H	1	0.63
(1,455)	1:505:A:LYS:HD3	1:506:A:ASP:H	1	0.63
(1,366)	1:502:A:TRP:HE1	1:515:A:ASN:HD22	3	0.63
(1,59)	1:468:A:GLY:HA3	1:516:A:GLU:HG2	6	0.63
(1,59)	1:468:A:GLY:HA3	1:516:A:GLU:HG3	6	0.63
(1,1227)	1:500:A:LYS:HE2	1:518:A:MET:HG2	5	0.62
(1,1227)	1:500:A:LYS:HE2	1:518:A:MET:HG3	5	0.62
(1,1227)	1:500:A:LYS:HE3	1:518:A:MET:HG2	5	0.62
(1,1227)	1:500:A:LYS:HE3	1:518:A:MET:HG3	5	0.62
(1,1219)	1:497:A:GLU:HG2	1:498:A:THR:HG21	1	0.62
(1,1219)	1:497:A:GLU:HG2	1:498:A:THR:HG22	1	0.62
(1,1219)	1:497:A:GLU:HG2	1:498:A:THR:HG23	1	0.62
(1,1219)	1:497:A:GLU:HG3	1:498:A:THR:HG21	1	0.62
(1,1219)	1:497:A:GLU:HG3	1:498:A:THR:HG22	1	0.62
(1,1219)	1:497:A:GLU:HG3	1:498:A:THR:HG23	1	0.62
(1,1042)	1:459:A:PRO:HB2	1:535:A:LEU:H	4	0.62
(1,1042)	1:459:A:PRO:HB3	1:535:A:LEU:H	4	0.62
(1,982)	1:502:A:TRP:HD1	1:515:A:ASN:H	8	0.62
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB1	6	0.62
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB2	6	0.62
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB3	6	0.62
(1,747)	1:460:A:LEU:H	1:534:A:ALA:HA	5	0.62
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG11	8	0.62
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG12	8	0.62
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG13	8	0.62
(1,544)	1:486:A:TRP:H	1:492:A:GLU:HA	7	0.62
(1,384)	1:486:A:TRP:HE1	1:510:A:HIS:HB3	4	0.62
(1,1024)	1:460:A:LEU:HB2	1:525:A:TYR:H	2	0.61
(1,1024)	1:460:A:LEU:HB3	1:525:A:TYR:H	2	0.61
(1,742)	1:468:A:GLY:H	1:516:A:GLU:HG2	4	0.61
(1,742)	1:468:A:GLY:H	1:516:A:GLU:HG3	4	0.61
(1,492)	1:464:A:LEU:HA	1:540:A:VAL:H	9	0.61
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD11	8	0.61
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD12	8	0.61
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD13	8	0.61
(1,1287)	1:527:A:LEU:H	1:533:A:GLN:HB2	9	0.6
(1,1287)	1:527:A:LEU:H	1:533:A:GLN:HB3	9	0.6
(1,973)	1:471:A:VAL:HB	1:514:A:ILE:H	7	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,911)	1:458:A:ARG:H	1:478:A:SER:H	9	0.6
(1,824)	1:456:A:ILE:HD11	1:533:A:GLN:H	10	0.6
(1,824)	1:456:A:ILE:HD12	1:533:A:GLN:H	10	0.6
(1,824)	1:456:A:ILE:HD13	1:533:A:GLN:H	10	0.6
(1,663)	1:474:A:GLU:H	1:486:A:TRP:HH2	6	0.6
(1,626)	1:462:A:ASP:HA	1:537:A:GLU:H	2	0.6
(1,561)	1:487:A:LEU:HA	1:491:A:VAL:H	3	0.6
(1,548)	1:486:A:TRP:H	1:493:A:LEU:H	3	0.6
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD21	10	0.6
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD22	10	0.6
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD23	10	0.6
(1,384)	1:486:A:TRP:HE1	1:510:A:HIS:HB3	5	0.6
(1,352)	1:464:A:LEU:HB2	1:539:A:ILE:H	10	0.6
(1,301)	1:503:A:PHE:HB2	1:503:A:PHE:HE1	8	0.6
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG21	7	0.6
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG22	7	0.6
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG23	7	0.6
(1,249)	1:460:A:LEU:HG	1:526:A:ALA:HA	6	0.6
(1,128)	1:453:A:PRO:HB2	1:531:A:GLY:HA2	5	0.6
(1,1146)	1:471:A:VAL:HG11	1:473:A:PHE:HD1	6	0.59
(1,1146)	1:471:A:VAL:HG12	1:473:A:PHE:HD1	6	0.59
(1,1146)	1:471:A:VAL:HG13	1:473:A:PHE:HD1	6	0.59
(1,1146)	1:471:A:VAL:HG21	1:473:A:PHE:HD1	6	0.59
(1,1146)	1:471:A:VAL:HG22	1:473:A:PHE:HD1	6	0.59
(1,1146)	1:471:A:VAL:HG23	1:473:A:PHE:HD1	6	0.59
(1,974)	1:513:A:ILE:HG13	1:514:A:ILE:H	2	0.59
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD21	4	0.59
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD22	4	0.59
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD23	4	0.59
(1,891)	1:475:A:CYS:H	1:510:A:HIS:H	1	0.59
(1,857)	1:462:A:ASP:H	1:463:A:GLN:HE21	5	0.59
(1,824)	1:456:A:ILE:HD11	1:533:A:GLN:H	1	0.59
(1,824)	1:456:A:ILE:HD12	1:533:A:GLN:H	1	0.59
(1,824)	1:456:A:ILE:HD13	1:533:A:GLN:H	1	0.59
(1,811)	1:465:A:VAL:HA	1:469:A:GLN:HE22	7	0.59
(1,794)	1:529:A:THR:HG21	1:532:A:GLY:H	10	0.59
(1,794)	1:529:A:THR:HG22	1:532:A:GLY:H	10	0.59
(1,794)	1:529:A:THR:HG23	1:532:A:GLY:H	10	0.59
(1,512)	1:522:A:ALA:HA	1:538:A:LEU:H	9	0.59
(1,439)	1:526:A:ALA:HA	1:534:A:ALA:H	7	0.59
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD11	6	0.59
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD12	6	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD13	6	0.59
(1,387)	1:486:A:TRP:HE1	1:503:A:PHE:HA	5	0.59
(1,302)	1:505:A:LYS:HB3	1:510:A:HIS:HE1	4	0.59
(1,301)	1:503:A:PHE:HB2	1:503:A:PHE:HE1	4	0.59
(1,301)	1:503:A:PHE:HB2	1:503:A:PHE:HE1	5	0.59
(1,301)	1:503:A:PHE:HB2	1:503:A:PHE:HE1	6	0.59
(1,301)	1:503:A:PHE:HB2	1:503:A:PHE:HE1	9	0.59
(1,19)	1:457:A:THR:HG21	1:478:A:SER:HB2	6	0.59
(1,19)	1:457:A:THR:HG21	1:478:A:SER:HB3	6	0.59
(1,19)	1:457:A:THR:HG22	1:478:A:SER:HB2	6	0.59
(1,19)	1:457:A:THR:HG22	1:478:A:SER:HB3	6	0.59
(1,19)	1:457:A:THR:HG23	1:478:A:SER:HB2	6	0.59
(1,19)	1:457:A:THR:HG23	1:478:A:SER:HB3	6	0.59
(1,1032)	1:529:A:THR:H	1:532:A:GLY:H	9	0.58
(1,1009)	1:517:A:ALA:HB1	1:521:A:ASP:H	9	0.58
(1,1009)	1:517:A:ALA:HB2	1:521:A:ASP:H	9	0.58
(1,1009)	1:517:A:ALA:HB3	1:521:A:ASP:H	9	0.58
(1,970)	1:470:A:ARG:HA	1:514:A:ILE:H	1	0.58
(1,970)	1:470:A:ARG:HA	1:514:A:ILE:H	9	0.58
(1,755)	1:463:A:GLN:HE21	1:464:A:LEU:H	4	0.58
(1,663)	1:474:A:GLU:H	1:486:A:TRP:HH2	7	0.58
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB2	5	0.58
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB3	5	0.58
(1,492)	1:464:A:LEU:HA	1:540:A:VAL:H	4	0.58
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD21	7	0.58
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD22	7	0.58
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD23	7	0.58
(1,308)	1:505:A:LYS:HE2	1:510:A:HIS:HE1	6	0.58
(1,308)	1:505:A:LYS:HE3	1:510:A:HIS:HE1	6	0.58
(1,301)	1:503:A:PHE:HB2	1:503:A:PHE:HE1	1	0.58
(1,301)	1:503:A:PHE:HB2	1:503:A:PHE:HE1	2	0.58
(1,930)	1:487:A:LEU:HB3	1:488:A:LYS:H	9	0.57
(1,897)	1:459:A:PRO:HA	1:476:A:GLU:H	3	0.57
(1,719)	1:500:A:LYS:HD2	1:501:A:TYR:H	10	0.57
(1,719)	1:500:A:LYS:HD3	1:501:A:TYR:H	10	0.57
(1,624)	1:462:A:ASP:HB3	1:537:A:GLU:H	10	0.57
(1,624)	1:462:A:ASP:HB2	1:537:A:GLU:H	10	0.57
(1,384)	1:486:A:TRP:HE1	1:510:A:HIS:HB3	1	0.57
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB1	10	0.57
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB2	10	0.57
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB3	10	0.57
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB1	10	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB2	10	0.57
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB3	10	0.57
(1,330)	1:456:A:ILE:HG21	1:459:A:PRO:HB2	7	0.57
(1,330)	1:456:A:ILE:HG21	1:459:A:PRO:HB3	7	0.57
(1,330)	1:456:A:ILE:HG22	1:459:A:PRO:HB2	7	0.57
(1,330)	1:456:A:ILE:HG22	1:459:A:PRO:HB3	7	0.57
(1,330)	1:456:A:ILE:HG23	1:459:A:PRO:HB2	7	0.57
(1,330)	1:456:A:ILE:HG23	1:459:A:PRO:HB3	7	0.57
(1,306)	1:505:A:LYS:HG2	1:510:A:HIS:HE1	9	0.57
(1,306)	1:505:A:LYS:HG3	1:510:A:HIS:HE1	9	0.57
(1,303)	1:509:A:ARG:HD2	1:511:A:HIS:HE1	10	0.57
(1,303)	1:509:A:ARG:HD3	1:511:A:HIS:HE1	10	0.57
(1,294)	1:474:A:GLU:HA	1:486:A:TRP:HZ2	8	0.57
(1,235)	1:519:A:LEU:HB2	1:520:A:GLU:HA	6	0.57
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD11	9	0.57
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD12	9	0.57
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD13	9	0.57
(1,29)	1:456:A:ILE:HD11	1:533:A:GLN:HA	5	0.57
(1,29)	1:456:A:ILE:HD12	1:533:A:GLN:HA	5	0.57
(1,29)	1:456:A:ILE:HD13	1:533:A:GLN:HA	5	0.57
(1,1226)	1:500:A:LYS:HE2	1:518:A:MET:H	8	0.56
(1,1226)	1:500:A:LYS:HE3	1:518:A:MET:H	8	0.56
(1,974)	1:513:A:ILE:HG13	1:514:A:ILE:H	8	0.56
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD21	6	0.56
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD22	6	0.56
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD23	6	0.56
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD21	5	0.56
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD22	5	0.56
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD23	5	0.56
(1,592)	1:519:A:LEU:H	1:540:A:VAL:HG11	7	0.56
(1,592)	1:519:A:LEU:H	1:540:A:VAL:HG12	7	0.56
(1,592)	1:519:A:LEU:H	1:540:A:VAL:HG13	7	0.56
(1,388)	1:486:A:TRP:HE1	1:510:A:HIS:HA	9	0.56
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG2	4	0.56
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG3	4	0.56
(1,150)	1:486:A:TRP:HZ2	1:503:A:PHE:HB3	2	0.56
(1,930)	1:487:A:LEU:HB3	1:488:A:LYS:H	8	0.55
(1,921)	1:487:A:LEU:H	1:493:A:LEU:H	6	0.55
(1,754)	1:463:A:GLN:HA	1:463:A:GLN:HE21	4	0.55
(1,747)	1:460:A:LEU:H	1:534:A:ALA:HA	4	0.55
(1,747)	1:460:A:LEU:H	1:534:A:ALA:HA	8	0.55
(1,742)	1:468:A:GLY:H	1:516:A:GLU:HG2	3	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,742)	1:468:A:GLY:H	1:516:A:GLU:HG3	3	0.55
(1,626)	1:462:A:ASP:HA	1:537:A:GLU:H	4	0.55
(1,626)	1:462:A:ASP:HA	1:537:A:GLU:H	7	0.55
(1,306)	1:505:A:LYS:HG2	1:510:A:HIS:HE1	6	0.55
(1,306)	1:505:A:LYS:HG3	1:510:A:HIS:HE1	6	0.55
(1,199)	1:537:A:GLU:HB2	1:539:A:ILE:HD11	5	0.55
(1,199)	1:537:A:GLU:HB2	1:539:A:ILE:HD12	5	0.55
(1,199)	1:537:A:GLU:HB2	1:539:A:ILE:HD13	5	0.55
(1,199)	1:537:A:GLU:HB3	1:539:A:ILE:HD11	5	0.55
(1,199)	1:537:A:GLU:HB3	1:539:A:ILE:HD12	5	0.55
(1,199)	1:537:A:GLU:HB3	1:539:A:ILE:HD13	5	0.55
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD11	1	0.55
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD12	1	0.55
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD13	1	0.55
(1,43)	1:465:A:VAL:HG21	1:471:A:VAL:HA	7	0.55
(1,43)	1:465:A:VAL:HG22	1:471:A:VAL:HA	7	0.55
(1,43)	1:465:A:VAL:HG23	1:471:A:VAL:HA	7	0.55
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD11	8	0.54
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD12	8	0.54
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD13	8	0.54
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD21	8	0.54
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD22	8	0.54
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD23	8	0.54
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD11	8	0.54
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD12	8	0.54
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD13	8	0.54
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD21	8	0.54
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD22	8	0.54
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD23	8	0.54
(1,1271)	1:519:A:LEU:HD11	1:542:A:GLU:H	4	0.54
(1,1271)	1:519:A:LEU:HD12	1:542:A:GLU:H	4	0.54
(1,1271)	1:519:A:LEU:HD13	1:542:A:GLU:H	4	0.54
(1,1271)	1:519:A:LEU:HD21	1:542:A:GLU:H	4	0.54
(1,1271)	1:519:A:LEU:HD22	1:542:A:GLU:H	4	0.54
(1,1271)	1:519:A:LEU:HD23	1:542:A:GLU:H	4	0.54
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD11	4	0.54
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD12	4	0.54
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD13	4	0.54
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD21	4	0.54
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD22	4	0.54
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD23	4	0.54
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD11	4	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD12	4	0.54
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD13	4	0.54
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD21	4	0.54
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD22	4	0.54
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD23	4	0.54
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD21	5	0.54
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD22	5	0.54
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD23	5	0.54
(1,921)	1:487:A:LEU:H	1:493:A:LEU:H	3	0.54
(1,794)	1:529:A:THR:HG21	1:532:A:GLY:H	5	0.54
(1,794)	1:529:A:THR:HG22	1:532:A:GLY:H	5	0.54
(1,794)	1:529:A:THR:HG23	1:532:A:GLY:H	5	0.54
(1,742)	1:468:A:GLY:H	1:516:A:GLU:HG2	8	0.54
(1,742)	1:468:A:GLY:H	1:516:A:GLU:HG3	8	0.54
(1,726)	1:492:A:GLU:HG2	1:494:A:THR:H	8	0.54
(1,726)	1:492:A:GLU:HG3	1:494:A:THR:H	8	0.54
(1,663)	1:474:A:GLU:H	1:486:A:TRP:HH2	1	0.54
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB2	6	0.54
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB3	6	0.54
(1,592)	1:519:A:LEU:H	1:540:A:VAL:HG11	4	0.54
(1,592)	1:519:A:LEU:H	1:540:A:VAL:HG12	4	0.54
(1,592)	1:519:A:LEU:H	1:540:A:VAL:HG13	4	0.54
(1,525)	1:525:A:TYR:HA	1:536:A:ALA:H	4	0.54
(1,470)	1:512:A:LEU:H	1:513:A:ILE:HD11	2	0.54
(1,470)	1:512:A:LEU:H	1:513:A:ILE:HD12	2	0.54
(1,470)	1:512:A:LEU:H	1:513:A:ILE:HD13	2	0.54
(1,388)	1:486:A:TRP:HE1	1:510:A:HIS:HA	6	0.54
(1,319)	1:486:A:TRP:HD1	1:503:A:PHE:HD2	6	0.54
(1,41)	1:463:A:GLN:HG2	1:465:A:VAL:HG21	5	0.54
(1,41)	1:463:A:GLN:HG2	1:465:A:VAL:HG22	5	0.54
(1,41)	1:463:A:GLN:HG2	1:465:A:VAL:HG23	5	0.54
(1,41)	1:463:A:GLN:HG3	1:465:A:VAL:HG21	5	0.54
(1,41)	1:463:A:GLN:HG3	1:465:A:VAL:HG22	5	0.54
(1,41)	1:463:A:GLN:HG3	1:465:A:VAL:HG23	5	0.54
(1,1242)	1:506:A:ASP:H	1:509:A:ARG:HB2	1	0.53
(1,1242)	1:506:A:ASP:H	1:509:A:ARG:HB3	1	0.53
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD11	3	0.53
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD12	3	0.53
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD13	3	0.53
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD21	3	0.53
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD22	3	0.53
(1,1172)	1:485:A:LYS:HD2	1:487:A:LEU:HD23	3	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD11	3	0.53
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD12	3	0.53
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD13	3	0.53
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD21	3	0.53
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD22	3	0.53
(1,1172)	1:485:A:LYS:HD3	1:487:A:LEU:HD23	3	0.53
(1,1009)	1:517:A:ALA:HB1	1:521:A:ASP:H	3	0.53
(1,1009)	1:517:A:ALA:HB2	1:521:A:ASP:H	3	0.53
(1,1009)	1:517:A:ALA:HB3	1:521:A:ASP:H	3	0.53
(1,897)	1:459:A:PRO:HA	1:476:A:GLU:H	5	0.53
(1,890)	1:475:A:CYS:H	1:486:A:TRP:HZ2	4	0.53
(1,794)	1:529:A:THR:HG21	1:532:A:GLY:H	3	0.53
(1,794)	1:529:A:THR:HG22	1:532:A:GLY:H	3	0.53
(1,794)	1:529:A:THR:HG23	1:532:A:GLY:H	3	0.53
(1,590)	1:467:A:VAL:HG11	1:519:A:LEU:H	9	0.53
(1,590)	1:467:A:VAL:HG12	1:519:A:LEU:H	9	0.53
(1,590)	1:467:A:VAL:HG13	1:519:A:LEU:H	9	0.53
(1,426)	1:525:A:TYR:H	1:537:A:GLU:HA	4	0.53
(1,316)	1:501:A:TYR:HB2	1:502:A:TRP:HD1	1	0.53
(1,316)	1:501:A:TYR:HB3	1:502:A:TRP:HD1	1	0.53
(1,238)	1:522:A:ALA:HB1	1:540:A:VAL:HG21	7	0.53
(1,238)	1:522:A:ALA:HB1	1:540:A:VAL:HG22	7	0.53
(1,238)	1:522:A:ALA:HB1	1:540:A:VAL:HG23	7	0.53
(1,238)	1:522:A:ALA:HB2	1:540:A:VAL:HG21	7	0.53
(1,238)	1:522:A:ALA:HB2	1:540:A:VAL:HG22	7	0.53
(1,238)	1:522:A:ALA:HB2	1:540:A:VAL:HG23	7	0.53
(1,238)	1:522:A:ALA:HB3	1:540:A:VAL:HG21	7	0.53
(1,238)	1:522:A:ALA:HB3	1:540:A:VAL:HG22	7	0.53
(1,238)	1:522:A:ALA:HB3	1:540:A:VAL:HG23	7	0.53
(1,1261)	1:518:A:MET:HB2	1:518:A:MET:HE1	4	0.52
(1,1261)	1:518:A:MET:HB2	1:518:A:MET:HE2	4	0.52
(1,1261)	1:518:A:MET:HB2	1:518:A:MET:HE3	4	0.52
(1,1261)	1:518:A:MET:HB3	1:518:A:MET:HE1	4	0.52
(1,1261)	1:518:A:MET:HB3	1:518:A:MET:HE2	4	0.52
(1,1261)	1:518:A:MET:HB3	1:518:A:MET:HE3	4	0.52
(1,1023)	1:488:A:LYS:HG2	1:524:A:HIS:H	2	0.52
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD21	3	0.52
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD22	3	0.52
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD23	3	0.52
(1,656)	1:457:A:THR:H	1:476:A:GLU:HG2	2	0.52
(1,650)	1:497:A:GLU:HB2	1:500:A:LYS:H	4	0.52
(1,650)	1:497:A:GLU:HB3	1:500:A:LYS:H	4	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG11	1	0.52
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG12	1	0.52
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG13	1	0.52
(1,611)	1:458:A:ARG:H	1:476:A:GLU:HG3	6	0.52
(1,610)	1:458:A:ARG:H	1:459:A:PRO:HB2	10	0.52
(1,610)	1:458:A:ARG:H	1:459:A:PRO:HB3	10	0.52
(1,548)	1:486:A:TRP:H	1:493:A:LEU:H	9	0.52
(1,390)	1:484:A:VAL:HB	1:486:A:TRP:HE1	1	0.52
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB1	6	0.52
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB2	6	0.52
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB3	6	0.52
(1,311)	1:502:A:TRP:HD1	1:503:A:PHE:H	7	0.52
(1,1261)	1:518:A:MET:HB2	1:518:A:MET:HE1	3	0.51
(1,1261)	1:518:A:MET:HB2	1:518:A:MET:HE2	3	0.51
(1,1261)	1:518:A:MET:HB2	1:518:A:MET:HE3	3	0.51
(1,1261)	1:518:A:MET:HB3	1:518:A:MET:HE1	3	0.51
(1,1261)	1:518:A:MET:HB3	1:518:A:MET:HE2	3	0.51
(1,1261)	1:518:A:MET:HB3	1:518:A:MET:HE3	3	0.51
(1,1261)	1:518:A:MET:HB2	1:518:A:MET:HE1	9	0.51
(1,1261)	1:518:A:MET:HB2	1:518:A:MET:HE2	9	0.51
(1,1261)	1:518:A:MET:HB2	1:518:A:MET:HE3	9	0.51
(1,1261)	1:518:A:MET:HB3	1:518:A:MET:HE1	9	0.51
(1,1261)	1:518:A:MET:HB3	1:518:A:MET:HE2	9	0.51
(1,1261)	1:518:A:MET:HB3	1:518:A:MET:HE3	9	0.51
(1,1072)	1:454:A:VAL:HG11	1:529:A:THR:HB	1	0.51
(1,1072)	1:454:A:VAL:HG12	1:529:A:THR:HB	1	0.51
(1,1072)	1:454:A:VAL:HG13	1:529:A:THR:HB	1	0.51
(1,1072)	1:454:A:VAL:HG21	1:529:A:THR:HB	1	0.51
(1,1072)	1:454:A:VAL:HG22	1:529:A:THR:HB	1	0.51
(1,1072)	1:454:A:VAL:HG23	1:529:A:THR:HB	1	0.51
(1,1001)	1:518:A:MET:H	1:520:A:GLU:H	9	0.51
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD21	7	0.51
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD22	7	0.51
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD23	7	0.51
(1,754)	1:463:A:GLN:HA	1:463:A:GLN:HE21	2	0.51
(1,649)	1:498:A:THR:HG21	1:500:A:LYS:H	8	0.51
(1,649)	1:498:A:THR:HG22	1:500:A:LYS:H	8	0.51
(1,649)	1:498:A:THR:HG23	1:500:A:LYS:H	8	0.51
(1,626)	1:462:A:ASP:HA	1:537:A:GLU:H	10	0.51
(1,561)	1:487:A:LEU:HA	1:491:A:VAL:H	10	0.51
(1,470)	1:512:A:LEU:H	1:513:A:ILE:HD11	8	0.51
(1,470)	1:512:A:LEU:H	1:513:A:ILE:HD12	8	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:512:A:LEU:H	1:513:A:ILE:HD13	8	0.51
(1,316)	1:501:A:TYR:HB2	1:502:A:TRP:HD1	10	0.51
(1,316)	1:501:A:TYR:HB3	1:502:A:TRP:HD1	10	0.51
(1,311)	1:502:A:TRP:HD1	1:503:A:PHE:H	5	0.51
(1,1242)	1:506:A:ASP:H	1:509:A:ARG:HB2	2	0.5
(1,1242)	1:506:A:ASP:H	1:509:A:ARG:HB3	2	0.5
(1,1135)	1:467:A:VAL:HG11	1:542:A:GLU:HG2	5	0.5
(1,1135)	1:467:A:VAL:HG11	1:542:A:GLU:HG3	5	0.5
(1,1135)	1:467:A:VAL:HG12	1:542:A:GLU:HG2	5	0.5
(1,1135)	1:467:A:VAL:HG12	1:542:A:GLU:HG3	5	0.5
(1,1135)	1:467:A:VAL:HG13	1:542:A:GLU:HG2	5	0.5
(1,1135)	1:467:A:VAL:HG13	1:542:A:GLU:HG3	5	0.5
(1,1135)	1:467:A:VAL:HG21	1:542:A:GLU:HG2	5	0.5
(1,1135)	1:467:A:VAL:HG21	1:542:A:GLU:HG3	5	0.5
(1,1135)	1:467:A:VAL:HG22	1:542:A:GLU:HG2	5	0.5
(1,1135)	1:467:A:VAL:HG22	1:542:A:GLU:HG3	5	0.5
(1,1135)	1:467:A:VAL:HG23	1:542:A:GLU:HG2	5	0.5
(1,1135)	1:467:A:VAL:HG23	1:542:A:GLU:HG3	5	0.5
(1,1012)	1:522:A:ALA:H	1:538:A:LEU:HG	4	0.5
(1,784)	1:476:A:GLU:HG3	1:508:A:GLN:HE22	6	0.5
(1,760)	1:465:A:VAL:HA	1:469:A:GLN:HE21	10	0.5
(1,663)	1:474:A:GLU:H	1:486:A:TRP:HH2	2	0.5
(1,650)	1:497:A:GLU:HB2	1:500:A:LYS:H	6	0.5
(1,650)	1:497:A:GLU:HB3	1:500:A:LYS:H	6	0.5
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB2	7	0.5
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB3	7	0.5
(1,477)	1:486:A:TRP:HH2	1:512:A:LEU:H	8	0.5
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD21	3	0.5
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD22	3	0.5
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD23	3	0.5
(1,361)	1:488:A:LYS:HD2	1:489:A:ASP:H	2	0.5
(1,333)	1:456:A:ILE:HG21	1:460:A:LEU:H	7	0.5
(1,333)	1:456:A:ILE:HG22	1:460:A:LEU:H	7	0.5
(1,333)	1:456:A:ILE:HG23	1:460:A:LEU:H	7	0.5
(1,305)	1:505:A:LYS:HB2	1:510:A:HIS:HE1	3	0.5
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD11	4	0.5
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD12	4	0.5
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD13	4	0.5
(1,128)	1:453:A:PRO:HB2	1:531:A:GLY:HA2	4	0.5
(1,1249)	1:509:A:ARG:HG2	1:510:A:HIS:H	10	0.49
(1,1249)	1:509:A:ARG:HG3	1:510:A:HIS:H	10	0.49
(1,1085)	1:456:A:ILE:HD11	1:532:A:GLY:HA2	3	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1085)	1:456:A:ILE:HD11	1:532:A:GLY:HA3	3	0.49
(1,1085)	1:456:A:ILE:HD12	1:532:A:GLY:HA2	3	0.49
(1,1085)	1:456:A:ILE:HD12	1:532:A:GLY:HA3	3	0.49
(1,1085)	1:456:A:ILE:HD13	1:532:A:GLY:HA2	3	0.49
(1,1085)	1:456:A:ILE:HD13	1:532:A:GLY:HA3	3	0.49
(1,1042)	1:459:A:PRO:HB2	1:535:A:LEU:H	2	0.49
(1,1042)	1:459:A:PRO:HB3	1:535:A:LEU:H	2	0.49
(1,1012)	1:522:A:ALA:H	1:538:A:LEU:HG	5	0.49
(1,1012)	1:522:A:ALA:H	1:538:A:LEU:HG	7	0.49
(1,886)	1:475:A:CYS:H	1:509:A:ARG:HA	1	0.49
(1,794)	1:529:A:THR:HG21	1:532:A:GLY:H	7	0.49
(1,794)	1:529:A:THR:HG22	1:532:A:GLY:H	7	0.49
(1,794)	1:529:A:THR:HG23	1:532:A:GLY:H	7	0.49
(1,719)	1:500:A:LYS:HD2	1:501:A:TYR:H	8	0.49
(1,719)	1:500:A:LYS:HD3	1:501:A:TYR:H	8	0.49
(1,514)	1:523:A:GLY:HA2	1:538:A:LEU:H	1	0.49
(1,512)	1:522:A:ALA:HA	1:538:A:LEU:H	7	0.49
(1,463)	1:473:A:PHE:H	1:511:A:HIS:HA	1	0.49
(1,447)	1:472:A:GLU:H	1:513:A:ILE:HA	7	0.49
(1,365)	1:489:A:ASP:H	1:524:A:HIS:H	4	0.49
(1,330)	1:456:A:ILE:HG21	1:459:A:PRO:HB2	1	0.49
(1,330)	1:456:A:ILE:HG21	1:459:A:PRO:HB3	1	0.49
(1,330)	1:456:A:ILE:HG22	1:459:A:PRO:HB2	1	0.49
(1,330)	1:456:A:ILE:HG22	1:459:A:PRO:HB3	1	0.49
(1,330)	1:456:A:ILE:HG23	1:459:A:PRO:HB2	1	0.49
(1,330)	1:456:A:ILE:HG23	1:459:A:PRO:HB3	1	0.49
(1,311)	1:502:A:TRP:HD1	1:503:A:PHE:H	1	0.49
(1,101)	1:457:A:THR:HG21	1:478:A:SER:HA	5	0.49
(1,101)	1:457:A:THR:HG22	1:478:A:SER:HA	5	0.49
(1,101)	1:457:A:THR:HG23	1:478:A:SER:HA	5	0.49
(1,1275)	1:520:A:GLU:H	1:520:A:GLU:HG2	5	0.48
(1,1275)	1:520:A:GLU:H	1:520:A:GLU:HG3	5	0.48
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD11	1	0.48
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD12	1	0.48
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD13	1	0.48
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD21	1	0.48
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD22	1	0.48
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD23	1	0.48
(1,1097)	1:460:A:LEU:HD11	1:476:A:GLU:H	2	0.48
(1,1097)	1:460:A:LEU:HD12	1:476:A:GLU:H	2	0.48
(1,1097)	1:460:A:LEU:HD13	1:476:A:GLU:H	2	0.48
(1,1097)	1:460:A:LEU:HD21	1:476:A:GLU:H	2	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1097)	1:460:A:LEU:HD22	1:476:A:GLU:H	2	0.48
(1,1097)	1:460:A:LEU:HD23	1:476:A:GLU:H	2	0.48
(1,1063)	1:453:A:PRO:HB2	1:531:A:GLY:H	2	0.48
(1,1063)	1:453:A:PRO:HB3	1:531:A:GLY:H	2	0.48
(1,930)	1:487:A:LEU:HB3	1:488:A:LYS:H	7	0.48
(1,843)	1:456:A:ILE:H	1:458:A:ARG:H	9	0.48
(1,802)	1:523:A:GLY:H	1:539:A:ILE:HA	2	0.48
(1,754)	1:463:A:GLN:HA	1:463:A:GLN:HE21	1	0.48
(1,754)	1:463:A:GLN:HA	1:463:A:GLN:HE21	3	0.48
(1,754)	1:463:A:GLN:HA	1:463:A:GLN:HE21	7	0.48
(1,684)	1:504:A:LYS:H	1:513:A:ILE:HD11	2	0.48
(1,684)	1:504:A:LYS:H	1:513:A:ILE:HD12	2	0.48
(1,684)	1:504:A:LYS:H	1:513:A:ILE:HD13	2	0.48
(1,548)	1:486:A:TRP:H	1:493:A:LEU:H	5	0.48
(1,492)	1:464:A:LEU:HA	1:540:A:VAL:H	10	0.48
(1,463)	1:473:A:PHE:H	1:511:A:HIS:HA	5	0.48
(1,434)	1:456:A:ILE:HD11	1:534:A:ALA:H	5	0.48
(1,434)	1:456:A:ILE:HD12	1:534:A:ALA:H	5	0.48
(1,434)	1:456:A:ILE:HD13	1:534:A:ALA:H	5	0.48
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD21	1	0.48
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD22	1	0.48
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD23	1	0.48
(1,384)	1:486:A:TRP:HE1	1:510:A:HIS:HB3	7	0.48
(1,374)	1:490:A:GLY:H	1:525:A:TYR:HA	10	0.48
(1,369)	1:502:A:TRP:HE1	1:513:A:ILE:HD11	9	0.48
(1,369)	1:502:A:TRP:HE1	1:513:A:ILE:HD12	9	0.48
(1,369)	1:502:A:TRP:HE1	1:513:A:ILE:HD13	9	0.48
(1,311)	1:502:A:TRP:HD1	1:503:A:PHE:H	10	0.48
(1,248)	1:460:A:LEU:HB2	1:526:A:ALA:HA	8	0.48
(1,248)	1:460:A:LEU:HB3	1:526:A:ALA:HA	8	0.48
(1,143)	1:495:A:ARG:HA	1:495:A:ARG:HD2	4	0.48
(1,143)	1:495:A:ARG:HA	1:495:A:ARG:HD3	4	0.48
(1,1313)	1:542:A:GLU:HB2	1:543:A:LYS:H	2	0.47
(1,1313)	1:542:A:GLU:HB3	1:543:A:LYS:H	2	0.47
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD11	8	0.47
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD12	8	0.47
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD13	8	0.47
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD21	8	0.47
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD22	8	0.47
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD23	8	0.47
(1,985)	1:470:A:ARG:HB2	1:516:A:GLU:H	3	0.47
(1,879)	1:470:A:ARG:H	1:516:A:GLU:HA	4	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,843)	1:456:A:ILE:H	1:458:A:ARG:H	6	0.47
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG21	7	0.47
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG22	7	0.47
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG23	7	0.47
(1,656)	1:457:A:THR:H	1:476:A:GLU:HG2	5	0.47
(1,626)	1:462:A:ASP:HA	1:537:A:GLU:H	8	0.47
(1,583)	1:528:A:CYS:H	1:533:A:GLN:HA	7	0.47
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG21	3	0.47
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG22	3	0.47
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG23	3	0.47
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD21	4	0.47
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD22	4	0.47
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD23	4	0.47
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD11	7	0.47
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD12	7	0.47
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD13	7	0.47
(1,158)	1:508:A:GLN:HA	1:510:A:HIS:HD2	1	0.47
(1,1158)	1:473:A:PHE:HB2	1:512:A:LEU:H	9	0.46
(1,1158)	1:473:A:PHE:HB3	1:512:A:LEU:H	9	0.46
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA2	7	0.46
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA3	7	0.46
(1,1032)	1:529:A:THR:H	1:532:A:GLY:H	2	0.46
(1,970)	1:470:A:ARG:HA	1:514:A:ILE:H	2	0.46
(1,818)	1:523:A:GLY:H	1:538:A:LEU:HB3	2	0.46
(1,818)	1:523:A:GLY:H	1:538:A:LEU:HB3	8	0.46
(1,771)	1:457:A:THR:HG21	1:478:A:SER:H	5	0.46
(1,771)	1:457:A:THR:HG22	1:478:A:SER:H	5	0.46
(1,771)	1:457:A:THR:HG23	1:478:A:SER:H	5	0.46
(1,754)	1:463:A:GLN:HA	1:463:A:GLN:HE21	10	0.46
(1,636)	1:487:A:LEU:HB2	1:526:A:ALA:H	3	0.46
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG21	9	0.46
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG22	9	0.46
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG23	9	0.46
(1,561)	1:487:A:LEU:HA	1:491:A:VAL:H	2	0.46
(1,455)	1:505:A:LYS:HD2	1:506:A:ASP:H	10	0.46
(1,455)	1:505:A:LYS:HD3	1:506:A:ASP:H	10	0.46
(1,449)	1:463:A:GLN:HE22	1:472:A:GLU:H	6	0.46
(1,360)	1:487:A:LEU:HG	1:489:A:ASP:H	7	0.46
(1,330)	1:456:A:ILE:HG21	1:459:A:PRO:HB2	5	0.46
(1,330)	1:456:A:ILE:HG21	1:459:A:PRO:HB3	5	0.46
(1,330)	1:456:A:ILE:HG22	1:459:A:PRO:HB2	5	0.46
(1,330)	1:456:A:ILE:HG22	1:459:A:PRO:HB3	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:456:A:ILE:HG23	1:459:A:PRO:HB2	5	0.46
(1,330)	1:456:A:ILE:HG23	1:459:A:PRO:HB3	5	0.46
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG21	1	0.46
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG22	1	0.46
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG23	1	0.46
(1,43)	1:465:A:VAL:HG21	1:471:A:VAL:HA	6	0.46
(1,43)	1:465:A:VAL:HG22	1:471:A:VAL:HA	6	0.46
(1,43)	1:465:A:VAL:HG23	1:471:A:VAL:HA	6	0.46
(1,1083)	1:456:A:ILE:HD11	1:527:A:LEU:HB2	8	0.45
(1,1083)	1:456:A:ILE:HD11	1:527:A:LEU:HB3	8	0.45
(1,1083)	1:456:A:ILE:HD12	1:527:A:LEU:HB2	8	0.45
(1,1083)	1:456:A:ILE:HD12	1:527:A:LEU:HB3	8	0.45
(1,1083)	1:456:A:ILE:HD13	1:527:A:LEU:HB2	8	0.45
(1,1083)	1:456:A:ILE:HD13	1:527:A:LEU:HB3	8	0.45
(1,996)	1:516:A:GLU:HG2	1:517:A:ALA:H	3	0.45
(1,996)	1:516:A:GLU:HG3	1:517:A:ALA:H	3	0.45
(1,843)	1:456:A:ILE:H	1:458:A:ARG:H	10	0.45
(1,791)	1:529:A:THR:HB	1:532:A:GLY:H	3	0.45
(1,624)	1:462:A:ASP:HB3	1:537:A:GLU:H	8	0.45
(1,624)	1:462:A:ASP:HB2	1:537:A:GLU:H	8	0.45
(1,610)	1:458:A:ARG:H	1:459:A:PRO:HB2	2	0.45
(1,610)	1:458:A:ARG:H	1:459:A:PRO:HB3	2	0.45
(1,601)	1:458:A:ARG:H	1:459:A:PRO:HD2	7	0.45
(1,502)	1:473:A:PHE:H	1:513:A:ILE:HD11	3	0.45
(1,502)	1:473:A:PHE:H	1:513:A:ILE:HD12	3	0.45
(1,502)	1:473:A:PHE:H	1:513:A:ILE:HD13	3	0.45
(1,361)	1:488:A:LYS:HD2	1:489:A:ASP:H	4	0.45
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB1	5	0.45
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB2	5	0.45
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB3	5	0.45
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB1	5	0.45
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB2	5	0.45
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB3	5	0.45
(1,321)	1:493:A:LEU:HD11	1:501:A:TYR:HE2	6	0.45
(1,321)	1:493:A:LEU:HD12	1:501:A:TYR:HE2	6	0.45
(1,321)	1:493:A:LEU:HD13	1:501:A:TYR:HE2	6	0.45
(1,220)	1:468:A:GLY:HA2	1:516:A:GLU:HG2	4	0.45
(1,220)	1:468:A:GLY:HA2	1:516:A:GLU:HG3	4	0.45
(1,144)	1:519:A:LEU:H	1:519:A:LEU:HG	6	0.45
(1,85)	1:457:A:THR:HG21	1:477:A:VAL:HA	7	0.45
(1,85)	1:457:A:THR:HG22	1:477:A:VAL:HA	7	0.45
(1,85)	1:457:A:THR:HG23	1:477:A:VAL:HA	7	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD11	10	0.44
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD12	10	0.44
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD13	10	0.44
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD21	10	0.44
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD22	10	0.44
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD23	10	0.44
(1,1014)	1:524:A:HIS:H	1:537:A:GLU:HA	8	0.44
(1,1012)	1:522:A:ALA:H	1:538:A:LEU:HG	6	0.44
(1,985)	1:470:A:ARG:HB2	1:516:A:GLU:H	7	0.44
(1,863)	1:463:A:GLN:H	1:538:A:LEU:HD11	9	0.44
(1,863)	1:463:A:GLN:H	1:538:A:LEU:HD12	9	0.44
(1,863)	1:463:A:GLN:H	1:538:A:LEU:HD13	9	0.44
(1,602)	1:458:A:ARG:H	1:477:A:VAL:HA	2	0.44
(1,502)	1:473:A:PHE:H	1:513:A:ILE:HD11	8	0.44
(1,502)	1:473:A:PHE:H	1:513:A:ILE:HD12	8	0.44
(1,502)	1:473:A:PHE:H	1:513:A:ILE:HD13	8	0.44
(1,472)	1:472:A:GLU:HG2	1:512:A:LEU:H	6	0.44
(1,472)	1:472:A:GLU:HG3	1:512:A:LEU:H	6	0.44
(1,463)	1:473:A:PHE:H	1:511:A:HIS:HA	7	0.44
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD21	2	0.44
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD22	2	0.44
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD23	2	0.44
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB1	6	0.44
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB2	6	0.44
(1,342)	1:459:A:PRO:HB2	1:534:A:ALA:HB3	6	0.44
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB1	6	0.44
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB2	6	0.44
(1,342)	1:459:A:PRO:HB3	1:534:A:ALA:HB3	6	0.44
(1,331)	1:456:A:ILE:HG21	1:459:A:PRO:HA	9	0.44
(1,331)	1:456:A:ILE:HG22	1:459:A:PRO:HA	9	0.44
(1,331)	1:456:A:ILE:HG23	1:459:A:PRO:HA	9	0.44
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB2	1	0.44
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB3	1	0.44
(1,85)	1:457:A:THR:HG21	1:477:A:VAL:HA	1	0.44
(1,85)	1:457:A:THR:HG22	1:477:A:VAL:HA	1	0.44
(1,85)	1:457:A:THR:HG23	1:477:A:VAL:HA	1	0.44
(1,59)	1:468:A:GLY:HA3	1:516:A:GLU:HG2	3	0.44
(1,59)	1:468:A:GLY:HA3	1:516:A:GLU:HG3	3	0.44
(1,19)	1:457:A:THR:HG21	1:478:A:SER:HB2	2	0.44
(1,19)	1:457:A:THR:HG21	1:478:A:SER:HB3	2	0.44
(1,19)	1:457:A:THR:HG22	1:478:A:SER:HB2	2	0.44
(1,19)	1:457:A:THR:HG22	1:478:A:SER:HB3	2	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:457:A:THR:HG23	1:478:A:SER:HB2	2	0.44
(1,19)	1:457:A:THR:HG23	1:478:A:SER:HB3	2	0.44
(1,1243)	1:506:A:ASP:H	1:509:A:ARG:HG2	3	0.43
(1,1243)	1:506:A:ASP:H	1:509:A:ARG:HG3	3	0.43
(1,1227)	1:500:A:LYS:HE2	1:518:A:MET:HG2	10	0.43
(1,1227)	1:500:A:LYS:HE2	1:518:A:MET:HG3	10	0.43
(1,1227)	1:500:A:LYS:HE3	1:518:A:MET:HG2	10	0.43
(1,1227)	1:500:A:LYS:HE3	1:518:A:MET:HG3	10	0.43
(1,1123)	1:466:A:MET:HG2	1:469:A:GLN:HG2	2	0.43
(1,1123)	1:466:A:MET:HG2	1:469:A:GLN:HG3	2	0.43
(1,1123)	1:466:A:MET:HG3	1:469:A:GLN:HG2	2	0.43
(1,1123)	1:466:A:MET:HG3	1:469:A:GLN:HG3	2	0.43
(1,1097)	1:460:A:LEU:HD11	1:476:A:GLU:H	8	0.43
(1,1097)	1:460:A:LEU:HD12	1:476:A:GLU:H	8	0.43
(1,1097)	1:460:A:LEU:HD13	1:476:A:GLU:H	8	0.43
(1,1097)	1:460:A:LEU:HD21	1:476:A:GLU:H	8	0.43
(1,1097)	1:460:A:LEU:HD22	1:476:A:GLU:H	8	0.43
(1,1097)	1:460:A:LEU:HD23	1:476:A:GLU:H	8	0.43
(1,1023)	1:488:A:LYS:HG2	1:524:A:HIS:H	9	0.43
(1,996)	1:516:A:GLU:HG2	1:517:A:ALA:H	9	0.43
(1,996)	1:516:A:GLU:HG3	1:517:A:ALA:H	9	0.43
(1,985)	1:470:A:ARG:HB2	1:516:A:GLU:H	9	0.43
(1,911)	1:458:A:ARG:H	1:478:A:SER:H	1	0.43
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD21	6	0.43
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD22	6	0.43
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD23	6	0.43
(1,765)	1:502:A:TRP:HZ2	1:515:A:ASN:HD22	7	0.43
(1,760)	1:465:A:VAL:HA	1:469:A:GLN:HE21	8	0.43
(1,754)	1:463:A:GLN:HA	1:463:A:GLN:HE21	6	0.43
(1,754)	1:463:A:GLN:HA	1:463:A:GLN:HE21	8	0.43
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG21	9	0.43
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG22	9	0.43
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG23	9	0.43
(1,428)	1:525:A:TYR:H	1:537:A:GLU:HB2	4	0.43
(1,428)	1:525:A:TYR:H	1:537:A:GLU:HB3	4	0.43
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB2	9	0.43
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB3	9	0.43
(1,248)	1:460:A:LEU:HB2	1:526:A:ALA:HA	5	0.43
(1,248)	1:460:A:LEU:HB3	1:526:A:ALA:HA	5	0.43
(1,220)	1:468:A:GLY:HA2	1:516:A:GLU:HG2	8	0.43
(1,220)	1:468:A:GLY:HA2	1:516:A:GLU:HG3	8	0.43
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG11	1	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG12	1	0.43
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG13	1	0.43
(1,1242)	1:506:A:ASP:H	1:509:A:ARG:HB2	10	0.42
(1,1242)	1:506:A:ASP:H	1:509:A:ARG:HB3	10	0.42
(1,1217)	1:496:A:GLU:H	1:496:A:GLU:HB2	1	0.42
(1,1217)	1:496:A:GLU:H	1:496:A:GLU:HB3	1	0.42
(1,1037)	1:456:A:ILE:HD11	1:529:A:THR:H	7	0.42
(1,1037)	1:456:A:ILE:HD12	1:529:A:THR:H	7	0.42
(1,1037)	1:456:A:ILE:HD13	1:529:A:THR:H	7	0.42
(1,911)	1:458:A:ARG:H	1:478:A:SER:H	6	0.42
(1,897)	1:459:A:PRO:HA	1:476:A:GLU:H	1	0.42
(1,791)	1:529:A:THR:HB	1:532:A:GLY:H	5	0.42
(1,719)	1:500:A:LYS:HD2	1:501:A:TYR:H	5	0.42
(1,719)	1:500:A:LYS:HD3	1:501:A:TYR:H	5	0.42
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG21	7	0.42
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG22	7	0.42
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG23	7	0.42
(1,562)	1:488:A:LYS:H	1:491:A:VAL:H	5	0.42
(1,514)	1:523:A:GLY:HA2	1:538:A:LEU:H	10	0.42
(1,472)	1:472:A:GLU:HG2	1:512:A:LEU:H	4	0.42
(1,472)	1:472:A:GLU:HG3	1:512:A:LEU:H	4	0.42
(1,309)	1:524:A:HIS:HE1	1:537:A:GLU:HB2	3	0.42
(1,309)	1:524:A:HIS:HE1	1:537:A:GLU:HB3	3	0.42
(1,29)	1:456:A:ILE:HD11	1:533:A:GLN:HA	4	0.42
(1,29)	1:456:A:ILE:HD12	1:533:A:GLN:HA	4	0.42
(1,29)	1:456:A:ILE:HD13	1:533:A:GLN:HA	4	0.42
(1,1295)	1:532:A:GLY:H	1:533:A:GLN:HB2	5	0.41
(1,1295)	1:532:A:GLY:H	1:533:A:GLN:HB3	5	0.41
(1,1270)	1:519:A:LEU:HD11	1:541:A:GLN:HA	7	0.41
(1,1270)	1:519:A:LEU:HD12	1:541:A:GLN:HA	7	0.41
(1,1270)	1:519:A:LEU:HD13	1:541:A:GLN:HA	7	0.41
(1,1270)	1:519:A:LEU:HD21	1:541:A:GLN:HA	7	0.41
(1,1270)	1:519:A:LEU:HD22	1:541:A:GLN:HA	7	0.41
(1,1270)	1:519:A:LEU:HD23	1:541:A:GLN:HA	7	0.41
(1,1194)	1:488:A:LYS:HB2	1:493:A:LEU:HD11	6	0.41
(1,1194)	1:488:A:LYS:HB2	1:493:A:LEU:HD12	6	0.41
(1,1194)	1:488:A:LYS:HB2	1:493:A:LEU:HD13	6	0.41
(1,1194)	1:488:A:LYS:HB2	1:493:A:LEU:HD21	6	0.41
(1,1194)	1:488:A:LYS:HB2	1:493:A:LEU:HD22	6	0.41
(1,1194)	1:488:A:LYS:HB2	1:493:A:LEU:HD23	6	0.41
(1,1194)	1:488:A:LYS:HB3	1:493:A:LEU:HD11	6	0.41
(1,1194)	1:488:A:LYS:HB3	1:493:A:LEU:HD12	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1194)	1:488:A:LYS:HB3	1:493:A:LEU:HD13	6	0.41
(1,1194)	1:488:A:LYS:HB3	1:493:A:LEU:HD21	6	0.41
(1,1194)	1:488:A:LYS:HB3	1:493:A:LEU:HD22	6	0.41
(1,1194)	1:488:A:LYS:HB3	1:493:A:LEU:HD23	6	0.41
(1,1185)	1:487:A:LEU:HD11	1:492:A:GLU:H	2	0.41
(1,1185)	1:487:A:LEU:HD12	1:492:A:GLU:H	2	0.41
(1,1185)	1:487:A:LEU:HD13	1:492:A:GLU:H	2	0.41
(1,1185)	1:487:A:LEU:HD21	1:492:A:GLU:H	2	0.41
(1,1185)	1:487:A:LEU:HD22	1:492:A:GLU:H	2	0.41
(1,1185)	1:487:A:LEU:HD23	1:492:A:GLU:H	2	0.41
(1,1032)	1:529:A:THR:H	1:532:A:GLY:H	3	0.41
(1,985)	1:470:A:ARG:HB2	1:516:A:GLU:H	5	0.41
(1,897)	1:459:A:PRO:HA	1:476:A:GLU:H	6	0.41
(1,890)	1:475:A:CYS:H	1:486:A:TRP:HZ2	6	0.41
(1,871)	1:487:A:LEU:HG	1:488:A:LYS:H	7	0.41
(1,754)	1:463:A:GLN:HA	1:463:A:GLN:HE21	9	0.41
(1,747)	1:460:A:LEU:H	1:534:A:ALA:HA	7	0.41
(1,601)	1:458:A:ARG:H	1:459:A:PRO:HD2	2	0.41
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD21	6	0.41
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD22	6	0.41
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD23	6	0.41
(1,1313)	1:542:A:GLU:HB2	1:543:A:LYS:H	9	0.4
(1,1313)	1:542:A:GLU:HB3	1:543:A:LYS:H	9	0.4
(1,1186)	1:487:A:LEU:HD11	1:492:A:GLU:HA	2	0.4
(1,1186)	1:487:A:LEU:HD12	1:492:A:GLU:HA	2	0.4
(1,1186)	1:487:A:LEU:HD13	1:492:A:GLU:HA	2	0.4
(1,1186)	1:487:A:LEU:HD21	1:492:A:GLU:HA	2	0.4
(1,1186)	1:487:A:LEU:HD22	1:492:A:GLU:HA	2	0.4
(1,1186)	1:487:A:LEU:HD23	1:492:A:GLU:HA	2	0.4
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD11	8	0.4
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD12	8	0.4
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD13	8	0.4
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD21	8	0.4
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD22	8	0.4
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD23	8	0.4
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD11	8	0.4
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD12	8	0.4
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD13	8	0.4
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD21	8	0.4
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD22	8	0.4
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD23	8	0.4
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD11	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD12	8	0.4
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD13	8	0.4
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD21	8	0.4
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD22	8	0.4
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD23	8	0.4
(1,1020)	1:524:A:HIS:H	1:524:A:HIS:HD2	2	0.4
(1,937)	1:496:A:GLU:H	1:497:A:GLU:H	1	0.4
(1,610)	1:458:A:ARG:H	1:459:A:PRO:HB2	6	0.4
(1,610)	1:458:A:ARG:H	1:459:A:PRO:HB3	6	0.4
(1,562)	1:488:A:LYS:H	1:491:A:VAL:H	8	0.4
(1,511)	1:525:A:TYR:HB2	1:538:A:LEU:H	4	0.4
(1,449)	1:463:A:GLN:HE22	1:472:A:GLU:H	3	0.4
(1,434)	1:456:A:ILE:HD11	1:534:A:ALA:H	7	0.4
(1,434)	1:456:A:ILE:HD12	1:534:A:ALA:H	7	0.4
(1,434)	1:456:A:ILE:HD13	1:534:A:ALA:H	7	0.4
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD21	8	0.4
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD22	8	0.4
(1,418)	1:464:A:LEU:H	1:464:A:LEU:HD23	8	0.4
(1,408)	1:487:A:LEU:HA	1:493:A:LEU:H	6	0.4
(1,387)	1:486:A:TRP:HE1	1:503:A:PHE:HA	8	0.4
(1,383)	1:486:A:TRP:HE1	1:511:A:HIS:H	3	0.4
(1,382)	1:455:A:LEU:H	1:479:A:GLU:H	4	0.4
(1,374)	1:490:A:GLY:H	1:525:A:TYR:HA	5	0.4
(1,352)	1:464:A:LEU:HB2	1:539:A:ILE:H	1	0.4
(1,352)	1:464:A:LEU:HB2	1:539:A:ILE:H	2	0.4
(1,352)	1:464:A:LEU:HB2	1:539:A:ILE:H	6	0.4
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG21	8	0.4
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG22	8	0.4
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG23	8	0.4
(1,214)	1:500:A:LYS:HG2	1:514:A:ILE:HG21	3	0.4
(1,214)	1:500:A:LYS:HG2	1:514:A:ILE:HG22	3	0.4
(1,214)	1:500:A:LYS:HG2	1:514:A:ILE:HG23	3	0.4
(1,214)	1:500:A:LYS:HG3	1:514:A:ILE:HG21	3	0.4
(1,214)	1:500:A:LYS:HG3	1:514:A:ILE:HG22	3	0.4
(1,214)	1:500:A:LYS:HG3	1:514:A:ILE:HG23	3	0.4
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG11	7	0.4
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG12	7	0.4
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG13	7	0.4
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG11	8	0.4
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG12	8	0.4
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG13	8	0.4
(1,1238)	1:505:A:LYS:HB2	1:505:A:LYS:HE2	9	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1238)	1:505:A:LYS:HB2	1:505:A:LYS:HE3	9	0.39
(1,1238)	1:505:A:LYS:HB3	1:505:A:LYS:HE2	9	0.39
(1,1238)	1:505:A:LYS:HB3	1:505:A:LYS:HE3	9	0.39
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD11	3	0.39
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD12	3	0.39
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD13	3	0.39
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD21	3	0.39
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD22	3	0.39
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD23	3	0.39
(1,970)	1:470:A:ARG:HA	1:514:A:ILE:H	3	0.39
(1,795)	1:456:A:ILE:HD11	1:532:A:GLY:H	6	0.39
(1,795)	1:456:A:ILE:HD12	1:532:A:GLY:H	6	0.39
(1,795)	1:456:A:ILE:HD13	1:532:A:GLY:H	6	0.39
(1,730)	1:498:A:THR:H	1:498:A:THR:HG21	8	0.39
(1,730)	1:498:A:THR:H	1:498:A:THR:HG22	8	0.39
(1,730)	1:498:A:THR:H	1:498:A:THR:HG23	8	0.39
(1,652)	1:457:A:THR:H	1:457:A:THR:HG21	7	0.39
(1,652)	1:457:A:THR:H	1:457:A:THR:HG22	7	0.39
(1,652)	1:457:A:THR:H	1:457:A:THR:HG23	7	0.39
(1,650)	1:497:A:GLU:HB2	1:500:A:LYS:H	1	0.39
(1,650)	1:497:A:GLU:HB3	1:500:A:LYS:H	1	0.39
(1,583)	1:528:A:CYS:H	1:533:A:GLN:HA	1	0.39
(1,562)	1:488:A:LYS:H	1:491:A:VAL:H	7	0.39
(1,514)	1:523:A:GLY:HA2	1:538:A:LEU:H	2	0.39
(1,438)	1:471:A:VAL:H	1:471:A:VAL:HB	8	0.39
(1,1037)	1:456:A:ILE:HD11	1:529:A:THR:H	8	0.38
(1,1037)	1:456:A:ILE:HD12	1:529:A:THR:H	8	0.38
(1,1037)	1:456:A:ILE:HD13	1:529:A:THR:H	8	0.38
(1,1024)	1:460:A:LEU:HB2	1:525:A:TYR:H	3	0.38
(1,1024)	1:460:A:LEU:HB3	1:525:A:TYR:H	3	0.38
(1,996)	1:516:A:GLU:HG2	1:517:A:ALA:H	4	0.38
(1,996)	1:516:A:GLU:HG3	1:517:A:ALA:H	4	0.38
(1,921)	1:487:A:LEU:H	1:493:A:LEU:H	8	0.38
(1,803)	1:523:A:GLY:H	1:525:A:TYR:HD1	6	0.38
(1,802)	1:523:A:GLY:H	1:539:A:ILE:HA	7	0.38
(1,726)	1:492:A:GLU:HG2	1:494:A:THR:H	6	0.38
(1,726)	1:492:A:GLU:HG3	1:494:A:THR:H	6	0.38
(1,652)	1:457:A:THR:H	1:457:A:THR:HG21	10	0.38
(1,652)	1:457:A:THR:H	1:457:A:THR:HG22	10	0.38
(1,652)	1:457:A:THR:H	1:457:A:THR:HG23	10	0.38
(1,492)	1:464:A:LEU:HA	1:540:A:VAL:H	8	0.38
(1,481)	1:472:A:GLU:HA	1:512:A:LEU:H	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,480)	1:473:A:PHE:H	1:512:A:LEU:H	9	0.38
(1,477)	1:486:A:TRP:HH2	1:512:A:LEU:H	5	0.38
(1,444)	1:472:A:GLU:H	1:514:A:ILE:HB	1	0.38
(1,434)	1:456:A:ILE:HD11	1:534:A:ALA:H	4	0.38
(1,434)	1:456:A:ILE:HD12	1:534:A:ALA:H	4	0.38
(1,434)	1:456:A:ILE:HD13	1:534:A:ALA:H	4	0.38
(1,387)	1:486:A:TRP:HE1	1:503:A:PHE:HA	1	0.38
(1,387)	1:486:A:TRP:HE1	1:503:A:PHE:HA	7	0.38
(1,318)	1:486:A:TRP:HD1	1:503:A:PHE:HE2	8	0.38
(1,272)	1:539:A:ILE:HG21	1:541:A:GLN:HG2	5	0.38
(1,272)	1:539:A:ILE:HG21	1:541:A:GLN:HG3	5	0.38
(1,272)	1:539:A:ILE:HG22	1:541:A:GLN:HG2	5	0.38
(1,272)	1:539:A:ILE:HG22	1:541:A:GLN:HG3	5	0.38
(1,272)	1:539:A:ILE:HG23	1:541:A:GLN:HG2	5	0.38
(1,272)	1:539:A:ILE:HG23	1:541:A:GLN:HG3	5	0.38
(1,181)	1:470:A:ARG:HB3	1:513:A:ILE:HG21	5	0.38
(1,181)	1:470:A:ARG:HB3	1:513:A:ILE:HG22	5	0.38
(1,181)	1:470:A:ARG:HB3	1:513:A:ILE:HG23	5	0.38
(1,150)	1:486:A:TRP:HZ2	1:503:A:PHE:HB3	5	0.38
(1,82)	1:529:A:THR:HG21	1:533:A:GLN:HA	9	0.38
(1,82)	1:529:A:THR:HG22	1:533:A:GLN:HA	9	0.38
(1,82)	1:529:A:THR:HG23	1:533:A:GLN:HA	9	0.38
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB1	8	0.38
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB2	8	0.38
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB3	8	0.38
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB1	8	0.38
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB2	8	0.38
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB3	8	0.38
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB1	8	0.38
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB2	8	0.38
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB3	8	0.38
(1,16)	1:459:A:PRO:HA	1:534:A:ALA:HB1	8	0.38
(1,16)	1:459:A:PRO:HA	1:534:A:ALA:HB2	8	0.38
(1,16)	1:459:A:PRO:HA	1:534:A:ALA:HB3	8	0.38
(1,1300)	1:533:A:GLN:HB2	1:535:A:LEU:H	9	0.37
(1,1300)	1:533:A:GLN:HB3	1:535:A:LEU:H	9	0.37
(1,1295)	1:532:A:GLY:H	1:533:A:GLN:HB2	2	0.37
(1,1295)	1:532:A:GLY:H	1:533:A:GLN:HB3	2	0.37
(1,1052)	1:465:A:VAL:H	1:539:A:ILE:H	6	0.37
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB1	2	0.37
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB2	2	0.37
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB3	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB1	10	0.37
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB2	10	0.37
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB3	10	0.37
(1,777)	1:455:A:LEU:H	1:478:A:SER:H	8	0.37
(1,752)	1:459:A:PRO:HG2	1:460:A:LEU:H	10	0.37
(1,752)	1:459:A:PRO:HG3	1:460:A:LEU:H	10	0.37
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG21	4	0.37
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG22	4	0.37
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG23	4	0.37
(1,601)	1:458:A:ARG:H	1:459:A:PRO:HD2	10	0.37
(1,504)	1:473:A:PHE:H	1:512:A:LEU:HB2	2	0.37
(1,503)	1:473:A:PHE:H	1:513:A:ILE:HG13	3	0.37
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD11	4	0.37
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD12	4	0.37
(1,432)	1:525:A:TYR:H	1:538:A:LEU:HD13	4	0.37
(1,426)	1:525:A:TYR:H	1:537:A:GLU:HA	7	0.37
(1,376)	1:487:A:LEU:HB3	1:490:A:GLY:H	10	0.37
(1,374)	1:490:A:GLY:H	1:525:A:TYR:HA	4	0.37
(1,352)	1:464:A:LEU:HB2	1:539:A:ILE:H	7	0.37
(1,316)	1:501:A:TYR:HB2	1:502:A:TRP:HD1	6	0.37
(1,316)	1:501:A:TYR:HB3	1:502:A:TRP:HD1	6	0.37
(1,220)	1:468:A:GLY:HA2	1:516:A:GLU:HG2	7	0.37
(1,220)	1:468:A:GLY:HA2	1:516:A:GLU:HG3	7	0.37
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD21	5	0.37
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD22	5	0.37
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD23	5	0.37
(1,142)	1:460:A:LEU:HD11	1:475:A:CYS:HB3	2	0.37
(1,142)	1:460:A:LEU:HD12	1:475:A:CYS:HB3	2	0.37
(1,142)	1:460:A:LEU:HD13	1:475:A:CYS:HB3	2	0.37
(1,61)	1:488:A:LYS:HA	1:488:A:LYS:HD3	4	0.37
(1,56)	1:467:A:VAL:HG11	1:518:A:MET:HA	9	0.37
(1,56)	1:467:A:VAL:HG12	1:518:A:MET:HA	9	0.37
(1,56)	1:467:A:VAL:HG13	1:518:A:MET:HA	9	0.37
(1,50)	1:465:A:VAL:HG11	1:471:A:VAL:HB	6	0.37
(1,50)	1:465:A:VAL:HG12	1:471:A:VAL:HB	6	0.37
(1,50)	1:465:A:VAL:HG13	1:471:A:VAL:HB	6	0.37
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD11	2	0.36
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD12	2	0.36
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD13	2	0.36
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD21	2	0.36
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD22	2	0.36
(1,1302)	1:533:A:GLN:HE21	1:535:A:LEU:HD23	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD11	2	0.36
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD12	2	0.36
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD13	2	0.36
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD21	2	0.36
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD22	2	0.36
(1,1302)	1:533:A:GLN:HE22	1:535:A:LEU:HD23	2	0.36
(1,1300)	1:533:A:GLN:HB2	1:535:A:LEU:H	8	0.36
(1,1300)	1:533:A:GLN:HB3	1:535:A:LEU:H	8	0.36
(1,1264)	1:518:A:MET:HG2	1:519:A:LEU:H	8	0.36
(1,1264)	1:518:A:MET:HG3	1:519:A:LEU:H	8	0.36
(1,1248)	1:509:A:ARG:HB2	1:511:A:HIS:HE1	8	0.36
(1,1248)	1:509:A:ARG:HB3	1:511:A:HIS:HE1	8	0.36
(1,1238)	1:505:A:LYS:HB2	1:505:A:LYS:HE2	5	0.36
(1,1238)	1:505:A:LYS:HB2	1:505:A:LYS:HE3	5	0.36
(1,1238)	1:505:A:LYS:HB3	1:505:A:LYS:HE2	5	0.36
(1,1238)	1:505:A:LYS:HB3	1:505:A:LYS:HE3	5	0.36
(1,1143)	1:471:A:VAL:HG11	1:472:A:GLU:H	8	0.36
(1,1143)	1:471:A:VAL:HG12	1:472:A:GLU:H	8	0.36
(1,1143)	1:471:A:VAL:HG13	1:472:A:GLU:H	8	0.36
(1,1143)	1:471:A:VAL:HG21	1:472:A:GLU:H	8	0.36
(1,1143)	1:471:A:VAL:HG22	1:472:A:GLU:H	8	0.36
(1,1143)	1:471:A:VAL:HG23	1:472:A:GLU:H	8	0.36
(1,958)	1:474:A:GLU:HA	1:511:A:HIS:H	6	0.36
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB1	4	0.36
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB2	4	0.36
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB3	4	0.36
(1,843)	1:456:A:ILE:H	1:458:A:ARG:H	1	0.36
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD21	2	0.36
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD22	2	0.36
(1,820)	1:523:A:GLY:H	1:538:A:LEU:HD23	2	0.36
(1,792)	1:454:A:VAL:HB	1:532:A:GLY:H	7	0.36
(1,778)	1:478:A:SER:HA	1:508:A:GLN:HE21	1	0.36
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG21	1	0.36
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG22	1	0.36
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG23	1	0.36
(1,652)	1:457:A:THR:H	1:457:A:THR:HG21	2	0.36
(1,652)	1:457:A:THR:H	1:457:A:THR:HG22	2	0.36
(1,652)	1:457:A:THR:H	1:457:A:THR:HG23	2	0.36
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB2	8	0.36
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB3	8	0.36
(1,610)	1:458:A:ARG:H	1:459:A:PRO:HB2	1	0.36
(1,610)	1:458:A:ARG:H	1:459:A:PRO:HB3	1	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	1:458:A:ARG:H	1:459:A:PRO:HB2	7	0.36
(1,610)	1:458:A:ARG:H	1:459:A:PRO:HB3	7	0.36
(1,492)	1:464:A:LEU:HA	1:540:A:VAL:H	1	0.36
(1,384)	1:486:A:TRP:HE1	1:510:A:HIS:HB3	9	0.36
(1,383)	1:486:A:TRP:HE1	1:511:A:HIS:H	6	0.36
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB1	8	0.36
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB2	8	0.36
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB3	8	0.36
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG21	1	0.36
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG22	1	0.36
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG23	1	0.36
(1,220)	1:468:A:GLY:HA2	1:516:A:GLU:HG2	6	0.36
(1,220)	1:468:A:GLY:HA2	1:516:A:GLU:HG3	6	0.36
(1,61)	1:488:A:LYS:HA	1:488:A:LYS:HD3	2	0.36
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB1	1	0.36
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB2	1	0.36
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB3	1	0.36
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB1	1	0.36
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB2	1	0.36
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB3	1	0.36
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB1	1	0.36
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB2	1	0.36
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB3	1	0.36
(1,1295)	1:532:A:GLY:H	1:533:A:GLN:HB2	9	0.35
(1,1295)	1:532:A:GLY:H	1:533:A:GLN:HB3	9	0.35
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD11	2	0.35
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD12	2	0.35
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD13	2	0.35
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD21	2	0.35
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD22	2	0.35
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD23	2	0.35
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD11	2	0.35
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD12	2	0.35
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD13	2	0.35
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD21	2	0.35
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD22	2	0.35
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD23	2	0.35
(1,1011)	1:519:A:LEU:HB3	1:522:A:ALA:H	6	0.35
(1,921)	1:487:A:LEU:H	1:493:A:LEU:H	5	0.35
(1,889)	1:475:A:CYS:H	1:486:A:TRP:HH2	10	0.35
(1,843)	1:456:A:ILE:H	1:458:A:ARG:H	8	0.35
(1,824)	1:456:A:ILE:HD11	1:533:A:GLN:H	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,824)	1:456:A:ILE:HD12	1:533:A:GLN:H	8	0.35
(1,824)	1:456:A:ILE:HD13	1:533:A:GLN:H	8	0.35
(1,754)	1:463:A:GLN:HA	1:463:A:GLN:HE21	5	0.35
(1,716)	1:466:A:MET:H	1:466:A:MET:HE1	10	0.35
(1,716)	1:466:A:MET:H	1:466:A:MET:HE2	10	0.35
(1,716)	1:466:A:MET:H	1:466:A:MET:HE3	10	0.35
(1,652)	1:457:A:THR:H	1:457:A:THR:HG21	6	0.35
(1,652)	1:457:A:THR:H	1:457:A:THR:HG22	6	0.35
(1,652)	1:457:A:THR:H	1:457:A:THR:HG23	6	0.35
(1,561)	1:487:A:LEU:HA	1:491:A:VAL:H	1	0.35
(1,544)	1:486:A:TRP:H	1:492:A:GLU:HA	10	0.35
(1,539)	1:515:A:ASN:H	1:515:A:ASN:HD21	3	0.35
(1,514)	1:523:A:GLY:HA2	1:538:A:LEU:H	9	0.35
(1,503)	1:473:A:PHE:H	1:513:A:ILE:HG13	8	0.35
(1,492)	1:464:A:LEU:HA	1:540:A:VAL:H	2	0.35
(1,473)	1:512:A:LEU:H	1:513:A:ILE:HG13	5	0.35
(1,404)	1:487:A:LEU:HA	1:492:A:GLU:H	3	0.35
(1,352)	1:464:A:LEU:HB2	1:539:A:ILE:H	3	0.35
(1,316)	1:501:A:TYR:HB2	1:502:A:TRP:HD1	5	0.35
(1,316)	1:501:A:TYR:HB3	1:502:A:TRP:HD1	5	0.35
(1,311)	1:502:A:TRP:HD1	1:503:A:PHE:H	3	0.35
(1,220)	1:468:A:GLY:HA2	1:516:A:GLU:HG2	9	0.35
(1,220)	1:468:A:GLY:HA2	1:516:A:GLU:HG3	9	0.35
(1,43)	1:465:A:VAL:HG21	1:471:A:VAL:HA	3	0.35
(1,43)	1:465:A:VAL:HG22	1:471:A:VAL:HA	3	0.35
(1,43)	1:465:A:VAL:HG23	1:471:A:VAL:HA	3	0.35
(1,28)	1:456:A:ILE:HD11	1:534:A:ALA:HA	6	0.35
(1,28)	1:456:A:ILE:HD12	1:534:A:ALA:HA	6	0.35
(1,28)	1:456:A:ILE:HD13	1:534:A:ALA:HA	6	0.35
(1,1314)	1:542:A:GLU:HG2	1:543:A:LYS:H	6	0.34
(1,1314)	1:542:A:GLU:HG3	1:543:A:LYS:H	6	0.34
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD11	1	0.34
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD12	1	0.34
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD13	1	0.34
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD21	1	0.34
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD22	1	0.34
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD23	1	0.34
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD11	1	0.34
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD12	1	0.34
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD13	1	0.34
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD21	1	0.34
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD22	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD23	1	0.34
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD11	7	0.34
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD12	7	0.34
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD13	7	0.34
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD21	7	0.34
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD22	7	0.34
(1,1171)	1:485:A:LYS:HG2	1:487:A:LEU:HD23	7	0.34
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD11	7	0.34
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD12	7	0.34
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD13	7	0.34
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD21	7	0.34
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD22	7	0.34
(1,1171)	1:485:A:LYS:HG3	1:487:A:LEU:HD23	7	0.34
(1,1121)	1:466:A:MET:HB2	1:469:A:GLN:HG2	8	0.34
(1,1121)	1:466:A:MET:HB2	1:469:A:GLN:HG3	8	0.34
(1,1121)	1:466:A:MET:HB3	1:469:A:GLN:HG2	8	0.34
(1,1121)	1:466:A:MET:HB3	1:469:A:GLN:HG3	8	0.34
(1,1101)	1:460:A:LEU:HD11	1:527:A:LEU:H	8	0.34
(1,1101)	1:460:A:LEU:HD12	1:527:A:LEU:H	8	0.34
(1,1101)	1:460:A:LEU:HD13	1:527:A:LEU:H	8	0.34
(1,1101)	1:460:A:LEU:HD21	1:527:A:LEU:H	8	0.34
(1,1101)	1:460:A:LEU:HD22	1:527:A:LEU:H	8	0.34
(1,1101)	1:460:A:LEU:HD23	1:527:A:LEU:H	8	0.34
(1,1083)	1:456:A:ILE:HD11	1:527:A:LEU:HB2	9	0.34
(1,1083)	1:456:A:ILE:HD11	1:527:A:LEU:HB3	9	0.34
(1,1083)	1:456:A:ILE:HD12	1:527:A:LEU:HB2	9	0.34
(1,1083)	1:456:A:ILE:HD12	1:527:A:LEU:HB3	9	0.34
(1,1083)	1:456:A:ILE:HD13	1:527:A:LEU:HB2	9	0.34
(1,1083)	1:456:A:ILE:HD13	1:527:A:LEU:HB3	9	0.34
(1,936)	1:496:A:GLU:HA	1:497:A:GLU:H	8	0.34
(1,926)	1:487:A:LEU:H	1:492:A:GLU:HA	9	0.34
(1,857)	1:462:A:ASP:H	1:463:A:GLN:HE21	10	0.34
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB1	1	0.34
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB2	1	0.34
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB3	1	0.34
(1,663)	1:474:A:GLU:H	1:486:A:TRP:HH2	10	0.34
(1,652)	1:457:A:THR:H	1:457:A:THR:HG21	1	0.34
(1,652)	1:457:A:THR:H	1:457:A:THR:HG22	1	0.34
(1,652)	1:457:A:THR:H	1:457:A:THR:HG23	1	0.34
(1,652)	1:457:A:THR:H	1:457:A:THR:HG21	8	0.34
(1,652)	1:457:A:THR:H	1:457:A:THR:HG22	8	0.34
(1,652)	1:457:A:THR:H	1:457:A:THR:HG23	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG11	9	0.34
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG12	9	0.34
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG13	9	0.34
(1,601)	1:458:A:ARG:H	1:459:A:PRO:HD2	6	0.34
(1,544)	1:486:A:TRP:H	1:492:A:GLU:HA	5	0.34
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB2	4	0.34
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB3	4	0.34
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG11	3	0.34
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG12	3	0.34
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG13	3	0.34
(1,29)	1:456:A:ILE:HD11	1:533:A:GLN:HA	6	0.34
(1,29)	1:456:A:ILE:HD12	1:533:A:GLN:HA	6	0.34
(1,29)	1:456:A:ILE:HD13	1:533:A:GLN:HA	6	0.34
(1,18)	1:453:A:PRO:HB3	1:531:A:GLY:HA2	2	0.34
(1,1037)	1:456:A:ILE:HD11	1:529:A:THR:H	6	0.33
(1,1037)	1:456:A:ILE:HD12	1:529:A:THR:H	6	0.33
(1,1037)	1:456:A:ILE:HD13	1:529:A:THR:H	6	0.33
(1,958)	1:474:A:GLU:HA	1:511:A:HIS:H	2	0.33
(1,851)	1:461:A:GLU:HG2	1:462:A:ASP:H	4	0.33
(1,851)	1:461:A:GLU:HG3	1:462:A:ASP:H	4	0.33
(1,843)	1:456:A:ILE:H	1:458:A:ARG:H	4	0.33
(1,824)	1:456:A:ILE:HD11	1:533:A:GLN:H	4	0.33
(1,824)	1:456:A:ILE:HD12	1:533:A:GLN:H	4	0.33
(1,824)	1:456:A:ILE:HD13	1:533:A:GLN:H	4	0.33
(1,816)	1:478:A:SER:H	1:508:A:GLN:HE22	4	0.33
(1,752)	1:459:A:PRO:HG2	1:460:A:LEU:H	5	0.33
(1,752)	1:459:A:PRO:HG3	1:460:A:LEU:H	5	0.33
(1,641)	1:479:A:GLU:HG2	1:482:A:ALA:H	3	0.33
(1,641)	1:479:A:GLU:HG3	1:482:A:ALA:H	3	0.33
(1,610)	1:458:A:ARG:H	1:459:A:PRO:HB2	9	0.33
(1,610)	1:458:A:ARG:H	1:459:A:PRO:HB3	9	0.33
(1,602)	1:458:A:ARG:H	1:477:A:VAL:HA	3	0.33
(1,561)	1:487:A:LEU:HA	1:491:A:VAL:H	9	0.33
(1,544)	1:486:A:TRP:H	1:492:A:GLU:HA	4	0.33
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB1	2	0.33
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB2	2	0.33
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB3	2	0.33
(1,249)	1:460:A:LEU:HG	1:526:A:ALA:HA	10	0.33
(1,248)	1:460:A:LEU:HB2	1:526:A:ALA:HA	6	0.33
(1,248)	1:460:A:LEU:HB3	1:526:A:ALA:HA	6	0.33
(1,224)	1:519:A:LEU:HA	1:540:A:VAL:HB	4	0.33
(1,1295)	1:532:A:GLY:H	1:533:A:GLN:HB2	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1295)	1:532:A:GLY:H	1:533:A:GLN:HB3	3	0.32
(1,1265)	1:518:A:MET:HG2	1:520:A:GLU:H	6	0.32
(1,1265)	1:518:A:MET:HG3	1:520:A:GLU:H	6	0.32
(1,1225)	1:500:A:LYS:HE2	1:514:A:ILE:HG21	9	0.32
(1,1225)	1:500:A:LYS:HE2	1:514:A:ILE:HG22	9	0.32
(1,1225)	1:500:A:LYS:HE2	1:514:A:ILE:HG23	9	0.32
(1,1225)	1:500:A:LYS:HE3	1:514:A:ILE:HG21	9	0.32
(1,1225)	1:500:A:LYS:HE3	1:514:A:ILE:HG22	9	0.32
(1,1225)	1:500:A:LYS:HE3	1:514:A:ILE:HG23	9	0.32
(1,1189)	1:487:A:LEU:HD11	1:493:A:LEU:H	6	0.32
(1,1189)	1:487:A:LEU:HD12	1:493:A:LEU:H	6	0.32
(1,1189)	1:487:A:LEU:HD13	1:493:A:LEU:H	6	0.32
(1,1189)	1:487:A:LEU:HD21	1:493:A:LEU:H	6	0.32
(1,1189)	1:487:A:LEU:HD22	1:493:A:LEU:H	6	0.32
(1,1189)	1:487:A:LEU:HD23	1:493:A:LEU:H	6	0.32
(1,1156)	1:473:A:PHE:HB2	1:486:A:TRP:HZ2	4	0.32
(1,1156)	1:473:A:PHE:HB3	1:486:A:TRP:HZ2	4	0.32
(1,996)	1:516:A:GLU:HG2	1:517:A:ALA:H	6	0.32
(1,996)	1:516:A:GLU:HG3	1:517:A:ALA:H	6	0.32
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD21	8	0.32
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD22	8	0.32
(1,945)	1:503:A:PHE:H	1:512:A:LEU:HD23	8	0.32
(1,774)	1:456:A:ILE:HA	1:478:A:SER:H	8	0.32
(1,698)	1:496:A:GLU:H	1:496:A:GLU:HG2	5	0.32
(1,698)	1:496:A:GLU:H	1:496:A:GLU:HG3	5	0.32
(1,636)	1:487:A:LEU:HB2	1:526:A:ALA:H	5	0.32
(1,626)	1:462:A:ASP:HA	1:537:A:GLU:H	3	0.32
(1,624)	1:462:A:ASP:HB3	1:537:A:GLU:H	6	0.32
(1,624)	1:462:A:ASP:HB2	1:537:A:GLU:H	6	0.32
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB2	1	0.32
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB3	1	0.32
(1,478)	1:474:A:GLU:HA	1:512:A:LEU:H	2	0.32
(1,448)	1:472:A:GLU:H	1:473:A:PHE:HD1	9	0.32
(1,331)	1:456:A:ILE:HG21	1:459:A:PRO:HA	7	0.32
(1,331)	1:456:A:ILE:HG22	1:459:A:PRO:HA	7	0.32
(1,331)	1:456:A:ILE:HG23	1:459:A:PRO:HA	7	0.32
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB2	8	0.32
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB3	8	0.32
(1,1243)	1:506:A:ASP:H	1:509:A:ARG:HG2	6	0.31
(1,1243)	1:506:A:ASP:H	1:509:A:ARG:HG3	6	0.31
(1,1212)	1:493:A:LEU:HD11	1:512:A:LEU:HD11	9	0.31
(1,1212)	1:493:A:LEU:HD11	1:512:A:LEU:HD12	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1212)	1:493:A:LEU:HD11	1:512:A:LEU:HD13	9	0.31
(1,1212)	1:493:A:LEU:HD12	1:512:A:LEU:HD11	9	0.31
(1,1212)	1:493:A:LEU:HD12	1:512:A:LEU:HD12	9	0.31
(1,1212)	1:493:A:LEU:HD12	1:512:A:LEU:HD13	9	0.31
(1,1212)	1:493:A:LEU:HD13	1:512:A:LEU:HD11	9	0.31
(1,1212)	1:493:A:LEU:HD13	1:512:A:LEU:HD12	9	0.31
(1,1212)	1:493:A:LEU:HD13	1:512:A:LEU:HD13	9	0.31
(1,1212)	1:493:A:LEU:HD21	1:512:A:LEU:HD11	9	0.31
(1,1212)	1:493:A:LEU:HD21	1:512:A:LEU:HD12	9	0.31
(1,1212)	1:493:A:LEU:HD21	1:512:A:LEU:HD13	9	0.31
(1,1212)	1:493:A:LEU:HD22	1:512:A:LEU:HD11	9	0.31
(1,1212)	1:493:A:LEU:HD22	1:512:A:LEU:HD12	9	0.31
(1,1212)	1:493:A:LEU:HD22	1:512:A:LEU:HD13	9	0.31
(1,1212)	1:493:A:LEU:HD23	1:512:A:LEU:HD11	9	0.31
(1,1212)	1:493:A:LEU:HD23	1:512:A:LEU:HD12	9	0.31
(1,1212)	1:493:A:LEU:HD23	1:512:A:LEU:HD13	9	0.31
(1,1090)	1:460:A:LEU:H	1:475:A:CYS:HB2	6	0.31
(1,1090)	1:460:A:LEU:H	1:475:A:CYS:HB3	6	0.31
(1,1037)	1:456:A:ILE:HD11	1:529:A:THR:H	2	0.31
(1,1037)	1:456:A:ILE:HD12	1:529:A:THR:H	2	0.31
(1,1037)	1:456:A:ILE:HD13	1:529:A:THR:H	2	0.31
(1,1012)	1:522:A:ALA:H	1:538:A:LEU:HG	8	0.31
(1,901)	1:476:A:GLU:H	1:477:A:VAL:HG21	5	0.31
(1,901)	1:476:A:GLU:H	1:477:A:VAL:HG22	5	0.31
(1,901)	1:476:A:GLU:H	1:477:A:VAL:HG23	5	0.31
(1,880)	1:470:A:ARG:H	1:470:A:ARG:HD2	4	0.31
(1,880)	1:470:A:ARG:H	1:470:A:ARG:HD3	4	0.31
(1,817)	1:523:A:GLY:H	1:540:A:VAL:HB	6	0.31
(1,726)	1:492:A:GLU:HG2	1:494:A:THR:H	5	0.31
(1,726)	1:492:A:GLU:HG3	1:494:A:THR:H	5	0.31
(1,656)	1:457:A:THR:H	1:476:A:GLU:HG2	9	0.31
(1,642)	1:482:A:ALA:H	1:508:A:GLN:HB3	3	0.31
(1,642)	1:482:A:ALA:H	1:508:A:GLN:HB2	3	0.31
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG21	1	0.31
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG22	1	0.31
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG23	1	0.31
(1,499)	1:473:A:PHE:H	1:512:A:LEU:HG	2	0.31
(1,426)	1:525:A:TYR:H	1:537:A:GLU:HA	9	0.31
(1,367)	1:502:A:TRP:HE1	1:515:A:ASN:HA	6	0.31
(1,311)	1:502:A:TRP:HD1	1:503:A:PHE:H	9	0.31
(1,286)	1:521:A:ASP:HB2	1:540:A:VAL:HG21	3	0.31
(1,286)	1:521:A:ASP:HB2	1:540:A:VAL:HG22	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,286)	1:521:A:ASP:HB2	1:540:A:VAL:HG23	3	0.31
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG11	4	0.31
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG12	4	0.31
(1,139)	1:519:A:LEU:HA	1:540:A:VAL:HG13	4	0.31
(1,43)	1:465:A:VAL:HG21	1:471:A:VAL:HA	8	0.31
(1,43)	1:465:A:VAL:HG22	1:471:A:VAL:HA	8	0.31
(1,43)	1:465:A:VAL:HG23	1:471:A:VAL:HA	8	0.31
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB1	5	0.31
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB2	5	0.31
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB3	5	0.31
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB1	5	0.31
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB2	5	0.31
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB3	5	0.31
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB1	5	0.31
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB2	5	0.31
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB3	5	0.31
(1,1314)	1:542:A:GLU:HG2	1:543:A:LYS:H	4	0.3
(1,1314)	1:542:A:GLU:HG3	1:543:A:LYS:H	4	0.3
(1,1090)	1:460:A:LEU:H	1:475:A:CYS:HB2	7	0.3
(1,1090)	1:460:A:LEU:H	1:475:A:CYS:HB3	7	0.3
(1,1014)	1:524:A:HIS:H	1:537:A:GLU:HA	7	0.3
(1,918)	1:486:A:TRP:HE1	1:504:A:LYS:H	4	0.3
(1,843)	1:456:A:ILE:H	1:458:A:ARG:H	2	0.3
(1,760)	1:465:A:VAL:HA	1:469:A:GLN:HE21	6	0.3
(1,672)	1:469:A:GLN:H	1:517:A:ALA:HA	4	0.3
(1,562)	1:488:A:LYS:H	1:491:A:VAL:H	3	0.3
(1,544)	1:486:A:TRP:H	1:492:A:GLU:HA	1	0.3
(1,481)	1:472:A:GLU:HA	1:512:A:LEU:H	7	0.3
(1,404)	1:487:A:LEU:HA	1:492:A:GLU:H	9	0.3
(1,333)	1:456:A:ILE:HG21	1:460:A:LEU:H	9	0.3
(1,333)	1:456:A:ILE:HG22	1:460:A:LEU:H	9	0.3
(1,333)	1:456:A:ILE:HG23	1:460:A:LEU:H	9	0.3
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB2	5	0.3
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB3	5	0.3
(1,67)	1:471:A:VAL:HB	1:514:A:ILE:HB	8	0.3
(1,29)	1:456:A:ILE:HD11	1:533:A:GLN:HA	3	0.3
(1,29)	1:456:A:ILE:HD12	1:533:A:GLN:HA	3	0.3
(1,29)	1:456:A:ILE:HD13	1:533:A:GLN:HA	3	0.3
(1,1295)	1:532:A:GLY:H	1:533:A:GLN:HB2	7	0.29
(1,1295)	1:532:A:GLY:H	1:533:A:GLN:HB3	7	0.29
(1,973)	1:471:A:VAL:HB	1:514:A:ILE:H	9	0.29
(1,958)	1:474:A:GLU:HA	1:511:A:HIS:H	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,921)	1:487:A:LEU:H	1:493:A:LEU:H	7	0.29
(1,890)	1:475:A:CYS:H	1:486:A:TRP:HZ2	2	0.29
(1,801)	1:529:A:THR:H	1:531:A:GLY:H	1	0.29
(1,752)	1:459:A:PRO:HG2	1:460:A:LEU:H	6	0.29
(1,752)	1:459:A:PRO:HG3	1:460:A:LEU:H	6	0.29
(1,663)	1:474:A:GLU:H	1:486:A:TRP:HH2	9	0.29
(1,657)	1:457:A:THR:H	1:477:A:VAL:HB	2	0.29
(1,601)	1:458:A:ARG:H	1:459:A:PRO:HD2	9	0.29
(1,548)	1:486:A:TRP:H	1:493:A:LEU:H	7	0.29
(1,386)	1:486:A:TRP:HE1	1:510:A:HIS:HB2	10	0.29
(1,384)	1:486:A:TRP:HE1	1:510:A:HIS:HB3	2	0.29
(1,302)	1:505:A:LYS:HB3	1:510:A:HIS:HE1	9	0.29
(1,215)	1:470:A:ARG:HB2	1:515:A:ASN:HA	7	0.29
(1,200)	1:514:A:ILE:HD11	1:521:A:ASP:HB2	9	0.29
(1,200)	1:514:A:ILE:HD12	1:521:A:ASP:HB2	9	0.29
(1,200)	1:514:A:ILE:HD13	1:521:A:ASP:HB2	9	0.29
(1,178)	1:470:A:ARG:HB2	1:513:A:ILE:HG21	6	0.29
(1,178)	1:470:A:ARG:HB2	1:513:A:ILE:HG22	6	0.29
(1,178)	1:470:A:ARG:HB2	1:513:A:ILE:HG23	6	0.29
(1,85)	1:457:A:THR:HG21	1:477:A:VAL:HA	6	0.29
(1,85)	1:457:A:THR:HG22	1:477:A:VAL:HA	6	0.29
(1,85)	1:457:A:THR:HG23	1:477:A:VAL:HA	6	0.29
(1,61)	1:488:A:LYS:HA	1:488:A:LYS:HD3	9	0.29
(1,41)	1:463:A:GLN:HG2	1:465:A:VAL:HG21	2	0.29
(1,41)	1:463:A:GLN:HG2	1:465:A:VAL:HG22	2	0.29
(1,41)	1:463:A:GLN:HG2	1:465:A:VAL:HG23	2	0.29
(1,41)	1:463:A:GLN:HG3	1:465:A:VAL:HG21	2	0.29
(1,41)	1:463:A:GLN:HG3	1:465:A:VAL:HG22	2	0.29
(1,41)	1:463:A:GLN:HG3	1:465:A:VAL:HG23	2	0.29
(1,1168)	1:485:A:LYS:H	1:527:A:LEU:HD11	1	0.28
(1,1168)	1:485:A:LYS:H	1:527:A:LEU:HD12	1	0.28
(1,1168)	1:485:A:LYS:H	1:527:A:LEU:HD13	1	0.28
(1,1168)	1:485:A:LYS:H	1:527:A:LEU:HD21	1	0.28
(1,1168)	1:485:A:LYS:H	1:527:A:LEU:HD22	1	0.28
(1,1168)	1:485:A:LYS:H	1:527:A:LEU:HD23	1	0.28
(1,1123)	1:466:A:MET:HG2	1:469:A:GLN:HG2	4	0.28
(1,1123)	1:466:A:MET:HG2	1:469:A:GLN:HG3	4	0.28
(1,1123)	1:466:A:MET:HG3	1:469:A:GLN:HG2	4	0.28
(1,1123)	1:466:A:MET:HG3	1:469:A:GLN:HG3	4	0.28
(1,1099)	1:460:A:LEU:HD11	1:486:A:TRP:HH2	9	0.28
(1,1099)	1:460:A:LEU:HD12	1:486:A:TRP:HH2	9	0.28
(1,1099)	1:460:A:LEU:HD13	1:486:A:TRP:HH2	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1099)	1:460:A:LEU:HD21	1:486:A:TRP:HH2	9	0.28
(1,1099)	1:460:A:LEU:HD22	1:486:A:TRP:HH2	9	0.28
(1,1099)	1:460:A:LEU:HD23	1:486:A:TRP:HH2	9	0.28
(1,1083)	1:456:A:ILE:HD11	1:527:A:LEU:HB2	2	0.28
(1,1083)	1:456:A:ILE:HD11	1:527:A:LEU:HB3	2	0.28
(1,1083)	1:456:A:ILE:HD12	1:527:A:LEU:HB2	2	0.28
(1,1083)	1:456:A:ILE:HD12	1:527:A:LEU:HB3	2	0.28
(1,1083)	1:456:A:ILE:HD13	1:527:A:LEU:HB2	2	0.28
(1,1083)	1:456:A:ILE:HD13	1:527:A:LEU:HB3	2	0.28
(1,1063)	1:453:A:PRO:HB2	1:531:A:GLY:H	5	0.28
(1,1063)	1:453:A:PRO:HB3	1:531:A:GLY:H	5	0.28
(1,1041)	1:526:A:ALA:HA	1:535:A:LEU:H	7	0.28
(1,1001)	1:518:A:MET:H	1:520:A:GLU:H	5	0.28
(1,921)	1:487:A:LEU:H	1:493:A:LEU:H	9	0.28
(1,880)	1:470:A:ARG:H	1:470:A:ARG:HD2	1	0.28
(1,880)	1:470:A:ARG:H	1:470:A:ARG:HD3	1	0.28
(1,879)	1:470:A:ARG:H	1:516:A:GLU:HA	8	0.28
(1,851)	1:461:A:GLU:HG2	1:462:A:ASP:H	2	0.28
(1,851)	1:461:A:GLU:HG3	1:462:A:ASP:H	2	0.28
(1,759)	1:462:A:ASP:H	1:463:A:GLN:HE22	5	0.28
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG21	10	0.28
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG22	10	0.28
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG23	10	0.28
(1,675)	1:467:A:VAL:HB	1:469:A:GLN:H	9	0.28
(1,566)	1:518:A:MET:H	1:522:A:ALA:H	6	0.28
(1,517)	1:535:A:LEU:HD11	1:536:A:ALA:H	7	0.28
(1,517)	1:535:A:LEU:HD12	1:536:A:ALA:H	7	0.28
(1,517)	1:535:A:LEU:HD13	1:536:A:ALA:H	7	0.28
(1,428)	1:525:A:TYR:H	1:537:A:GLU:HB2	9	0.28
(1,428)	1:525:A:TYR:H	1:537:A:GLU:HB3	9	0.28
(1,309)	1:524:A:HIS:HE1	1:537:A:GLU:HB2	2	0.28
(1,309)	1:524:A:HIS:HE1	1:537:A:GLU:HB3	2	0.28
(1,308)	1:505:A:LYS:HE2	1:510:A:HIS:HE1	4	0.28
(1,308)	1:505:A:LYS:HE3	1:510:A:HIS:HE1	4	0.28
(1,134)	1:487:A:LEU:HG	1:492:A:GLU:HA	1	0.28
(1,123)	1:462:A:ASP:HA	1:536:A:ALA:HB1	6	0.28
(1,123)	1:462:A:ASP:HA	1:536:A:ALA:HB2	6	0.28
(1,123)	1:462:A:ASP:HA	1:536:A:ALA:HB3	6	0.28
(1,1260)	1:518:A:MET:HA	1:519:A:LEU:HD11	6	0.27
(1,1260)	1:518:A:MET:HA	1:519:A:LEU:HD12	6	0.27
(1,1260)	1:518:A:MET:HA	1:519:A:LEU:HD13	6	0.27
(1,1260)	1:518:A:MET:HA	1:519:A:LEU:HD21	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1260)	1:518:A:MET:HA	1:519:A:LEU:HD22	6	0.27
(1,1260)	1:518:A:MET:HA	1:519:A:LEU:HD23	6	0.27
(1,1253)	1:514:A:ILE:HG12	1:515:A:ASN:H	5	0.27
(1,1253)	1:514:A:ILE:HG13	1:515:A:ASN:H	5	0.27
(1,1249)	1:509:A:ARG:HG2	1:510:A:HIS:H	9	0.27
(1,1249)	1:509:A:ARG:HG3	1:510:A:HIS:H	9	0.27
(1,1220)	1:497:A:GLU:HG2	1:500:A:LYS:H	6	0.27
(1,1220)	1:497:A:GLU:HG3	1:500:A:LYS:H	6	0.27
(1,1158)	1:473:A:PHE:HB2	1:512:A:LEU:H	8	0.27
(1,1158)	1:473:A:PHE:HB3	1:512:A:LEU:H	8	0.27
(1,1146)	1:471:A:VAL:HG11	1:473:A:PHE:HD1	2	0.27
(1,1146)	1:471:A:VAL:HG12	1:473:A:PHE:HD1	2	0.27
(1,1146)	1:471:A:VAL:HG13	1:473:A:PHE:HD1	2	0.27
(1,1146)	1:471:A:VAL:HG21	1:473:A:PHE:HD1	2	0.27
(1,1146)	1:471:A:VAL:HG22	1:473:A:PHE:HD1	2	0.27
(1,1146)	1:471:A:VAL:HG23	1:473:A:PHE:HD1	2	0.27
(1,1095)	1:460:A:LEU:HD11	1:475:A:CYS:H	10	0.27
(1,1095)	1:460:A:LEU:HD12	1:475:A:CYS:H	10	0.27
(1,1095)	1:460:A:LEU:HD13	1:475:A:CYS:H	10	0.27
(1,1095)	1:460:A:LEU:HD21	1:475:A:CYS:H	10	0.27
(1,1095)	1:460:A:LEU:HD22	1:475:A:CYS:H	10	0.27
(1,1095)	1:460:A:LEU:HD23	1:475:A:CYS:H	10	0.27
(1,991)	1:469:A:GLN:HA	1:517:A:ALA:H	4	0.27
(1,955)	1:510:A:HIS:H	1:511:A:HIS:HD2	6	0.27
(1,879)	1:470:A:ARG:H	1:516:A:GLU:HA	9	0.27
(1,816)	1:478:A:SER:H	1:508:A:GLN:HE22	10	0.27
(1,811)	1:465:A:VAL:HA	1:469:A:GLN:HE22	3	0.27
(1,780)	1:476:A:GLU:HG3	1:508:A:GLN:HE21	7	0.27
(1,774)	1:456:A:ILE:HA	1:478:A:SER:H	3	0.27
(1,765)	1:502:A:TRP:HZ2	1:515:A:ASN:HD22	10	0.27
(1,760)	1:465:A:VAL:HA	1:469:A:GLN:HE21	4	0.27
(1,726)	1:492:A:GLU:HG2	1:494:A:THR:H	10	0.27
(1,726)	1:492:A:GLU:HG3	1:494:A:THR:H	10	0.27
(1,663)	1:474:A:GLU:H	1:486:A:TRP:HH2	5	0.27
(1,444)	1:472:A:GLU:H	1:514:A:ILE:HB	2	0.27
(1,382)	1:455:A:LEU:H	1:479:A:GLU:H	1	0.27
(1,382)	1:455:A:LEU:H	1:479:A:GLU:H	8	0.27
(1,330)	1:456:A:ILE:HG21	1:459:A:PRO:HB2	2	0.27
(1,330)	1:456:A:ILE:HG21	1:459:A:PRO:HB3	2	0.27
(1,330)	1:456:A:ILE:HG22	1:459:A:PRO:HB2	2	0.27
(1,330)	1:456:A:ILE:HG22	1:459:A:PRO:HB3	2	0.27
(1,330)	1:456:A:ILE:HG23	1:459:A:PRO:HB2	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:456:A:ILE:HG23	1:459:A:PRO:HB3	2	0.27
(1,311)	1:502:A:TRP:HD1	1:503:A:PHE:H	2	0.27
(1,303)	1:509:A:ARG:HD2	1:511:A:HIS:HE1	7	0.27
(1,303)	1:509:A:ARG:HD3	1:511:A:HIS:HE1	7	0.27
(1,282)	1:464:A:LEU:HA	1:540:A:VAL:HG21	10	0.27
(1,282)	1:464:A:LEU:HA	1:540:A:VAL:HG22	10	0.27
(1,282)	1:464:A:LEU:HA	1:540:A:VAL:HG23	10	0.27
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG21	2	0.27
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG22	2	0.27
(1,270)	1:464:A:LEU:HB2	1:539:A:ILE:HG23	2	0.27
(1,248)	1:460:A:LEU:HB2	1:526:A:ALA:HA	10	0.27
(1,248)	1:460:A:LEU:HB3	1:526:A:ALA:HA	10	0.27
(1,224)	1:519:A:LEU:HA	1:540:A:VAL:HB	7	0.27
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD21	7	0.27
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD22	7	0.27
(1,172)	1:503:A:PHE:HD2	1:512:A:LEU:HD23	7	0.27
(1,120)	1:525:A:TYR:HB2	1:536:A:ALA:HB1	4	0.27
(1,120)	1:525:A:TYR:HB2	1:536:A:ALA:HB2	4	0.27
(1,120)	1:525:A:TYR:HB2	1:536:A:ALA:HB3	4	0.27
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB1	7	0.27
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB2	7	0.27
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB3	7	0.27
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB1	7	0.27
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB2	7	0.27
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB3	7	0.27
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB1	7	0.27
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB2	7	0.27
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB3	7	0.27
(1,1295)	1:532:A:GLY:H	1:533:A:GLN:HB2	10	0.26
(1,1295)	1:532:A:GLY:H	1:533:A:GLN:HB3	10	0.26
(1,1269)	1:519:A:LEU:HD11	1:540:A:VAL:HB	3	0.26
(1,1269)	1:519:A:LEU:HD12	1:540:A:VAL:HB	3	0.26
(1,1269)	1:519:A:LEU:HD13	1:540:A:VAL:HB	3	0.26
(1,1269)	1:519:A:LEU:HD21	1:540:A:VAL:HB	3	0.26
(1,1269)	1:519:A:LEU:HD22	1:540:A:VAL:HB	3	0.26
(1,1269)	1:519:A:LEU:HD23	1:540:A:VAL:HB	3	0.26
(1,1265)	1:518:A:MET:HG2	1:520:A:GLU:H	8	0.26
(1,1265)	1:518:A:MET:HG3	1:520:A:GLU:H	8	0.26
(1,1238)	1:505:A:LYS:HB2	1:505:A:LYS:HE2	1	0.26
(1,1238)	1:505:A:LYS:HB2	1:505:A:LYS:HE3	1	0.26
(1,1238)	1:505:A:LYS:HB3	1:505:A:LYS:HE2	1	0.26
(1,1238)	1:505:A:LYS:HB3	1:505:A:LYS:HE3	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD11	5	0.26
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD12	5	0.26
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD13	5	0.26
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD21	5	0.26
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD22	5	0.26
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD23	5	0.26
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD11	7	0.26
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD12	7	0.26
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD13	7	0.26
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD21	7	0.26
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD22	7	0.26
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD23	7	0.26
(1,1148)	1:471:A:VAL:HG11	1:514:A:ILE:HD11	1	0.26
(1,1148)	1:471:A:VAL:HG11	1:514:A:ILE:HD12	1	0.26
(1,1148)	1:471:A:VAL:HG11	1:514:A:ILE:HD13	1	0.26
(1,1148)	1:471:A:VAL:HG12	1:514:A:ILE:HD11	1	0.26
(1,1148)	1:471:A:VAL:HG12	1:514:A:ILE:HD12	1	0.26
(1,1148)	1:471:A:VAL:HG12	1:514:A:ILE:HD13	1	0.26
(1,1148)	1:471:A:VAL:HG13	1:514:A:ILE:HD11	1	0.26
(1,1148)	1:471:A:VAL:HG13	1:514:A:ILE:HD12	1	0.26
(1,1148)	1:471:A:VAL:HG13	1:514:A:ILE:HD13	1	0.26
(1,1148)	1:471:A:VAL:HG21	1:514:A:ILE:HD11	1	0.26
(1,1148)	1:471:A:VAL:HG21	1:514:A:ILE:HD12	1	0.26
(1,1148)	1:471:A:VAL:HG21	1:514:A:ILE:HD13	1	0.26
(1,1148)	1:471:A:VAL:HG22	1:514:A:ILE:HD11	1	0.26
(1,1148)	1:471:A:VAL:HG22	1:514:A:ILE:HD12	1	0.26
(1,1148)	1:471:A:VAL:HG22	1:514:A:ILE:HD13	1	0.26
(1,1148)	1:471:A:VAL:HG23	1:514:A:ILE:HD11	1	0.26
(1,1148)	1:471:A:VAL:HG23	1:514:A:ILE:HD12	1	0.26
(1,1148)	1:471:A:VAL:HG23	1:514:A:ILE:HD13	1	0.26
(1,1068)	1:454:A:VAL:HG11	1:478:A:SER:H	3	0.26
(1,1068)	1:454:A:VAL:HG12	1:478:A:SER:H	3	0.26
(1,1068)	1:454:A:VAL:HG13	1:478:A:SER:H	3	0.26
(1,1068)	1:454:A:VAL:HG21	1:478:A:SER:H	3	0.26
(1,1068)	1:454:A:VAL:HG22	1:478:A:SER:H	3	0.26
(1,1068)	1:454:A:VAL:HG23	1:478:A:SER:H	3	0.26
(1,1023)	1:488:A:LYS:HG2	1:524:A:HIS:H	3	0.26
(1,699)	1:495:A:ARG:HD2	1:496:A:GLU:H	10	0.26
(1,699)	1:495:A:ARG:HD3	1:496:A:GLU:H	10	0.26
(1,636)	1:487:A:LEU:HB2	1:526:A:ALA:H	2	0.26
(1,595)	1:518:A:MET:HE1	1:519:A:LEU:H	5	0.26
(1,595)	1:518:A:MET:HE2	1:519:A:LEU:H	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,595)	1:518:A:MET:HE3	1:519:A:LEU:H	5	0.26
(1,517)	1:535:A:LEU:HD11	1:536:A:ALA:H	6	0.26
(1,517)	1:535:A:LEU:HD12	1:536:A:ALA:H	6	0.26
(1,517)	1:535:A:LEU:HD13	1:536:A:ALA:H	6	0.26
(1,512)	1:522:A:ALA:HA	1:538:A:LEU:H	1	0.26
(1,472)	1:472:A:GLU:HG2	1:512:A:LEU:H	10	0.26
(1,472)	1:472:A:GLU:HG3	1:512:A:LEU:H	10	0.26
(1,455)	1:505:A:LYS:HD2	1:506:A:ASP:H	3	0.26
(1,455)	1:505:A:LYS:HD3	1:506:A:ASP:H	3	0.26
(1,452)	1:505:A:LYS:HG2	1:506:A:ASP:H	10	0.26
(1,452)	1:505:A:LYS:HG3	1:506:A:ASP:H	10	0.26
(1,376)	1:487:A:LEU:HB3	1:490:A:GLY:H	7	0.26
(1,352)	1:464:A:LEU:HB2	1:539:A:ILE:H	4	0.26
(1,333)	1:456:A:ILE:HG21	1:460:A:LEU:H	1	0.26
(1,333)	1:456:A:ILE:HG22	1:460:A:LEU:H	1	0.26
(1,333)	1:456:A:ILE:HG23	1:460:A:LEU:H	1	0.26
(1,316)	1:501:A:TYR:HB2	1:502:A:TRP:HD1	7	0.26
(1,316)	1:501:A:TYR:HB3	1:502:A:TRP:HD1	7	0.26
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB2	3	0.26
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB3	3	0.26
(1,238)	1:522:A:ALA:HB1	1:540:A:VAL:HG21	4	0.26
(1,238)	1:522:A:ALA:HB1	1:540:A:VAL:HG22	4	0.26
(1,238)	1:522:A:ALA:HB1	1:540:A:VAL:HG23	4	0.26
(1,238)	1:522:A:ALA:HB2	1:540:A:VAL:HG21	4	0.26
(1,238)	1:522:A:ALA:HB2	1:540:A:VAL:HG22	4	0.26
(1,238)	1:522:A:ALA:HB2	1:540:A:VAL:HG23	4	0.26
(1,238)	1:522:A:ALA:HB3	1:540:A:VAL:HG21	4	0.26
(1,238)	1:522:A:ALA:HB3	1:540:A:VAL:HG22	4	0.26
(1,238)	1:522:A:ALA:HB3	1:540:A:VAL:HG23	4	0.26
(1,181)	1:470:A:ARG:HB3	1:513:A:ILE:HG21	6	0.26
(1,181)	1:470:A:ARG:HB3	1:513:A:ILE:HG22	6	0.26
(1,181)	1:470:A:ARG:HB3	1:513:A:ILE:HG23	6	0.26
(1,151)	1:502:A:TRP:H	1:503:A:PHE:HB3	4	0.26
(1,151)	1:502:A:TRP:H	1:503:A:PHE:HB3	6	0.26
(1,134)	1:487:A:LEU:HG	1:492:A:GLU:HA	7	0.26
(1,115)	1:484:A:VAL:HG11	1:510:A:HIS:H	5	0.26
(1,115)	1:484:A:VAL:HG12	1:510:A:HIS:H	5	0.26
(1,115)	1:484:A:VAL:HG13	1:510:A:HIS:H	5	0.26
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB1	9	0.26
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB2	9	0.26
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB3	9	0.26
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB1	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB2	9	0.26
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB3	9	0.26
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB1	9	0.26
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB2	9	0.26
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB3	9	0.26
(1,1123)	1:466:A:MET:HG2	1:469:A:GLN:HG2	7	0.25
(1,1123)	1:466:A:MET:HG2	1:469:A:GLN:HG3	7	0.25
(1,1123)	1:466:A:MET:HG3	1:469:A:GLN:HG2	7	0.25
(1,1123)	1:466:A:MET:HG3	1:469:A:GLN:HG3	7	0.25
(1,996)	1:516:A:GLU:HG2	1:517:A:ALA:H	2	0.25
(1,996)	1:516:A:GLU:HG3	1:517:A:ALA:H	2	0.25
(1,851)	1:461:A:GLU:HG2	1:462:A:ASP:H	6	0.25
(1,851)	1:461:A:GLU:HG3	1:462:A:ASP:H	6	0.25
(1,819)	1:523:A:GLY:H	1:538:A:LEU:HG	9	0.25
(1,784)	1:476:A:GLU:HG3	1:508:A:GLN:HE22	4	0.25
(1,636)	1:487:A:LEU:HB2	1:526:A:ALA:H	9	0.25
(1,569)	1:522:A:ALA:H	1:540:A:VAL:HB	5	0.25
(1,569)	1:522:A:ALA:H	1:540:A:VAL:HB	9	0.25
(1,561)	1:487:A:LEU:HA	1:491:A:VAL:H	6	0.25
(1,481)	1:472:A:GLU:HA	1:512:A:LEU:H	1	0.25
(1,472)	1:472:A:GLU:HG2	1:512:A:LEU:H	7	0.25
(1,472)	1:472:A:GLU:HG3	1:512:A:LEU:H	7	0.25
(1,449)	1:463:A:GLN:HE22	1:472:A:GLU:H	10	0.25
(1,384)	1:486:A:TRP:HE1	1:510:A:HIS:HB3	10	0.25
(1,181)	1:470:A:ARG:HB3	1:513:A:ILE:HG21	10	0.25
(1,181)	1:470:A:ARG:HB3	1:513:A:ILE:HG22	10	0.25
(1,181)	1:470:A:ARG:HB3	1:513:A:ILE:HG23	10	0.25
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD21	7	0.25
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD22	7	0.25
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD23	7	0.25
(1,28)	1:456:A:ILE:HD11	1:534:A:ALA:HA	4	0.25
(1,28)	1:456:A:ILE:HD12	1:534:A:ALA:HA	4	0.25
(1,28)	1:456:A:ILE:HD13	1:534:A:ALA:HA	4	0.25
(1,1291)	1:527:A:LEU:HD11	1:528:A:CYS:H	1	0.24
(1,1291)	1:527:A:LEU:HD12	1:528:A:CYS:H	1	0.24
(1,1291)	1:527:A:LEU:HD13	1:528:A:CYS:H	1	0.24
(1,1291)	1:527:A:LEU:HD21	1:528:A:CYS:H	1	0.24
(1,1291)	1:527:A:LEU:HD22	1:528:A:CYS:H	1	0.24
(1,1291)	1:527:A:LEU:HD23	1:528:A:CYS:H	1	0.24
(1,1262)	1:518:A:MET:HB2	1:520:A:GLU:HB2	10	0.24
(1,1262)	1:518:A:MET:HB2	1:520:A:GLU:HB3	10	0.24
(1,1262)	1:518:A:MET:HB3	1:520:A:GLU:HB2	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1262)	1:518:A:MET:HB3	1:520:A:GLU:HB3	10	0.24
(1,1188)	1:487:A:LEU:HD11	1:492:A:GLU:HG2	2	0.24
(1,1188)	1:487:A:LEU:HD11	1:492:A:GLU:HG3	2	0.24
(1,1188)	1:487:A:LEU:HD12	1:492:A:GLU:HG2	2	0.24
(1,1188)	1:487:A:LEU:HD12	1:492:A:GLU:HG3	2	0.24
(1,1188)	1:487:A:LEU:HD13	1:492:A:GLU:HG2	2	0.24
(1,1188)	1:487:A:LEU:HD13	1:492:A:GLU:HG3	2	0.24
(1,1188)	1:487:A:LEU:HD21	1:492:A:GLU:HG2	2	0.24
(1,1188)	1:487:A:LEU:HD21	1:492:A:GLU:HG3	2	0.24
(1,1188)	1:487:A:LEU:HD22	1:492:A:GLU:HG2	2	0.24
(1,1188)	1:487:A:LEU:HD22	1:492:A:GLU:HG3	2	0.24
(1,1188)	1:487:A:LEU:HD23	1:492:A:GLU:HG2	2	0.24
(1,1188)	1:487:A:LEU:HD23	1:492:A:GLU:HG3	2	0.24
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD11	9	0.24
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD12	9	0.24
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD13	9	0.24
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD21	9	0.24
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD22	9	0.24
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD23	9	0.24
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG11	5	0.24
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG12	5	0.24
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG13	5	0.24
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG21	5	0.24
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG22	5	0.24
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG23	5	0.24
(1,1052)	1:465:A:VAL:H	1:539:A:ILE:H	3	0.24
(1,901)	1:476:A:GLU:H	1:477:A:VAL:HG21	2	0.24
(1,901)	1:476:A:GLU:H	1:477:A:VAL:HG22	2	0.24
(1,901)	1:476:A:GLU:H	1:477:A:VAL:HG23	2	0.24
(1,866)	1:463:A:GLN:HG2	1:465:A:VAL:H	4	0.24
(1,866)	1:463:A:GLN:HG3	1:465:A:VAL:H	4	0.24
(1,788)	1:531:A:GLY:H	1:532:A:GLY:H	7	0.24
(1,755)	1:463:A:GLN:HE21	1:464:A:LEU:H	2	0.24
(1,752)	1:459:A:PRO:HG2	1:460:A:LEU:H	2	0.24
(1,752)	1:459:A:PRO:HG3	1:460:A:LEU:H	2	0.24
(1,752)	1:459:A:PRO:HG2	1:460:A:LEU:H	7	0.24
(1,752)	1:459:A:PRO:HG3	1:460:A:LEU:H	7	0.24
(1,705)	1:467:A:VAL:H	1:542:A:GLU:HA	6	0.24
(1,672)	1:469:A:GLN:H	1:517:A:ALA:HA	9	0.24
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG11	7	0.24
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG12	7	0.24
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG13	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,552)	1:486:A:TRP:H	1:492:A:GLU:HG2	1	0.24
(1,552)	1:486:A:TRP:H	1:492:A:GLU:HG3	1	0.24
(1,481)	1:472:A:GLU:HA	1:512:A:LEU:H	2	0.24
(1,316)	1:501:A:TYR:HB2	1:502:A:TRP:HD1	2	0.24
(1,316)	1:501:A:TYR:HB3	1:502:A:TRP:HD1	2	0.24
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG2	7	0.24
(1,310)	1:524:A:HIS:HE1	1:537:A:GLU:HG3	7	0.24
(1,307)	1:505:A:LYS:HD2	1:510:A:HIS:HE1	8	0.24
(1,307)	1:505:A:LYS:HD3	1:510:A:HIS:HE1	8	0.24
(1,274)	1:464:A:LEU:HA	1:539:A:ILE:HG21	4	0.24
(1,274)	1:464:A:LEU:HA	1:539:A:ILE:HG22	4	0.24
(1,274)	1:464:A:LEU:HA	1:539:A:ILE:HG23	4	0.24
(1,115)	1:484:A:VAL:HG11	1:510:A:HIS:H	7	0.24
(1,115)	1:484:A:VAL:HG12	1:510:A:HIS:H	7	0.24
(1,115)	1:484:A:VAL:HG13	1:510:A:HIS:H	7	0.24
(1,1298)	1:533:A:GLN:HB2	1:533:A:GLN:HE21	9	0.23
(1,1298)	1:533:A:GLN:HB2	1:533:A:GLN:HE22	9	0.23
(1,1298)	1:533:A:GLN:HB3	1:533:A:GLN:HE21	9	0.23
(1,1298)	1:533:A:GLN:HB3	1:533:A:GLN:HE22	9	0.23
(1,1239)	1:505:A:LYS:HB2	1:506:A:ASP:H	2	0.23
(1,1239)	1:505:A:LYS:HB3	1:506:A:ASP:H	2	0.23
(1,1090)	1:460:A:LEU:H	1:475:A:CYS:HB2	3	0.23
(1,1090)	1:460:A:LEU:H	1:475:A:CYS:HB3	3	0.23
(1,1085)	1:456:A:ILE:HD11	1:532:A:GLY:HA2	6	0.23
(1,1085)	1:456:A:ILE:HD11	1:532:A:GLY:HA3	6	0.23
(1,1085)	1:456:A:ILE:HD12	1:532:A:GLY:HA2	6	0.23
(1,1085)	1:456:A:ILE:HD12	1:532:A:GLY:HA3	6	0.23
(1,1085)	1:456:A:ILE:HD13	1:532:A:GLY:HA2	6	0.23
(1,1085)	1:456:A:ILE:HD13	1:532:A:GLY:HA3	6	0.23
(1,1063)	1:453:A:PRO:HB2	1:531:A:GLY:H	3	0.23
(1,1063)	1:453:A:PRO:HB3	1:531:A:GLY:H	3	0.23
(1,1023)	1:488:A:LYS:HG2	1:524:A:HIS:H	10	0.23
(1,1022)	1:524:A:HIS:H	1:537:A:GLU:HB2	4	0.23
(1,1022)	1:524:A:HIS:H	1:537:A:GLU:HB3	4	0.23
(1,991)	1:469:A:GLN:HA	1:517:A:ALA:H	10	0.23
(1,989)	1:469:A:GLN:H	1:517:A:ALA:H	4	0.23
(1,989)	1:469:A:GLN:H	1:517:A:ALA:H	9	0.23
(1,857)	1:462:A:ASP:H	1:463:A:GLN:HE21	8	0.23
(1,811)	1:465:A:VAL:HA	1:469:A:GLN:HE22	1	0.23
(1,803)	1:523:A:GLY:H	1:525:A:TYR:HD1	3	0.23
(1,782)	1:457:A:THR:HG21	1:508:A:GLN:HE21	6	0.23
(1,782)	1:457:A:THR:HG22	1:508:A:GLN:HE21	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,782)	1:457:A:THR:HG23	1:508:A:GLN:HE21	6	0.23
(1,726)	1:492:A:GLU:HG2	1:494:A:THR:H	1	0.23
(1,726)	1:492:A:GLU:HG3	1:494:A:THR:H	1	0.23
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG21	4	0.23
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG22	4	0.23
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG23	4	0.23
(1,504)	1:473:A:PHE:H	1:512:A:LEU:HB2	1	0.23
(1,473)	1:512:A:LEU:H	1:513:A:ILE:HG13	7	0.23
(1,331)	1:456:A:ILE:HG21	1:459:A:PRO:HA	1	0.23
(1,331)	1:456:A:ILE:HG22	1:459:A:PRO:HA	1	0.23
(1,331)	1:456:A:ILE:HG23	1:459:A:PRO:HA	1	0.23
(1,330)	1:456:A:ILE:HG21	1:459:A:PRO:HB2	10	0.23
(1,330)	1:456:A:ILE:HG21	1:459:A:PRO:HB3	10	0.23
(1,330)	1:456:A:ILE:HG22	1:459:A:PRO:HB2	10	0.23
(1,330)	1:456:A:ILE:HG22	1:459:A:PRO:HB3	10	0.23
(1,330)	1:456:A:ILE:HG23	1:459:A:PRO:HB2	10	0.23
(1,330)	1:456:A:ILE:HG23	1:459:A:PRO:HB3	10	0.23
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD11	9	0.23
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD12	9	0.23
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD13	9	0.23
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB2	7	0.23
(1,291)	1:477:A:VAL:HB	1:479:A:GLU:HB3	7	0.23
(1,200)	1:514:A:ILE:HD11	1:521:A:ASP:HB2	6	0.23
(1,200)	1:514:A:ILE:HD12	1:521:A:ASP:HB2	6	0.23
(1,200)	1:514:A:ILE:HD13	1:521:A:ASP:HB2	6	0.23
(1,142)	1:460:A:LEU:HD11	1:475:A:CYS:HB3	3	0.23
(1,142)	1:460:A:LEU:HD12	1:475:A:CYS:HB3	3	0.23
(1,142)	1:460:A:LEU:HD13	1:475:A:CYS:HB3	3	0.23
(1,41)	1:463:A:GLN:HG2	1:465:A:VAL:HG21	10	0.23
(1,41)	1:463:A:GLN:HG2	1:465:A:VAL:HG22	10	0.23
(1,41)	1:463:A:GLN:HG2	1:465:A:VAL:HG23	10	0.23
(1,41)	1:463:A:GLN:HG3	1:465:A:VAL:HG21	10	0.23
(1,41)	1:463:A:GLN:HG3	1:465:A:VAL:HG22	10	0.23
(1,41)	1:463:A:GLN:HG3	1:465:A:VAL:HG23	10	0.23
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB1	2	0.23
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB2	2	0.23
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB3	2	0.23
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB1	2	0.23
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB2	2	0.23
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB3	2	0.23
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB1	2	0.23
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB2	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB3	2	0.23
(1,1298)	1:533:A:GLN:HB2	1:533:A:GLN:HE21	4	0.22
(1,1298)	1:533:A:GLN:HB2	1:533:A:GLN:HE22	4	0.22
(1,1298)	1:533:A:GLN:HB3	1:533:A:GLN:HE21	4	0.22
(1,1298)	1:533:A:GLN:HB3	1:533:A:GLN:HE22	4	0.22
(1,1238)	1:505:A:LYS:HB2	1:505:A:LYS:HE2	8	0.22
(1,1238)	1:505:A:LYS:HB2	1:505:A:LYS:HE3	8	0.22
(1,1238)	1:505:A:LYS:HB3	1:505:A:LYS:HE2	8	0.22
(1,1238)	1:505:A:LYS:HB3	1:505:A:LYS:HE3	8	0.22
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD11	2	0.22
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD12	2	0.22
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD13	2	0.22
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD21	2	0.22
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD22	2	0.22
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD23	2	0.22
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD11	2	0.22
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD12	2	0.22
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD13	2	0.22
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD21	2	0.22
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD22	2	0.22
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD23	2	0.22
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD11	2	0.22
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD12	2	0.22
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD13	2	0.22
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD21	2	0.22
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD22	2	0.22
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD23	2	0.22
(1,1121)	1:466:A:MET:HB2	1:469:A:GLN:HG2	3	0.22
(1,1121)	1:466:A:MET:HB2	1:469:A:GLN:HG3	3	0.22
(1,1121)	1:466:A:MET:HB3	1:469:A:GLN:HG2	3	0.22
(1,1121)	1:466:A:MET:HB3	1:469:A:GLN:HG3	3	0.22
(1,1098)	1:460:A:LEU:HD11	1:486:A:TRP:HZ2	6	0.22
(1,1098)	1:460:A:LEU:HD12	1:486:A:TRP:HZ2	6	0.22
(1,1098)	1:460:A:LEU:HD13	1:486:A:TRP:HZ2	6	0.22
(1,1098)	1:460:A:LEU:HD21	1:486:A:TRP:HZ2	6	0.22
(1,1098)	1:460:A:LEU:HD22	1:486:A:TRP:HZ2	6	0.22
(1,1098)	1:460:A:LEU:HD23	1:486:A:TRP:HZ2	6	0.22
(1,1092)	1:460:A:LEU:HB2	1:475:A:CYS:HB2	7	0.22
(1,1092)	1:460:A:LEU:HB2	1:475:A:CYS:HB3	7	0.22
(1,1092)	1:460:A:LEU:HB3	1:475:A:CYS:HB2	7	0.22
(1,1092)	1:460:A:LEU:HB3	1:475:A:CYS:HB3	7	0.22
(1,1090)	1:460:A:LEU:H	1:475:A:CYS:HB2	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	1:460:A:LEU:H	1:475:A:CYS:HB3	10	0.22
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA2	8	0.22
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA3	8	0.22
(1,1014)	1:524:A:HIS:H	1:537:A:GLU:HA	6	0.22
(1,960)	1:486:A:TRP:HZ2	1:511:A:HIS:H	5	0.22
(1,926)	1:487:A:LEU:H	1:492:A:GLU:HA	3	0.22
(1,906)	1:476:A:GLU:HG3	1:477:A:VAL:H	8	0.22
(1,906)	1:476:A:GLU:HG2	1:477:A:VAL:H	8	0.22
(1,889)	1:475:A:CYS:H	1:486:A:TRP:HH2	2	0.22
(1,880)	1:470:A:ARG:H	1:470:A:ARG:HD2	6	0.22
(1,880)	1:470:A:ARG:H	1:470:A:ARG:HD3	6	0.22
(1,857)	1:462:A:ASP:H	1:463:A:GLN:HE21	1	0.22
(1,851)	1:461:A:GLU:HG2	1:462:A:ASP:H	3	0.22
(1,851)	1:461:A:GLU:HG3	1:462:A:ASP:H	3	0.22
(1,851)	1:461:A:GLU:HG2	1:462:A:ASP:H	7	0.22
(1,851)	1:461:A:GLU:HG3	1:462:A:ASP:H	7	0.22
(1,828)	1:479:A:GLU:H	1:508:A:GLN:HE21	2	0.22
(1,818)	1:523:A:GLY:H	1:538:A:LEU:HB3	5	0.22
(1,817)	1:523:A:GLY:H	1:540:A:VAL:HB	1	0.22
(1,721)	1:500:A:LYS:HG2	1:501:A:TYR:H	9	0.22
(1,721)	1:500:A:LYS:HG3	1:501:A:TYR:H	9	0.22
(1,672)	1:469:A:GLN:H	1:517:A:ALA:HA	10	0.22
(1,608)	1:458:A:ARG:H	1:476:A:GLU:HG2	5	0.22
(1,473)	1:512:A:LEU:H	1:513:A:ILE:HG13	9	0.22
(1,376)	1:487:A:LEU:HB3	1:490:A:GLY:H	3	0.22
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB1	4	0.22
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB2	4	0.22
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB3	4	0.22
(1,309)	1:524:A:HIS:HE1	1:537:A:GLU:HB2	6	0.22
(1,309)	1:524:A:HIS:HE1	1:537:A:GLU:HB3	6	0.22
(1,304)	1:484:A:VAL:HG11	1:510:A:HIS:HE1	3	0.22
(1,304)	1:484:A:VAL:HG12	1:510:A:HIS:HE1	3	0.22
(1,304)	1:484:A:VAL:HG13	1:510:A:HIS:HE1	3	0.22
(1,304)	1:484:A:VAL:HG21	1:510:A:HIS:HE1	3	0.22
(1,304)	1:484:A:VAL:HG22	1:510:A:HIS:HE1	3	0.22
(1,304)	1:484:A:VAL:HG23	1:510:A:HIS:HE1	3	0.22
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG21	8	0.22
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG22	8	0.22
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG23	8	0.22
(1,282)	1:464:A:LEU:HA	1:540:A:VAL:HG21	6	0.22
(1,282)	1:464:A:LEU:HA	1:540:A:VAL:HG22	6	0.22
(1,282)	1:464:A:LEU:HA	1:540:A:VAL:HG23	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,142)	1:460:A:LEU:HD11	1:475:A:CYS:HB3	6	0.22
(1,142)	1:460:A:LEU:HD12	1:475:A:CYS:HB3	6	0.22
(1,142)	1:460:A:LEU:HD13	1:475:A:CYS:HB3	6	0.22
(1,77)	1:471:A:VAL:HA	1:472:A:GLU:HG2	5	0.22
(1,77)	1:471:A:VAL:HA	1:472:A:GLU:HG3	5	0.22
(1,1300)	1:533:A:GLN:HB2	1:535:A:LEU:H	5	0.21
(1,1300)	1:533:A:GLN:HB3	1:535:A:LEU:H	5	0.21
(1,1263)	1:518:A:MET:HB2	1:521:A:ASP:H	2	0.21
(1,1263)	1:518:A:MET:HB3	1:521:A:ASP:H	2	0.21
(1,1262)	1:518:A:MET:HB2	1:520:A:GLU:HB2	2	0.21
(1,1262)	1:518:A:MET:HB2	1:520:A:GLU:HB3	2	0.21
(1,1262)	1:518:A:MET:HB3	1:520:A:GLU:HB2	2	0.21
(1,1262)	1:518:A:MET:HB3	1:520:A:GLU:HB3	2	0.21
(1,1210)	1:493:A:LEU:HD11	1:494:A:THR:H	3	0.21
(1,1210)	1:493:A:LEU:HD12	1:494:A:THR:H	3	0.21
(1,1210)	1:493:A:LEU:HD13	1:494:A:THR:H	3	0.21
(1,1210)	1:493:A:LEU:HD21	1:494:A:THR:H	3	0.21
(1,1210)	1:493:A:LEU:HD22	1:494:A:THR:H	3	0.21
(1,1210)	1:493:A:LEU:HD23	1:494:A:THR:H	3	0.21
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG11	2	0.21
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG12	2	0.21
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG13	2	0.21
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG21	2	0.21
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG22	2	0.21
(1,1137)	1:468:A:GLY:H	1:471:A:VAL:HG23	2	0.21
(1,1098)	1:460:A:LEU:HD11	1:486:A:TRP:HZ2	3	0.21
(1,1098)	1:460:A:LEU:HD12	1:486:A:TRP:HZ2	3	0.21
(1,1098)	1:460:A:LEU:HD13	1:486:A:TRP:HZ2	3	0.21
(1,1098)	1:460:A:LEU:HD21	1:486:A:TRP:HZ2	3	0.21
(1,1098)	1:460:A:LEU:HD22	1:486:A:TRP:HZ2	3	0.21
(1,1098)	1:460:A:LEU:HD23	1:486:A:TRP:HZ2	3	0.21
(1,1021)	1:488:A:LYS:HG3	1:524:A:HIS:H	7	0.21
(1,890)	1:475:A:CYS:H	1:486:A:TRP:HZ2	10	0.21
(1,887)	1:475:A:CYS:H	1:510:A:HIS:HB3	6	0.21
(1,880)	1:470:A:ARG:H	1:470:A:ARG:HD2	9	0.21
(1,880)	1:470:A:ARG:H	1:470:A:ARG:HD3	9	0.21
(1,828)	1:479:A:GLU:H	1:508:A:GLN:HE21	4	0.21
(1,755)	1:463:A:GLN:HE21	1:464:A:LEU:H	1	0.21
(1,755)	1:463:A:GLN:HE21	1:464:A:LEU:H	9	0.21
(1,747)	1:460:A:LEU:H	1:534:A:ALA:HA	2	0.21
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG21	2	0.21
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG22	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG23	2	0.21
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG21	5	0.21
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG22	5	0.21
(1,744)	1:468:A:GLY:H	1:514:A:ILE:HG23	5	0.21
(1,721)	1:500:A:LYS:HG2	1:501:A:TYR:H	4	0.21
(1,721)	1:500:A:LYS:HG3	1:501:A:TYR:H	4	0.21
(1,721)	1:500:A:LYS:HG2	1:501:A:TYR:H	7	0.21
(1,721)	1:500:A:LYS:HG3	1:501:A:TYR:H	7	0.21
(1,716)	1:466:A:MET:H	1:466:A:MET:HE1	7	0.21
(1,716)	1:466:A:MET:H	1:466:A:MET:HE2	7	0.21
(1,716)	1:466:A:MET:H	1:466:A:MET:HE3	7	0.21
(1,592)	1:519:A:LEU:H	1:540:A:VAL:HG11	3	0.21
(1,592)	1:519:A:LEU:H	1:540:A:VAL:HG12	3	0.21
(1,592)	1:519:A:LEU:H	1:540:A:VAL:HG13	3	0.21
(1,562)	1:488:A:LYS:H	1:491:A:VAL:H	2	0.21
(1,479)	1:486:A:TRP:HZ2	1:512:A:LEU:H	7	0.21
(1,463)	1:473:A:PHE:H	1:511:A:HIS:HA	6	0.21
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD11	8	0.21
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD12	8	0.21
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD13	8	0.21
(1,200)	1:514:A:ILE:HD11	1:521:A:ASP:HB2	7	0.21
(1,200)	1:514:A:ILE:HD12	1:521:A:ASP:HB2	7	0.21
(1,200)	1:514:A:ILE:HD13	1:521:A:ASP:HB2	7	0.21
(1,151)	1:502:A:TRP:H	1:503:A:PHE:HB3	2	0.21
(1,79)	1:485:A:LYS:HB2	1:485:A:LYS:HE2	7	0.21
(1,79)	1:485:A:LYS:HB2	1:485:A:LYS:HE3	7	0.21
(1,79)	1:485:A:LYS:HB3	1:485:A:LYS:HE2	7	0.21
(1,79)	1:485:A:LYS:HB3	1:485:A:LYS:HE3	7	0.21
(1,1226)	1:500:A:LYS:HE2	1:518:A:MET:H	1	0.2
(1,1226)	1:500:A:LYS:HE3	1:518:A:MET:H	1	0.2
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD11	4	0.2
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD12	4	0.2
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD13	4	0.2
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD21	4	0.2
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD22	4	0.2
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD23	4	0.2
(1,1097)	1:460:A:LEU:HD11	1:476:A:GLU:H	10	0.2
(1,1097)	1:460:A:LEU:HD12	1:476:A:GLU:H	10	0.2
(1,1097)	1:460:A:LEU:HD13	1:476:A:GLU:H	10	0.2
(1,1097)	1:460:A:LEU:HD21	1:476:A:GLU:H	10	0.2
(1,1097)	1:460:A:LEU:HD22	1:476:A:GLU:H	10	0.2
(1,1097)	1:460:A:LEU:HD23	1:476:A:GLU:H	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1041)	1:526:A:ALA:HA	1:535:A:LEU:H	4	0.2
(1,996)	1:516:A:GLU:HG2	1:517:A:ALA:H	1	0.2
(1,996)	1:516:A:GLU:HG3	1:517:A:ALA:H	1	0.2
(1,996)	1:516:A:GLU:HG2	1:517:A:ALA:H	8	0.2
(1,996)	1:516:A:GLU:HG3	1:517:A:ALA:H	8	0.2
(1,985)	1:470:A:ARG:HB2	1:516:A:GLU:H	1	0.2
(1,906)	1:476:A:GLU:HG3	1:477:A:VAL:H	7	0.2
(1,906)	1:476:A:GLU:HG2	1:477:A:VAL:H	7	0.2
(1,879)	1:470:A:ARG:H	1:516:A:GLU:HA	3	0.2
(1,802)	1:523:A:GLY:H	1:539:A:ILE:HA	10	0.2
(1,782)	1:457:A:THR:HG21	1:508:A:GLN:HE21	10	0.2
(1,782)	1:457:A:THR:HG22	1:508:A:GLN:HE21	10	0.2
(1,782)	1:457:A:THR:HG23	1:508:A:GLN:HE21	10	0.2
(1,780)	1:476:A:GLU:HG3	1:508:A:GLN:HE21	8	0.2
(1,780)	1:476:A:GLU:HG3	1:508:A:GLN:HE21	9	0.2
(1,719)	1:500:A:LYS:HD2	1:501:A:TYR:H	1	0.2
(1,719)	1:500:A:LYS:HD3	1:501:A:TYR:H	1	0.2
(1,716)	1:466:A:MET:H	1:466:A:MET:HE1	6	0.2
(1,716)	1:466:A:MET:H	1:466:A:MET:HE2	6	0.2
(1,716)	1:466:A:MET:H	1:466:A:MET:HE3	6	0.2
(1,701)	1:495:A:ARG:H	1:496:A:GLU:H	1	0.2
(1,610)	1:458:A:ARG:H	1:459:A:PRO:HB2	8	0.2
(1,610)	1:458:A:ARG:H	1:459:A:PRO:HB3	8	0.2
(1,492)	1:464:A:LEU:HA	1:540:A:VAL:H	7	0.2
(1,481)	1:472:A:GLU:HA	1:512:A:LEU:H	8	0.2
(1,306)	1:505:A:LYS:HG2	1:510:A:HIS:HE1	5	0.2
(1,306)	1:505:A:LYS:HG3	1:510:A:HIS:HE1	5	0.2
(1,158)	1:508:A:GLN:HA	1:510:A:HIS:HD2	5	0.2
(1,143)	1:495:A:ARG:HA	1:495:A:ARG:HD2	10	0.2
(1,143)	1:495:A:ARG:HA	1:495:A:ARG:HD3	10	0.2
(1,101)	1:457:A:THR:HG21	1:478:A:SER:HA	3	0.2
(1,101)	1:457:A:THR:HG22	1:478:A:SER:HA	3	0.2
(1,101)	1:457:A:THR:HG23	1:478:A:SER:HA	3	0.2
(1,85)	1:457:A:THR:HG21	1:477:A:VAL:HA	10	0.2
(1,85)	1:457:A:THR:HG22	1:477:A:VAL:HA	10	0.2
(1,85)	1:457:A:THR:HG23	1:477:A:VAL:HA	10	0.2
(1,43)	1:465:A:VAL:HG21	1:471:A:VAL:HA	2	0.2
(1,43)	1:465:A:VAL:HG22	1:471:A:VAL:HA	2	0.2
(1,43)	1:465:A:VAL:HG23	1:471:A:VAL:HA	2	0.2
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB1	3	0.2
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB2	3	0.2
(1,26)	1:456:A:ILE:HD11	1:534:A:ALA:HB3	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB1	3	0.2
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB2	3	0.2
(1,26)	1:456:A:ILE:HD12	1:534:A:ALA:HB3	3	0.2
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB1	3	0.2
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB2	3	0.2
(1,26)	1:456:A:ILE:HD13	1:534:A:ALA:HB3	3	0.2
(1,16)	1:459:A:PRO:HA	1:534:A:ALA:HB1	2	0.2
(1,16)	1:459:A:PRO:HA	1:534:A:ALA:HB2	2	0.2
(1,16)	1:459:A:PRO:HA	1:534:A:ALA:HB3	2	0.2
(1,1300)	1:533:A:GLN:HB2	1:535:A:LEU:H	2	0.19
(1,1300)	1:533:A:GLN:HB3	1:535:A:LEU:H	2	0.19
(1,1249)	1:509:A:ARG:HG2	1:510:A:HIS:H	8	0.19
(1,1249)	1:509:A:ARG:HG3	1:510:A:HIS:H	8	0.19
(1,1146)	1:471:A:VAL:HG11	1:473:A:PHE:HD1	3	0.19
(1,1146)	1:471:A:VAL:HG12	1:473:A:PHE:HD1	3	0.19
(1,1146)	1:471:A:VAL:HG13	1:473:A:PHE:HD1	3	0.19
(1,1146)	1:471:A:VAL:HG21	1:473:A:PHE:HD1	3	0.19
(1,1146)	1:471:A:VAL:HG22	1:473:A:PHE:HD1	3	0.19
(1,1146)	1:471:A:VAL:HG23	1:473:A:PHE:HD1	3	0.19
(1,1093)	1:460:A:LEU:HG	1:475:A:CYS:HB2	7	0.19
(1,1093)	1:460:A:LEU:HG	1:475:A:CYS:HB3	7	0.19
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA2	4	0.19
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA3	4	0.19
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA2	9	0.19
(1,1080)	1:456:A:ILE:H	1:532:A:GLY:HA3	9	0.19
(1,1022)	1:524:A:HIS:H	1:537:A:GLU:HB2	6	0.19
(1,1022)	1:524:A:HIS:H	1:537:A:GLU:HB3	6	0.19
(1,1019)	1:524:A:HIS:H	1:525:A:TYR:HD1	6	0.19
(1,1014)	1:524:A:HIS:H	1:537:A:GLU:HA	4	0.19
(1,1011)	1:519:A:LEU:HB3	1:522:A:ALA:H	4	0.19
(1,996)	1:516:A:GLU:HG2	1:517:A:ALA:H	7	0.19
(1,996)	1:516:A:GLU:HG3	1:517:A:ALA:H	7	0.19
(1,996)	1:516:A:GLU:HG2	1:517:A:ALA:H	10	0.19
(1,996)	1:516:A:GLU:HG3	1:517:A:ALA:H	10	0.19
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB1	5	0.19
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB2	5	0.19
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB3	5	0.19
(1,731)	1:498:A:THR:H	1:501:A:TYR:H	7	0.19
(1,708)	1:467:A:VAL:H	1:541:A:GLN:H	4	0.19
(1,655)	1:457:A:THR:H	1:458:A:ARG:HB2	8	0.19
(1,655)	1:457:A:THR:H	1:458:A:ARG:HB3	8	0.19
(1,619)	1:466:A:MET:HA	1:542:A:GLU:H	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,583)	1:528:A:CYS:H	1:533:A:GLN:HA	8	0.19
(1,570)	1:520:A:GLU:HB2	1:522:A:ALA:H	9	0.19
(1,570)	1:520:A:GLU:HB3	1:522:A:ALA:H	9	0.19
(1,477)	1:486:A:TRP:HH2	1:512:A:LEU:H	10	0.19
(1,439)	1:526:A:ALA:HA	1:534:A:ALA:H	1	0.19
(1,390)	1:484:A:VAL:HB	1:486:A:TRP:HE1	7	0.19
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD21	1	0.19
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD22	1	0.19
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD23	1	0.19
(1,134)	1:487:A:LEU:HG	1:492:A:GLU:HA	3	0.19
(1,41)	1:463:A:GLN:HG2	1:465:A:VAL:HG21	4	0.19
(1,41)	1:463:A:GLN:HG2	1:465:A:VAL:HG22	4	0.19
(1,41)	1:463:A:GLN:HG2	1:465:A:VAL:HG23	4	0.19
(1,41)	1:463:A:GLN:HG3	1:465:A:VAL:HG21	4	0.19
(1,41)	1:463:A:GLN:HG3	1:465:A:VAL:HG22	4	0.19
(1,41)	1:463:A:GLN:HG3	1:465:A:VAL:HG23	4	0.19
(1,34)	1:460:A:LEU:HA	1:536:A:ALA:HB1	7	0.19
(1,34)	1:460:A:LEU:HA	1:536:A:ALA:HB2	7	0.19
(1,34)	1:460:A:LEU:HA	1:536:A:ALA:HB3	7	0.19
(1,1266)	1:519:A:LEU:H	1:519:A:LEU:HD11	6	0.18
(1,1266)	1:519:A:LEU:H	1:519:A:LEU:HD12	6	0.18
(1,1266)	1:519:A:LEU:H	1:519:A:LEU:HD13	6	0.18
(1,1266)	1:519:A:LEU:H	1:519:A:LEU:HD21	6	0.18
(1,1266)	1:519:A:LEU:H	1:519:A:LEU:HD22	6	0.18
(1,1266)	1:519:A:LEU:H	1:519:A:LEU:HD23	6	0.18
(1,1217)	1:496:A:GLU:H	1:496:A:GLU:HB2	10	0.18
(1,1217)	1:496:A:GLU:H	1:496:A:GLU:HB3	10	0.18
(1,1189)	1:487:A:LEU:HD11	1:493:A:LEU:H	10	0.18
(1,1189)	1:487:A:LEU:HD12	1:493:A:LEU:H	10	0.18
(1,1189)	1:487:A:LEU:HD13	1:493:A:LEU:H	10	0.18
(1,1189)	1:487:A:LEU:HD21	1:493:A:LEU:H	10	0.18
(1,1189)	1:487:A:LEU:HD22	1:493:A:LEU:H	10	0.18
(1,1189)	1:487:A:LEU:HD23	1:493:A:LEU:H	10	0.18
(1,1177)	1:486:A:TRP:HE1	1:527:A:LEU:HD11	6	0.18
(1,1177)	1:486:A:TRP:HE1	1:527:A:LEU:HD12	6	0.18
(1,1177)	1:486:A:TRP:HE1	1:527:A:LEU:HD13	6	0.18
(1,1177)	1:486:A:TRP:HE1	1:527:A:LEU:HD21	6	0.18
(1,1177)	1:486:A:TRP:HE1	1:527:A:LEU:HD22	6	0.18
(1,1177)	1:486:A:TRP:HE1	1:527:A:LEU:HD23	6	0.18
(1,1095)	1:460:A:LEU:HD11	1:475:A:CYS:H	7	0.18
(1,1095)	1:460:A:LEU:HD12	1:475:A:CYS:H	7	0.18
(1,1095)	1:460:A:LEU:HD13	1:475:A:CYS:H	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1095)	1:460:A:LEU:HD21	1:475:A:CYS:H	7	0.18
(1,1095)	1:460:A:LEU:HD22	1:475:A:CYS:H	7	0.18
(1,1095)	1:460:A:LEU:HD23	1:475:A:CYS:H	7	0.18
(1,1042)	1:459:A:PRO:HB2	1:535:A:LEU:H	1	0.18
(1,1042)	1:459:A:PRO:HB3	1:535:A:LEU:H	1	0.18
(1,1042)	1:459:A:PRO:HB2	1:535:A:LEU:H	3	0.18
(1,1042)	1:459:A:PRO:HB3	1:535:A:LEU:H	3	0.18
(1,1021)	1:488:A:LYS:HG3	1:524:A:HIS:H	2	0.18
(1,1012)	1:522:A:ALA:H	1:538:A:LEU:HG	9	0.18
(1,960)	1:486:A:TRP:HZ2	1:511:A:HIS:H	8	0.18
(1,843)	1:456:A:ILE:H	1:458:A:ARG:H	7	0.18
(1,731)	1:498:A:THR:H	1:501:A:TYR:H	4	0.18
(1,723)	1:499:A:PHE:HA	1:501:A:TYR:H	1	0.18
(1,708)	1:467:A:VAL:H	1:541:A:GLN:H	7	0.18
(1,562)	1:488:A:LYS:H	1:491:A:VAL:H	10	0.18
(1,517)	1:535:A:LEU:HD11	1:536:A:ALA:H	5	0.18
(1,517)	1:535:A:LEU:HD12	1:536:A:ALA:H	5	0.18
(1,517)	1:535:A:LEU:HD13	1:536:A:ALA:H	5	0.18
(1,479)	1:486:A:TRP:HZ2	1:512:A:LEU:H	4	0.18
(1,404)	1:487:A:LEU:HA	1:492:A:GLU:H	1	0.18
(1,385)	1:486:A:TRP:HE1	1:503:A:PHE:HB2	3	0.18
(1,385)	1:486:A:TRP:HE1	1:503:A:PHE:HB3	3	0.18
(1,374)	1:490:A:GLY:H	1:525:A:TYR:HA	7	0.18
(1,312)	1:502:A:TRP:HD1	1:515:A:ASN:HD21	7	0.18
(1,160)	1:509:A:ARG:HA	1:509:A:ARG:HD2	7	0.18
(1,160)	1:509:A:ARG:HA	1:509:A:ARG:HD3	7	0.18
(1,134)	1:487:A:LEU:HG	1:492:A:GLU:HA	6	0.18
(1,1287)	1:527:A:LEU:H	1:533:A:GLN:HB2	1	0.17
(1,1287)	1:527:A:LEU:H	1:533:A:GLN:HB3	1	0.17
(1,1234)	1:504:A:LYS:HB2	1:513:A:ILE:HD11	8	0.17
(1,1234)	1:504:A:LYS:HB2	1:513:A:ILE:HD12	8	0.17
(1,1234)	1:504:A:LYS:HB2	1:513:A:ILE:HD13	8	0.17
(1,1234)	1:504:A:LYS:HB3	1:513:A:ILE:HD11	8	0.17
(1,1234)	1:504:A:LYS:HB3	1:513:A:ILE:HD12	8	0.17
(1,1234)	1:504:A:LYS:HB3	1:513:A:ILE:HD13	8	0.17
(1,1217)	1:496:A:GLU:H	1:496:A:GLU:HB2	2	0.17
(1,1217)	1:496:A:GLU:H	1:496:A:GLU:HB3	2	0.17
(1,1086)	1:457:A:THR:HA	1:459:A:PRO:HD2	8	0.17
(1,1086)	1:457:A:THR:HA	1:459:A:PRO:HD3	8	0.17
(1,1082)	1:456:A:ILE:HG12	1:533:A:GLN:H	7	0.17
(1,1082)	1:456:A:ILE:HG13	1:533:A:GLN:H	7	0.17
(1,1022)	1:524:A:HIS:H	1:537:A:GLU:HB2	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1022)	1:524:A:HIS:H	1:537:A:GLU:HB3	9	0.17
(1,934)	1:495:A:ARG:H	1:495:A:ARG:HD2	6	0.17
(1,934)	1:495:A:ARG:H	1:495:A:ARG:HD3	6	0.17
(1,857)	1:462:A:ASP:H	1:463:A:GLN:HE21	6	0.17
(1,811)	1:465:A:VAL:HA	1:469:A:GLN:HE22	8	0.17
(1,801)	1:529:A:THR:H	1:531:A:GLY:H	8	0.17
(1,794)	1:529:A:THR:HG21	1:532:A:GLY:H	6	0.17
(1,794)	1:529:A:THR:HG22	1:532:A:GLY:H	6	0.17
(1,794)	1:529:A:THR:HG23	1:532:A:GLY:H	6	0.17
(1,742)	1:468:A:GLY:H	1:516:A:GLU:HG2	1	0.17
(1,742)	1:468:A:GLY:H	1:516:A:GLU:HG3	1	0.17
(1,709)	1:467:A:VAL:H	1:542:A:GLU:H	6	0.17
(1,606)	1:457:A:THR:HG21	1:458:A:ARG:H	3	0.17
(1,606)	1:457:A:THR:HG22	1:458:A:ARG:H	3	0.17
(1,606)	1:457:A:THR:HG23	1:458:A:ARG:H	3	0.17
(1,595)	1:518:A:MET:HE1	1:519:A:LEU:H	2	0.17
(1,595)	1:518:A:MET:HE2	1:519:A:LEU:H	2	0.17
(1,595)	1:518:A:MET:HE3	1:519:A:LEU:H	2	0.17
(1,552)	1:486:A:TRP:H	1:492:A:GLU:HG2	8	0.17
(1,552)	1:486:A:TRP:H	1:492:A:GLU:HG3	8	0.17
(1,503)	1:473:A:PHE:H	1:513:A:ILE:HG13	7	0.17
(1,442)	1:527:A:LEU:H	1:534:A:ALA:H	7	0.17
(1,333)	1:456:A:ILE:HG21	1:460:A:LEU:H	3	0.17
(1,333)	1:456:A:ILE:HG22	1:460:A:LEU:H	3	0.17
(1,333)	1:456:A:ILE:HG23	1:460:A:LEU:H	3	0.17
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG21	2	0.17
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG22	2	0.17
(1,285)	1:519:A:LEU:HA	1:540:A:VAL:HG23	2	0.17
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD11	8	0.17
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD12	8	0.17
(1,198)	1:464:A:LEU:HB3	1:539:A:ILE:HD13	8	0.17
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD21	8	0.17
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD22	8	0.17
(1,174)	1:501:A:TYR:HE2	1:512:A:LEU:HD23	8	0.17
(1,128)	1:453:A:PRO:HB2	1:531:A:GLY:HA2	3	0.17
(1,101)	1:457:A:THR:HG21	1:478:A:SER:HA	1	0.17
(1,101)	1:457:A:THR:HG22	1:478:A:SER:HA	1	0.17
(1,101)	1:457:A:THR:HG23	1:478:A:SER:HA	1	0.17
(1,34)	1:460:A:LEU:HA	1:536:A:ALA:HB1	4	0.17
(1,34)	1:460:A:LEU:HA	1:536:A:ALA:HB2	4	0.17
(1,34)	1:460:A:LEU:HA	1:536:A:ALA:HB3	4	0.17
(1,1249)	1:509:A:ARG:HG2	1:510:A:HIS:H	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1249)	1:509:A:ARG:HG3	1:510:A:HIS:H	5	0.16
(1,1227)	1:500:A:LYS:HE2	1:518:A:MET:HG2	7	0.16
(1,1227)	1:500:A:LYS:HE2	1:518:A:MET:HG3	7	0.16
(1,1227)	1:500:A:LYS:HE3	1:518:A:MET:HG2	7	0.16
(1,1227)	1:500:A:LYS:HE3	1:518:A:MET:HG3	7	0.16
(1,1185)	1:487:A:LEU:HD11	1:492:A:GLU:H	1	0.16
(1,1185)	1:487:A:LEU:HD12	1:492:A:GLU:H	1	0.16
(1,1185)	1:487:A:LEU:HD13	1:492:A:GLU:H	1	0.16
(1,1185)	1:487:A:LEU:HD21	1:492:A:GLU:H	1	0.16
(1,1185)	1:487:A:LEU:HD22	1:492:A:GLU:H	1	0.16
(1,1185)	1:487:A:LEU:HD23	1:492:A:GLU:H	1	0.16
(1,1184)	1:487:A:LEU:HD11	1:491:A:VAL:HA	2	0.16
(1,1184)	1:487:A:LEU:HD12	1:491:A:VAL:HA	2	0.16
(1,1184)	1:487:A:LEU:HD13	1:491:A:VAL:HA	2	0.16
(1,1184)	1:487:A:LEU:HD21	1:491:A:VAL:HA	2	0.16
(1,1184)	1:487:A:LEU:HD22	1:491:A:VAL:HA	2	0.16
(1,1184)	1:487:A:LEU:HD23	1:491:A:VAL:HA	2	0.16
(1,1160)	1:475:A:CYS:HB2	1:476:A:GLU:H	2	0.16
(1,1160)	1:475:A:CYS:HB3	1:476:A:GLU:H	2	0.16
(1,1160)	1:475:A:CYS:HB2	1:476:A:GLU:H	9	0.16
(1,1160)	1:475:A:CYS:HB3	1:476:A:GLU:H	9	0.16
(1,1097)	1:460:A:LEU:HD11	1:476:A:GLU:H	7	0.16
(1,1097)	1:460:A:LEU:HD12	1:476:A:GLU:H	7	0.16
(1,1097)	1:460:A:LEU:HD13	1:476:A:GLU:H	7	0.16
(1,1097)	1:460:A:LEU:HD21	1:476:A:GLU:H	7	0.16
(1,1097)	1:460:A:LEU:HD22	1:476:A:GLU:H	7	0.16
(1,1097)	1:460:A:LEU:HD23	1:476:A:GLU:H	7	0.16
(1,1095)	1:460:A:LEU:HD11	1:475:A:CYS:H	2	0.16
(1,1095)	1:460:A:LEU:HD12	1:475:A:CYS:H	2	0.16
(1,1095)	1:460:A:LEU:HD13	1:475:A:CYS:H	2	0.16
(1,1095)	1:460:A:LEU:HD21	1:475:A:CYS:H	2	0.16
(1,1095)	1:460:A:LEU:HD22	1:475:A:CYS:H	2	0.16
(1,1095)	1:460:A:LEU:HD23	1:475:A:CYS:H	2	0.16
(1,1069)	1:454:A:VAL:HG11	1:479:A:GLU:H	3	0.16
(1,1069)	1:454:A:VAL:HG12	1:479:A:GLU:H	3	0.16
(1,1069)	1:454:A:VAL:HG13	1:479:A:GLU:H	3	0.16
(1,1069)	1:454:A:VAL:HG21	1:479:A:GLU:H	3	0.16
(1,1069)	1:454:A:VAL:HG22	1:479:A:GLU:H	3	0.16
(1,1069)	1:454:A:VAL:HG23	1:479:A:GLU:H	3	0.16
(1,1052)	1:465:A:VAL:H	1:539:A:ILE:H	7	0.16
(1,1049)	1:541:A:GLN:H	1:542:A:GLU:HA	8	0.16
(1,960)	1:486:A:TRP:HZ2	1:511:A:HIS:H	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,930)	1:487:A:LEU:HB3	1:488:A:LYS:H	4	0.16
(1,912)	1:479:A:GLU:H	1:482:A:ALA:H	10	0.16
(1,866)	1:463:A:GLN:HG2	1:465:A:VAL:H	2	0.16
(1,866)	1:463:A:GLN:HG3	1:465:A:VAL:H	2	0.16
(1,857)	1:462:A:ASP:H	1:463:A:GLN:HE21	3	0.16
(1,747)	1:460:A:LEU:H	1:534:A:ALA:HA	9	0.16
(1,708)	1:467:A:VAL:H	1:541:A:GLN:H	8	0.16
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB2	3	0.16
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB3	3	0.16
(1,570)	1:520:A:GLU:HB2	1:522:A:ALA:H	3	0.16
(1,570)	1:520:A:GLU:HB3	1:522:A:ALA:H	3	0.16
(1,479)	1:486:A:TRP:HZ2	1:512:A:LEU:H	9	0.16
(1,376)	1:487:A:LEU:HB3	1:490:A:GLY:H	2	0.16
(1,323)	1:498:A:THR:HG21	1:501:A:TYR:HD1	3	0.16
(1,323)	1:498:A:THR:HG22	1:501:A:TYR:HD1	3	0.16
(1,323)	1:498:A:THR:HG23	1:501:A:TYR:HD1	3	0.16
(1,249)	1:460:A:LEU:HG	1:526:A:ALA:HA	2	0.16
(1,35)	1:522:A:ALA:HA	1:538:A:LEU:HD11	6	0.16
(1,35)	1:522:A:ALA:HA	1:538:A:LEU:HD12	6	0.16
(1,35)	1:522:A:ALA:HA	1:538:A:LEU:HD13	6	0.16
(1,17)	1:453:A:PRO:HA	1:531:A:GLY:HA3	9	0.16
(1,1300)	1:533:A:GLN:HB2	1:535:A:LEU:H	7	0.15
(1,1300)	1:533:A:GLN:HB3	1:535:A:LEU:H	7	0.15
(1,1248)	1:509:A:ARG:HB2	1:511:A:HIS:HE1	9	0.15
(1,1248)	1:509:A:ARG:HB3	1:511:A:HIS:HE1	9	0.15
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD11	3	0.15
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD12	3	0.15
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD13	3	0.15
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD21	3	0.15
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD22	3	0.15
(1,1161)	1:477:A:VAL:HG11	1:527:A:LEU:HD23	3	0.15
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD11	3	0.15
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD12	3	0.15
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD13	3	0.15
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD21	3	0.15
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD22	3	0.15
(1,1161)	1:477:A:VAL:HG12	1:527:A:LEU:HD23	3	0.15
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD11	3	0.15
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD12	3	0.15
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD13	3	0.15
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD21	3	0.15
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD22	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1161)	1:477:A:VAL:HG13	1:527:A:LEU:HD23	3	0.15
(1,1160)	1:475:A:CYS:HB2	1:476:A:GLU:H	1	0.15
(1,1160)	1:475:A:CYS:HB3	1:476:A:GLU:H	1	0.15
(1,1108)	1:461:A:GLU:HB2	1:471:A:VAL:HG11	8	0.15
(1,1108)	1:461:A:GLU:HB2	1:471:A:VAL:HG12	8	0.15
(1,1108)	1:461:A:GLU:HB2	1:471:A:VAL:HG13	8	0.15
(1,1108)	1:461:A:GLU:HB2	1:471:A:VAL:HG21	8	0.15
(1,1108)	1:461:A:GLU:HB2	1:471:A:VAL:HG22	8	0.15
(1,1108)	1:461:A:GLU:HB2	1:471:A:VAL:HG23	8	0.15
(1,1108)	1:461:A:GLU:HB3	1:471:A:VAL:HG11	8	0.15
(1,1108)	1:461:A:GLU:HB3	1:471:A:VAL:HG12	8	0.15
(1,1108)	1:461:A:GLU:HB3	1:471:A:VAL:HG13	8	0.15
(1,1108)	1:461:A:GLU:HB3	1:471:A:VAL:HG21	8	0.15
(1,1108)	1:461:A:GLU:HB3	1:471:A:VAL:HG22	8	0.15
(1,1108)	1:461:A:GLU:HB3	1:471:A:VAL:HG23	8	0.15
(1,1083)	1:456:A:ILE:HD11	1:527:A:LEU:HB2	7	0.15
(1,1083)	1:456:A:ILE:HD11	1:527:A:LEU:HB3	7	0.15
(1,1083)	1:456:A:ILE:HD12	1:527:A:LEU:HB2	7	0.15
(1,1083)	1:456:A:ILE:HD12	1:527:A:LEU:HB3	7	0.15
(1,1083)	1:456:A:ILE:HD13	1:527:A:LEU:HB2	7	0.15
(1,1083)	1:456:A:ILE:HD13	1:527:A:LEU:HB3	7	0.15
(1,1052)	1:465:A:VAL:H	1:539:A:ILE:H	5	0.15
(1,1011)	1:519:A:LEU:HB3	1:522:A:ALA:H	10	0.15
(1,991)	1:469:A:GLN:HA	1:517:A:ALA:H	8	0.15
(1,982)	1:502:A:TRP:HD1	1:515:A:ASN:H	6	0.15
(1,880)	1:470:A:ARG:H	1:470:A:ARG:HD2	2	0.15
(1,880)	1:470:A:ARG:H	1:470:A:ARG:HD3	2	0.15
(1,857)	1:462:A:ASP:H	1:463:A:GLN:HE21	7	0.15
(1,815)	1:477:A:VAL:H	1:508:A:GLN:HE21	1	0.15
(1,815)	1:477:A:VAL:H	1:508:A:GLN:HE22	1	0.15
(1,758)	1:461:A:GLU:H	1:463:A:GLN:HE22	7	0.15
(1,627)	1:524:A:HIS:HA	1:537:A:GLU:H	9	0.15
(1,624)	1:462:A:ASP:HB3	1:537:A:GLU:H	7	0.15
(1,624)	1:462:A:ASP:HB2	1:537:A:GLU:H	7	0.15
(1,595)	1:518:A:MET:HE1	1:519:A:LEU:H	10	0.15
(1,595)	1:518:A:MET:HE2	1:519:A:LEU:H	10	0.15
(1,595)	1:518:A:MET:HE3	1:519:A:LEU:H	10	0.15
(1,569)	1:522:A:ALA:H	1:540:A:VAL:HB	6	0.15
(1,566)	1:518:A:MET:H	1:522:A:ALA:H	5	0.15
(1,463)	1:473:A:PHE:H	1:511:A:HIS:HA	4	0.15
(1,447)	1:472:A:GLU:H	1:513:A:ILE:HA	2	0.15
(1,434)	1:456:A:ILE:HD11	1:534:A:ALA:H	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,434)	1:456:A:ILE:HD12	1:534:A:ALA:H	1	0.15
(1,434)	1:456:A:ILE:HD13	1:534:A:ALA:H	1	0.15
(1,404)	1:487:A:LEU:HA	1:492:A:GLU:H	8	0.15
(1,384)	1:486:A:TRP:HE1	1:510:A:HIS:HB3	6	0.15
(1,374)	1:490:A:GLY:H	1:525:A:TYR:HA	6	0.15
(1,294)	1:474:A:GLU:HA	1:486:A:TRP:HZ2	5	0.15
(1,249)	1:460:A:LEU:HG	1:526:A:ALA:HA	5	0.15
(1,171)	1:512:A:LEU:HD21	1:514:A:ILE:HD11	3	0.15
(1,171)	1:512:A:LEU:HD21	1:514:A:ILE:HD12	3	0.15
(1,171)	1:512:A:LEU:HD21	1:514:A:ILE:HD13	3	0.15
(1,171)	1:512:A:LEU:HD22	1:514:A:ILE:HD11	3	0.15
(1,171)	1:512:A:LEU:HD22	1:514:A:ILE:HD12	3	0.15
(1,171)	1:512:A:LEU:HD22	1:514:A:ILE:HD13	3	0.15
(1,171)	1:512:A:LEU:HD23	1:514:A:ILE:HD11	3	0.15
(1,171)	1:512:A:LEU:HD23	1:514:A:ILE:HD12	3	0.15
(1,171)	1:512:A:LEU:HD23	1:514:A:ILE:HD13	3	0.15
(1,151)	1:502:A:TRP:H	1:503:A:PHE:HB3	3	0.15
(1,128)	1:453:A:PRO:HB2	1:531:A:GLY:HA2	6	0.15
(1,1273)	1:519:A:LEU:HD11	1:542:A:GLU:HG2	2	0.14
(1,1273)	1:519:A:LEU:HD11	1:542:A:GLU:HG3	2	0.14
(1,1273)	1:519:A:LEU:HD12	1:542:A:GLU:HG2	2	0.14
(1,1273)	1:519:A:LEU:HD12	1:542:A:GLU:HG3	2	0.14
(1,1273)	1:519:A:LEU:HD13	1:542:A:GLU:HG2	2	0.14
(1,1273)	1:519:A:LEU:HD13	1:542:A:GLU:HG3	2	0.14
(1,1273)	1:519:A:LEU:HD21	1:542:A:GLU:HG2	2	0.14
(1,1273)	1:519:A:LEU:HD21	1:542:A:GLU:HG3	2	0.14
(1,1273)	1:519:A:LEU:HD22	1:542:A:GLU:HG2	2	0.14
(1,1273)	1:519:A:LEU:HD22	1:542:A:GLU:HG3	2	0.14
(1,1273)	1:519:A:LEU:HD23	1:542:A:GLU:HG2	2	0.14
(1,1273)	1:519:A:LEU:HD23	1:542:A:GLU:HG3	2	0.14
(1,1271)	1:519:A:LEU:HD11	1:542:A:GLU:H	7	0.14
(1,1271)	1:519:A:LEU:HD12	1:542:A:GLU:H	7	0.14
(1,1271)	1:519:A:LEU:HD13	1:542:A:GLU:H	7	0.14
(1,1271)	1:519:A:LEU:HD21	1:542:A:GLU:H	7	0.14
(1,1271)	1:519:A:LEU:HD22	1:542:A:GLU:H	7	0.14
(1,1271)	1:519:A:LEU:HD23	1:542:A:GLU:H	7	0.14
(1,1132)	1:467:A:VAL:HG11	1:541:A:GLN:H	9	0.14
(1,1132)	1:467:A:VAL:HG12	1:541:A:GLN:H	9	0.14
(1,1132)	1:467:A:VAL:HG13	1:541:A:GLN:H	9	0.14
(1,1132)	1:467:A:VAL:HG21	1:541:A:GLN:H	9	0.14
(1,1132)	1:467:A:VAL:HG22	1:541:A:GLN:H	9	0.14
(1,1132)	1:467:A:VAL:HG23	1:541:A:GLN:H	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1097)	1:460:A:LEU:HD11	1:476:A:GLU:H	3	0.14
(1,1097)	1:460:A:LEU:HD12	1:476:A:GLU:H	3	0.14
(1,1097)	1:460:A:LEU:HD13	1:476:A:GLU:H	3	0.14
(1,1097)	1:460:A:LEU:HD21	1:476:A:GLU:H	3	0.14
(1,1097)	1:460:A:LEU:HD22	1:476:A:GLU:H	3	0.14
(1,1097)	1:460:A:LEU:HD23	1:476:A:GLU:H	3	0.14
(1,1085)	1:456:A:ILE:HD11	1:532:A:GLY:HA2	5	0.14
(1,1085)	1:456:A:ILE:HD11	1:532:A:GLY:HA3	5	0.14
(1,1085)	1:456:A:ILE:HD12	1:532:A:GLY:HA2	5	0.14
(1,1085)	1:456:A:ILE:HD12	1:532:A:GLY:HA3	5	0.14
(1,1085)	1:456:A:ILE:HD13	1:532:A:GLY:HA2	5	0.14
(1,1085)	1:456:A:ILE:HD13	1:532:A:GLY:HA3	5	0.14
(1,1085)	1:456:A:ILE:HD11	1:532:A:GLY:HA2	10	0.14
(1,1085)	1:456:A:ILE:HD11	1:532:A:GLY:HA3	10	0.14
(1,1085)	1:456:A:ILE:HD12	1:532:A:GLY:HA2	10	0.14
(1,1085)	1:456:A:ILE:HD12	1:532:A:GLY:HA3	10	0.14
(1,1085)	1:456:A:ILE:HD13	1:532:A:GLY:HA2	10	0.14
(1,1085)	1:456:A:ILE:HD13	1:532:A:GLY:HA3	10	0.14
(1,1083)	1:456:A:ILE:HD11	1:527:A:LEU:HB2	5	0.14
(1,1083)	1:456:A:ILE:HD11	1:527:A:LEU:HB3	5	0.14
(1,1083)	1:456:A:ILE:HD12	1:527:A:LEU:HB2	5	0.14
(1,1083)	1:456:A:ILE:HD12	1:527:A:LEU:HB3	5	0.14
(1,1083)	1:456:A:ILE:HD13	1:527:A:LEU:HB2	5	0.14
(1,1083)	1:456:A:ILE:HD13	1:527:A:LEU:HB3	5	0.14
(1,1049)	1:541:A:GLN:H	1:542:A:GLU:HA	1	0.14
(1,1014)	1:524:A:HIS:H	1:537:A:GLU:HA	3	0.14
(1,1011)	1:519:A:LEU:HB3	1:522:A:ALA:H	9	0.14
(1,905)	1:477:A:VAL:H	1:508:A:GLN:HG2	5	0.14
(1,905)	1:477:A:VAL:H	1:508:A:GLN:HG3	5	0.14
(1,887)	1:475:A:CYS:H	1:510:A:HIS:HB3	4	0.14
(1,755)	1:463:A:GLN:HE21	1:464:A:LEU:H	7	0.14
(1,672)	1:469:A:GLN:H	1:517:A:ALA:HA	6	0.14
(1,657)	1:457:A:THR:H	1:477:A:VAL:HB	3	0.14
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB2	2	0.14
(1,614)	1:454:A:VAL:H	1:530:A:SER:HB3	2	0.14
(1,606)	1:457:A:THR:HG21	1:458:A:ARG:H	4	0.14
(1,606)	1:457:A:THR:HG22	1:458:A:ARG:H	4	0.14
(1,606)	1:457:A:THR:HG23	1:458:A:ARG:H	4	0.14
(1,604)	1:456:A:ILE:HA	1:458:A:ARG:H	1	0.14
(1,517)	1:535:A:LEU:HD11	1:536:A:ALA:H	1	0.14
(1,517)	1:535:A:LEU:HD12	1:536:A:ALA:H	1	0.14
(1,517)	1:535:A:LEU:HD13	1:536:A:ALA:H	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,445)	1:472:A:GLU:H	1:472:A:GLU:HG2	2	0.14
(1,445)	1:472:A:GLU:H	1:472:A:GLU:HG3	2	0.14
(1,404)	1:487:A:LEU:HA	1:492:A:GLU:H	7	0.14
(1,386)	1:486:A:TRP:HE1	1:510:A:HIS:HB2	3	0.14
(1,361)	1:488:A:LYS:HD2	1:489:A:ASP:H	7	0.14
(1,352)	1:464:A:LEU:HB2	1:539:A:ILE:H	8	0.14
(1,255)	1:484:A:VAL:HB	1:527:A:LEU:HD21	4	0.14
(1,255)	1:484:A:VAL:HB	1:527:A:LEU:HD22	4	0.14
(1,255)	1:484:A:VAL:HB	1:527:A:LEU:HD23	4	0.14
(1,218)	1:468:A:GLY:HA2	1:516:A:GLU:HA	8	0.14
(1,195)	1:514:A:ILE:HD11	1:521:A:ASP:HB3	8	0.14
(1,195)	1:514:A:ILE:HD12	1:521:A:ASP:HB3	8	0.14
(1,195)	1:514:A:ILE:HD13	1:521:A:ASP:HB3	8	0.14
(1,115)	1:484:A:VAL:HG11	1:510:A:HIS:H	2	0.14
(1,115)	1:484:A:VAL:HG12	1:510:A:HIS:H	2	0.14
(1,115)	1:484:A:VAL:HG13	1:510:A:HIS:H	2	0.14
(1,1249)	1:509:A:ARG:HG2	1:510:A:HIS:H	3	0.13
(1,1249)	1:509:A:ARG:HG3	1:510:A:HIS:H	3	0.13
(1,1189)	1:487:A:LEU:HD11	1:493:A:LEU:H	5	0.13
(1,1189)	1:487:A:LEU:HD12	1:493:A:LEU:H	5	0.13
(1,1189)	1:487:A:LEU:HD13	1:493:A:LEU:H	5	0.13
(1,1189)	1:487:A:LEU:HD21	1:493:A:LEU:H	5	0.13
(1,1189)	1:487:A:LEU:HD22	1:493:A:LEU:H	5	0.13
(1,1189)	1:487:A:LEU:HD23	1:493:A:LEU:H	5	0.13
(1,1156)	1:473:A:PHE:HB2	1:486:A:TRP:HZ2	6	0.13
(1,1156)	1:473:A:PHE:HB3	1:486:A:TRP:HZ2	6	0.13
(1,1090)	1:460:A:LEU:H	1:475:A:CYS:HB2	2	0.13
(1,1090)	1:460:A:LEU:H	1:475:A:CYS:HB3	2	0.13
(1,1068)	1:454:A:VAL:HG11	1:478:A:SER:H	8	0.13
(1,1068)	1:454:A:VAL:HG12	1:478:A:SER:H	8	0.13
(1,1068)	1:454:A:VAL:HG13	1:478:A:SER:H	8	0.13
(1,1068)	1:454:A:VAL:HG21	1:478:A:SER:H	8	0.13
(1,1068)	1:454:A:VAL:HG22	1:478:A:SER:H	8	0.13
(1,1068)	1:454:A:VAL:HG23	1:478:A:SER:H	8	0.13
(1,1011)	1:519:A:LEU:HB3	1:522:A:ALA:H	3	0.13
(1,859)	1:463:A:GLN:H	1:463:A:GLN:HE21	10	0.13
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB1	9	0.13
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB2	9	0.13
(1,853)	1:462:A:ASP:H	1:536:A:ALA:HB3	9	0.13
(1,816)	1:478:A:SER:H	1:508:A:GLN:HE22	2	0.13
(1,796)	1:529:A:THR:HG21	1:531:A:GLY:H	4	0.13
(1,796)	1:529:A:THR:HG22	1:531:A:GLY:H	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,796)	1:529:A:THR:HG23	1:531:A:GLY:H	4	0.13
(1,758)	1:461:A:GLU:H	1:463:A:GLN:HE22	10	0.13
(1,731)	1:498:A:THR:H	1:501:A:TYR:H	5	0.13
(1,709)	1:467:A:VAL:H	1:542:A:GLU:H	5	0.13
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG11	5	0.13
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG12	5	0.13
(1,643)	1:482:A:ALA:H	1:484:A:VAL:HG13	5	0.13
(1,636)	1:487:A:LEU:HB2	1:526:A:ALA:H	4	0.13
(1,624)	1:462:A:ASP:HB3	1:537:A:GLU:H	4	0.13
(1,624)	1:462:A:ASP:HB2	1:537:A:GLU:H	4	0.13
(1,620)	1:541:A:GLN:HG2	1:542:A:GLU:H	3	0.13
(1,620)	1:541:A:GLN:HG3	1:542:A:GLU:H	3	0.13
(1,517)	1:535:A:LEU:HD11	1:536:A:ALA:H	10	0.13
(1,517)	1:535:A:LEU:HD12	1:536:A:ALA:H	10	0.13
(1,517)	1:535:A:LEU:HD13	1:536:A:ALA:H	10	0.13
(1,439)	1:526:A:ALA:HA	1:534:A:ALA:H	4	0.13
(1,434)	1:456:A:ILE:HD11	1:534:A:ALA:H	6	0.13
(1,434)	1:456:A:ILE:HD12	1:534:A:ALA:H	6	0.13
(1,434)	1:456:A:ILE:HD13	1:534:A:ALA:H	6	0.13
(1,421)	1:525:A:TYR:H	1:536:A:ALA:H	9	0.13
(1,397)	1:513:A:ILE:H	1:513:A:ILE:HD11	2	0.13
(1,397)	1:513:A:ILE:H	1:513:A:ILE:HD12	2	0.13
(1,397)	1:513:A:ILE:H	1:513:A:ILE:HD13	2	0.13
(1,387)	1:486:A:TRP:HE1	1:503:A:PHE:HA	10	0.13
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB1	7	0.13
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB2	7	0.13
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB3	7	0.13
(1,282)	1:464:A:LEU:HA	1:540:A:VAL:HG21	9	0.13
(1,282)	1:464:A:LEU:HA	1:540:A:VAL:HG22	9	0.13
(1,282)	1:464:A:LEU:HA	1:540:A:VAL:HG23	9	0.13
(1,218)	1:468:A:GLY:HA2	1:516:A:GLU:HA	7	0.13
(1,175)	1:512:A:LEU:HG	1:514:A:ILE:HD11	3	0.13
(1,175)	1:512:A:LEU:HG	1:514:A:ILE:HD12	3	0.13
(1,175)	1:512:A:LEU:HG	1:514:A:ILE:HD13	3	0.13
(1,158)	1:508:A:GLN:HA	1:510:A:HIS:HD2	6	0.13
(1,35)	1:522:A:ALA:HA	1:538:A:LEU:HD11	10	0.13
(1,35)	1:522:A:ALA:HA	1:538:A:LEU:HD12	10	0.13
(1,35)	1:522:A:ALA:HA	1:538:A:LEU:HD13	10	0.13
(1,1287)	1:527:A:LEU:H	1:533:A:GLN:HB2	6	0.12
(1,1287)	1:527:A:LEU:H	1:533:A:GLN:HB3	6	0.12
(1,1240)	1:505:A:LYS:HB2	1:510:A:HIS:HE1	1	0.12
(1,1240)	1:505:A:LYS:HB3	1:510:A:HIS:HE1	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1185)	1:487:A:LEU:HD11	1:492:A:GLU:H	3	0.12
(1,1185)	1:487:A:LEU:HD12	1:492:A:GLU:H	3	0.12
(1,1185)	1:487:A:LEU:HD13	1:492:A:GLU:H	3	0.12
(1,1185)	1:487:A:LEU:HD21	1:492:A:GLU:H	3	0.12
(1,1185)	1:487:A:LEU:HD22	1:492:A:GLU:H	3	0.12
(1,1185)	1:487:A:LEU:HD23	1:492:A:GLU:H	3	0.12
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD11	6	0.12
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD12	6	0.12
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD13	6	0.12
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD21	6	0.12
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD22	6	0.12
(1,1173)	1:486:A:TRP:H	1:487:A:LEU:HD23	6	0.12
(1,979)	1:470:A:ARG:H	1:517:A:ALA:H	4	0.12
(1,898)	1:475:A:CYS:HB2	1:476:A:GLU:H	2	0.12
(1,859)	1:463:A:GLN:H	1:463:A:GLN:HE21	7	0.12
(1,834)	1:477:A:VAL:HG11	1:479:A:GLU:H	10	0.12
(1,834)	1:477:A:VAL:HG12	1:479:A:GLU:H	10	0.12
(1,834)	1:477:A:VAL:HG13	1:479:A:GLU:H	10	0.12
(1,817)	1:523:A:GLY:H	1:540:A:VAL:HB	8	0.12
(1,794)	1:529:A:THR:HG21	1:532:A:GLY:H	4	0.12
(1,794)	1:529:A:THR:HG22	1:532:A:GLY:H	4	0.12
(1,794)	1:529:A:THR:HG23	1:532:A:GLY:H	4	0.12
(1,755)	1:463:A:GLN:HE21	1:464:A:LEU:H	3	0.12
(1,722)	1:501:A:TYR:H	1:501:A:TYR:HD1	10	0.12
(1,699)	1:495:A:ARG:HD2	1:496:A:GLU:H	6	0.12
(1,699)	1:495:A:ARG:HD3	1:496:A:GLU:H	6	0.12
(1,659)	1:457:A:THR:H	1:477:A:VAL:HA	5	0.12
(1,633)	1:526:A:ALA:H	1:535:A:LEU:HA	7	0.12
(1,461)	1:472:A:GLU:HG2	1:473:A:PHE:H	8	0.12
(1,461)	1:472:A:GLU:HG3	1:473:A:PHE:H	8	0.12
(1,439)	1:526:A:ALA:HA	1:534:A:ALA:H	5	0.12
(1,405)	1:491:A:VAL:H	1:492:A:GLU:H	4	0.12
(1,374)	1:490:A:GLY:H	1:525:A:TYR:HA	1	0.12
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB1	5	0.12
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB2	5	0.12
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB3	5	0.12
(1,1299)	1:533:A:GLN:HB2	1:534:A:ALA:H	9	0.11
(1,1299)	1:533:A:GLN:HB3	1:534:A:ALA:H	9	0.11
(1,1226)	1:500:A:LYS:HE2	1:518:A:MET:H	3	0.11
(1,1226)	1:500:A:LYS:HE3	1:518:A:MET:H	3	0.11
(1,1216)	1:495:A:ARG:HG2	1:496:A:GLU:H	8	0.11
(1,1216)	1:495:A:ARG:HG3	1:496:A:GLU:H	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1019)	1:524:A:HIS:H	1:525:A:TYR:HD1	9	0.11
(1,1009)	1:517:A:ALA:HB1	1:521:A:ASP:H	8	0.11
(1,1009)	1:517:A:ALA:HB2	1:521:A:ASP:H	8	0.11
(1,1009)	1:517:A:ALA:HB3	1:521:A:ASP:H	8	0.11
(1,991)	1:469:A:GLN:HA	1:517:A:ALA:H	9	0.11
(1,912)	1:479:A:GLU:H	1:482:A:ALA:H	5	0.11
(1,912)	1:479:A:GLU:H	1:482:A:ALA:H	6	0.11
(1,901)	1:476:A:GLU:H	1:477:A:VAL:HG21	8	0.11
(1,901)	1:476:A:GLU:H	1:477:A:VAL:HG22	8	0.11
(1,901)	1:476:A:GLU:H	1:477:A:VAL:HG23	8	0.11
(1,859)	1:463:A:GLN:H	1:463:A:GLN:HE21	5	0.11
(1,719)	1:500:A:LYS:HD2	1:501:A:TYR:H	2	0.11
(1,719)	1:500:A:LYS:HD3	1:501:A:TYR:H	2	0.11
(1,711)	1:501:A:TYR:HB2	1:502:A:TRP:H	2	0.11
(1,711)	1:501:A:TYR:HB3	1:502:A:TRP:H	2	0.11
(1,665)	1:473:A:PHE:H	1:474:A:GLU:H	1	0.11
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG21	8	0.11
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG22	8	0.11
(1,571)	1:522:A:ALA:H	1:540:A:VAL:HG23	8	0.11
(1,565)	1:520:A:GLU:H	1:522:A:ALA:H	4	0.11
(1,519)	1:535:A:LEU:HG	1:536:A:ALA:H	7	0.11
(1,507)	1:537:A:GLU:HG2	1:538:A:LEU:H	10	0.11
(1,507)	1:537:A:GLU:HG3	1:538:A:LEU:H	10	0.11
(1,479)	1:486:A:TRP:HZ2	1:512:A:LEU:H	5	0.11
(1,475)	1:473:A:PHE:HA	1:512:A:LEU:H	8	0.11
(1,444)	1:472:A:GLU:H	1:514:A:ILE:HB	3	0.11
(1,329)	1:504:A:LYS:HD2	1:513:A:ILE:HD11	10	0.11
(1,329)	1:504:A:LYS:HD2	1:513:A:ILE:HD12	10	0.11
(1,329)	1:504:A:LYS:HD2	1:513:A:ILE:HD13	10	0.11
(1,329)	1:504:A:LYS:HD3	1:513:A:ILE:HD11	10	0.11
(1,329)	1:504:A:LYS:HD3	1:513:A:ILE:HD12	10	0.11
(1,329)	1:504:A:LYS:HD3	1:513:A:ILE:HD13	10	0.11
(1,278)	1:465:A:VAL:H	1:540:A:VAL:HG11	6	0.11
(1,278)	1:465:A:VAL:H	1:540:A:VAL:HG12	6	0.11
(1,278)	1:465:A:VAL:H	1:540:A:VAL:HG13	6	0.11
(1,224)	1:519:A:LEU:HA	1:540:A:VAL:HB	3	0.11
(1,215)	1:470:A:ARG:HB2	1:515:A:ASN:HA	10	0.11
(1,193)	1:471:A:VAL:HB	1:514:A:ILE:HD11	1	0.11
(1,193)	1:471:A:VAL:HB	1:514:A:ILE:HD12	1	0.11
(1,193)	1:471:A:VAL:HB	1:514:A:ILE:HD13	1	0.11
(1,59)	1:468:A:GLY:HA3	1:516:A:GLU:HG2	1	0.11
(1,59)	1:468:A:GLY:HA3	1:516:A:GLU:HG3	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:460:A:LEU:HA	1:536:A:ALA:HB1	8	0.11
(1,34)	1:460:A:LEU:HA	1:536:A:ALA:HB2	8	0.11
(1,34)	1:460:A:LEU:HA	1:536:A:ALA:HB3	8	0.11
(1,1314)	1:542:A:GLU:HG2	1:543:A:LYS:H	5	0.1
(1,1314)	1:542:A:GLU:HG3	1:543:A:LYS:H	5	0.1
(1,1299)	1:533:A:GLN:HB2	1:534:A:ALA:H	4	0.1
(1,1299)	1:533:A:GLN:HB3	1:534:A:ALA:H	4	0.1
(1,979)	1:470:A:ARG:H	1:517:A:ALA:H	10	0.1
(1,887)	1:475:A:CYS:H	1:510:A:HIS:HB3	2	0.1
(1,708)	1:467:A:VAL:H	1:541:A:GLN:H	1	0.1
(1,699)	1:495:A:ARG:HD2	1:496:A:GLU:H	9	0.1
(1,699)	1:495:A:ARG:HD3	1:496:A:GLU:H	9	0.1
(1,604)	1:456:A:ILE:HA	1:458:A:ARG:H	8	0.1
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB1	9	0.1
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB2	9	0.1
(1,339)	1:460:A:LEU:H	1:534:A:ALA:HB3	9	0.1
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD11	2	0.1
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD12	2	0.1
(1,300)	1:501:A:TYR:HD1	1:512:A:LEU:HD13	2	0.1
(1,282)	1:464:A:LEU:HA	1:540:A:VAL:HG21	5	0.1
(1,282)	1:464:A:LEU:HA	1:540:A:VAL:HG22	5	0.1
(1,282)	1:464:A:LEU:HA	1:540:A:VAL:HG23	5	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found