



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 03:48 PM UTC

PDB ID : 2KWH / pdb_00002kwh
BMRB ID : 15524
Title : Ral binding domain of RLIP76 (RalBP1)
Authors : Fenwick, R.B.; Campbell, L.J.; Rajasekar, K.; Prasannan, S.; Nietlispach, D.;
Camonis, J.; Owen, D.; Mott, H.R.
Deposited on : 2010-04-12

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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

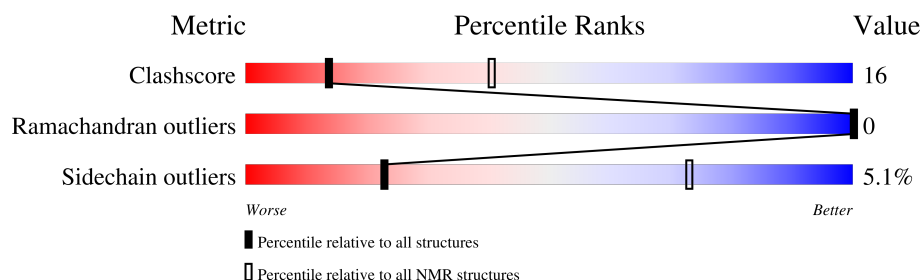
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 58%.

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	56	

2 Ensemble composition and analysis

This entry contains 50 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:395-A:416, A:422-A:443 (44)	0.47	14

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

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

The models can be grouped into 8 clusters and 12 single-model clusters were found.

Cluster number	Models
1	5, 7, 8, 14, 20, 21, 30, 37, 43, 50
2	1, 6, 10, 17, 34, 36, 39, 46
3	2, 28, 31, 42
4	9, 19, 32, 48
5	11, 15, 16
6	24, 26, 33
7	18, 38, 47
8	12, 29, 35
Single-model clusters	3; 4; 13; 22; 23; 25; 27; 40; 41; 44; 45; 49

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 951 atoms, of which 487 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RalA-binding protein 1.

Mol	Chain	Residues	Atoms					Trace
1	A	56	Total	C	H	N	O	0
			951	287	487	90	87	

There are 3 discrepancies between the modelled and reference sequences:

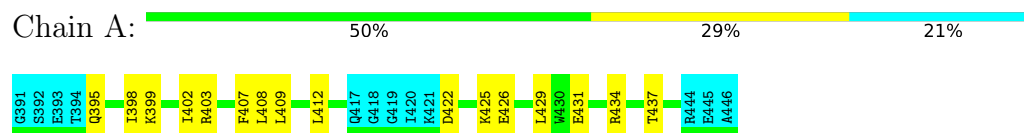
Chain	Residue	Modelled	Actual	Comment	Reference
A	391	GLY	-	expression tag	UNP Q15311
A	392	SER	-	expression tag	UNP Q15311
A	411	SER	CYS	engineered mutation	UNP Q15311

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: RalA-binding protein 1

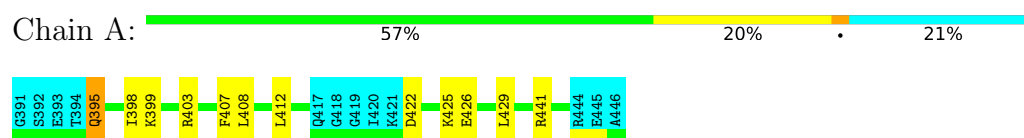


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

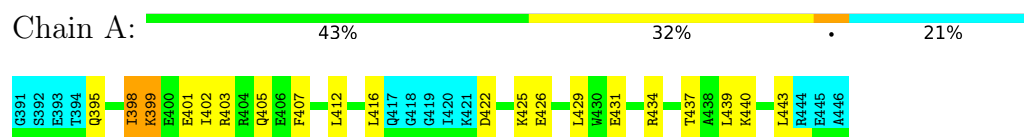
4.2.1 Score per residue for model 1

- Molecule 1: RalA-binding protein 1



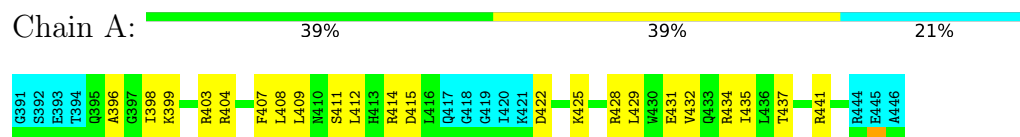
4.2.2 Score per residue for model 2

- Molecule 1: RalA-binding protein 1



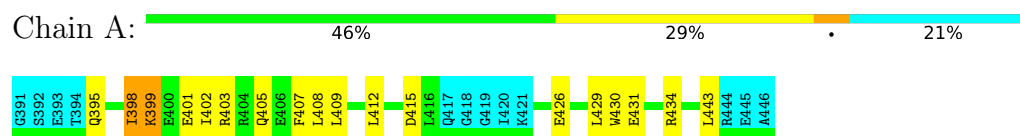
4.2.3 Score per residue for model 3

- Molecule 1: RalA-binding protein 1



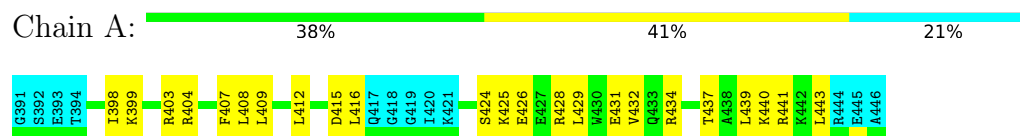
4.2.4 Score per residue for model 4

- Molecule 1: RalA-binding protein 1



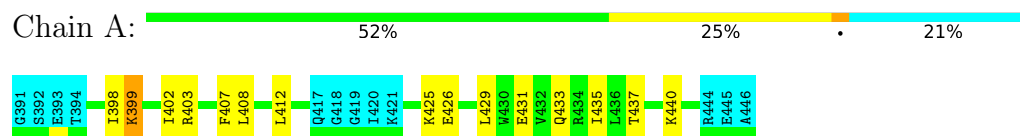
4.2.5 Score per residue for model 5

- Molecule 1: RalA-binding protein 1



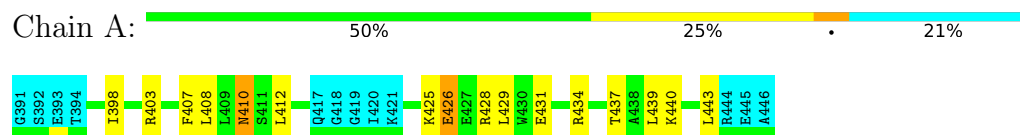
4.2.6 Score per residue for model 6

- Molecule 1: RalA-binding protein 1



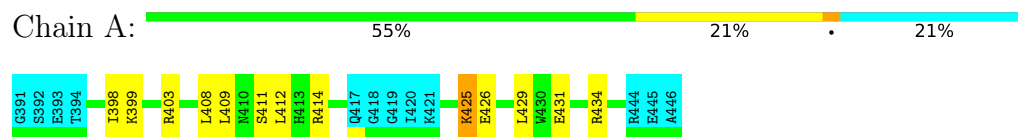
4.2.7 Score per residue for model 7

- Molecule 1: RalA-binding protein 1



4.2.8 Score per residue for model 8

- Molecule 1: RalA-binding protein 1



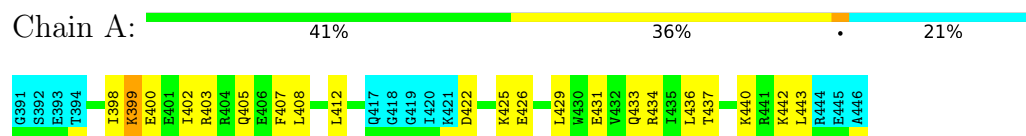
4.2.9 Score per residue for model 9

- Molecule 1: RalA-binding protein 1



4.2.10 Score per residue for model 10

- Molecule 1: RalA-binding protein 1



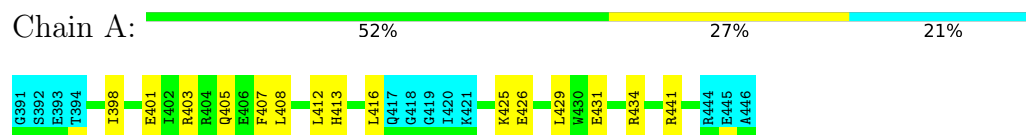
4.2.11 Score per residue for model 11

- Molecule 1: RalA-binding protein 1



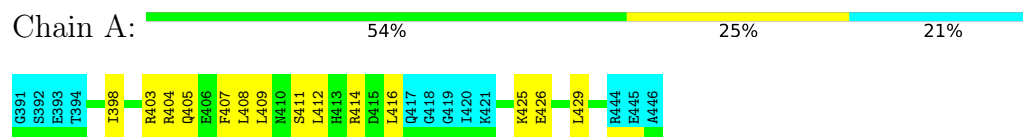
4.2.12 Score per residue for model 12

- Molecule 1: RalA-binding protein 1



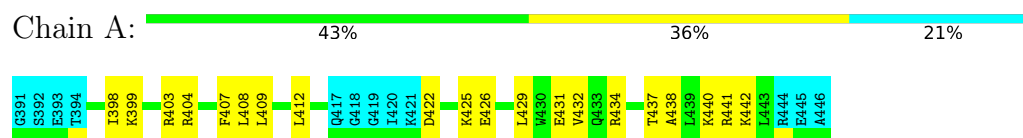
4.2.13 Score per residue for model 13

- Molecule 1: RalA-binding protein 1



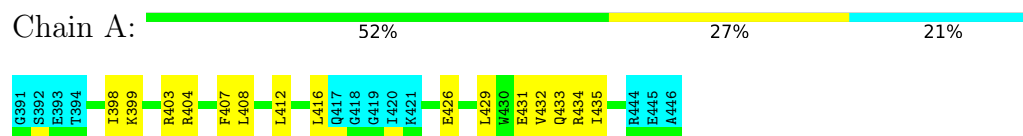
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: RalA-binding protein 1



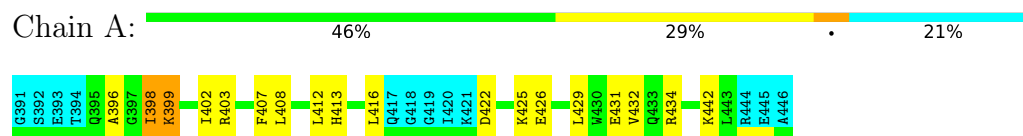
4.2.15 Score per residue for model 15

- Molecule 1: RalA-binding protein 1



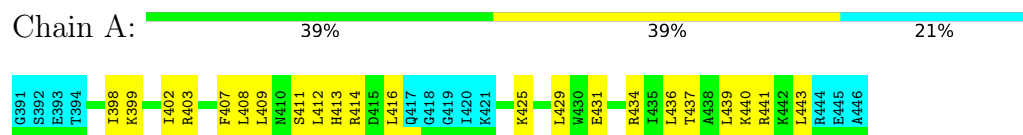
4.2.16 Score per residue for model 16

- Molecule 1: RalA-binding protein 1



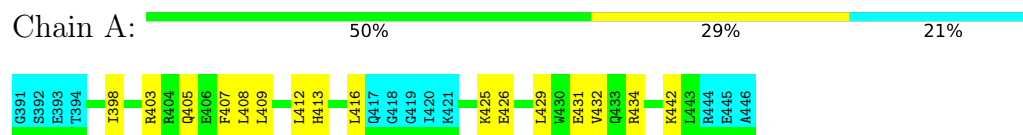
4.2.17 Score per residue for model 17

- Molecule 1: RalA-binding protein 1



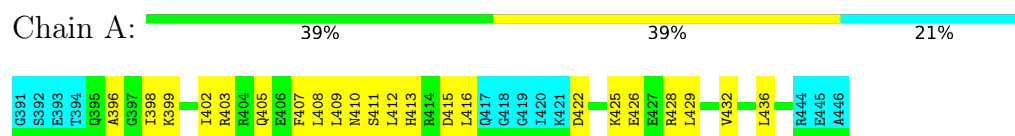
4.2.18 Score per residue for model 18

- Molecule 1: RalA-binding protein 1



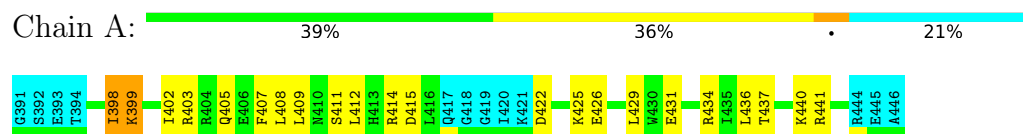
4.2.19 Score per residue for model 19

- Molecule 1: RalA-binding protein 1



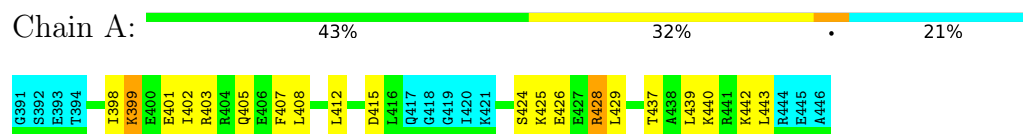
4.2.20 Score per residue for model 20

- Molecule 1: RalA-binding protein 1



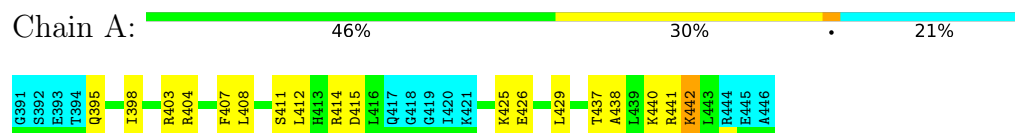
4.2.21 Score per residue for model 21

- Molecule 1: RalA-binding protein 1



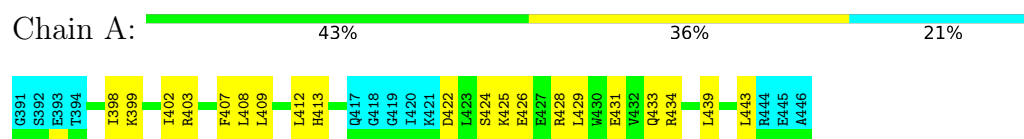
4.2.22 Score per residue for model 22

- Molecule 1: RalA-binding protein 1



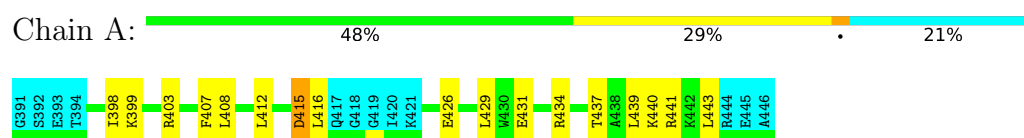
4.2.23 Score per residue for model 23

- Molecule 1: RalA-binding protein 1



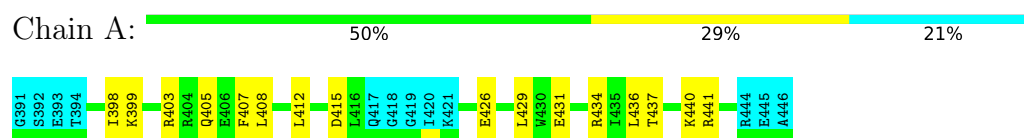
4.2.24 Score per residue for model 24

- Molecule 1: RalA-binding protein 1



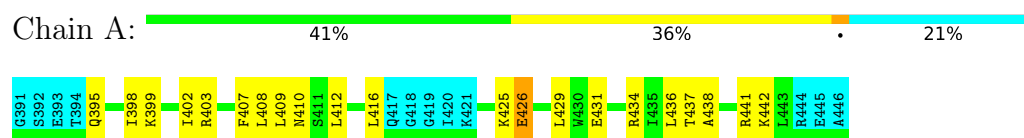
4.2.25 Score per residue for model 25

- Molecule 1: RalA-binding protein 1



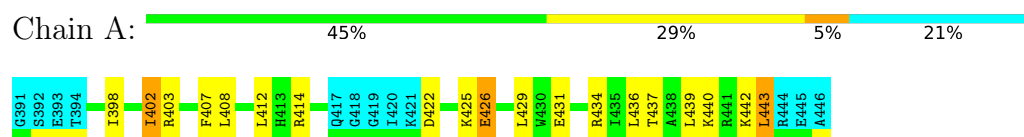
4.2.26 Score per residue for model 26

- Molecule 1: RalA-binding protein 1



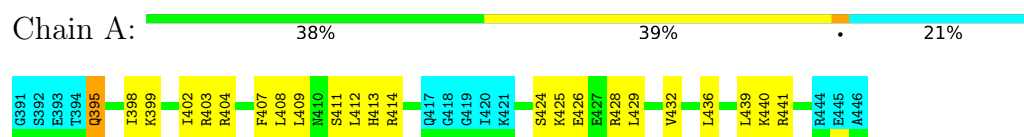
4.2.27 Score per residue for model 27

- Molecule 1: RalA-binding protein 1



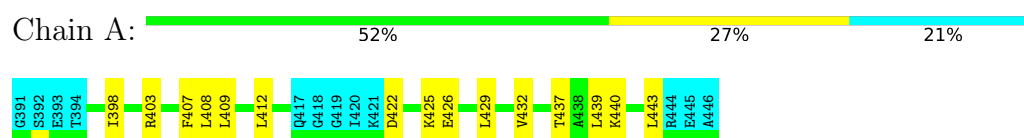
4.2.28 Score per residue for model 28

- Molecule 1: RalA-binding protein 1



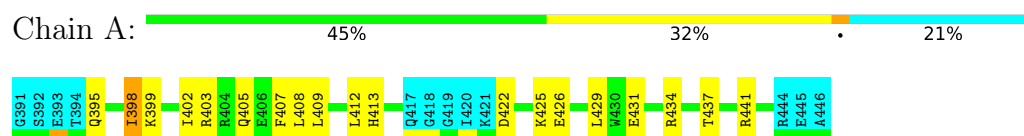
4.2.29 Score per residue for model 29

- Molecule 1: RalA-binding protein 1



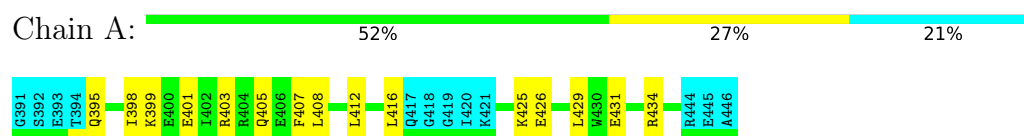
4.2.30 Score per residue for model 30

- Molecule 1: RalA-binding protein 1



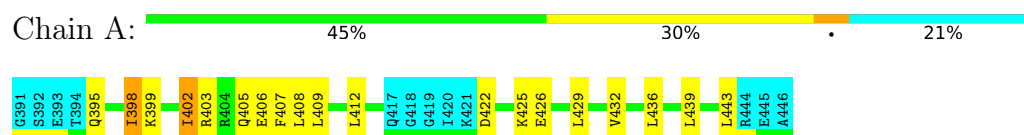
4.2.31 Score per residue for model 31

- Molecule 1: RalA-binding protein 1



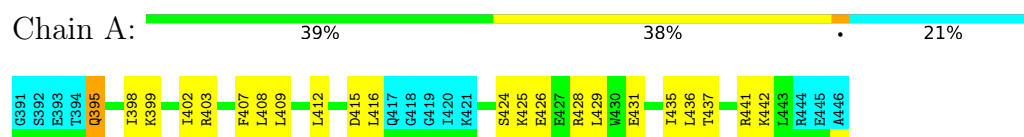
4.2.32 Score per residue for model 32

- Molecule 1: RalA-binding protein 1



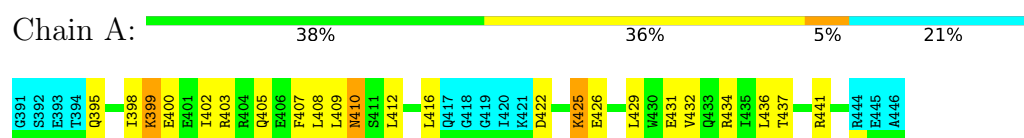
4.2.33 Score per residue for model 33

- Molecule 1: RalA-binding protein 1



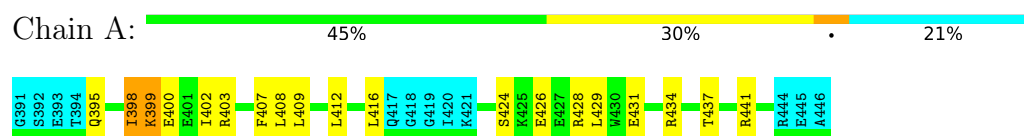
4.2.34 Score per residue for model 34

- Molecule 1: RalA-binding protein 1



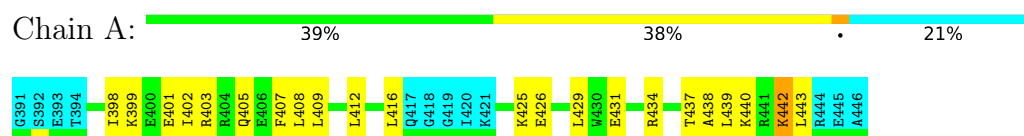
4.2.35 Score per residue for model 35

- Molecule 1: RalA-binding protein 1



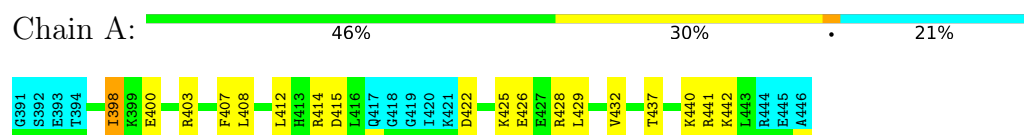
4.2.36 Score per residue for model 36

- Molecule 1: RalA-binding protein 1



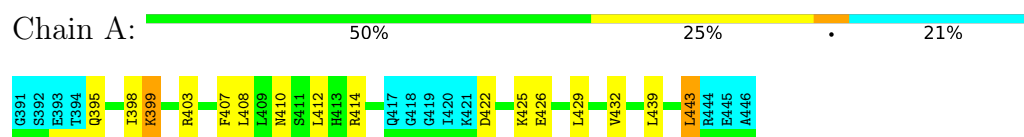
4.2.37 Score per residue for model 37

- Molecule 1: RalA-binding protein 1



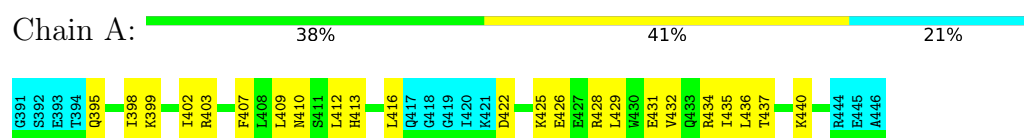
4.2.38 Score per residue for model 38

- Molecule 1: RalA-binding protein 1



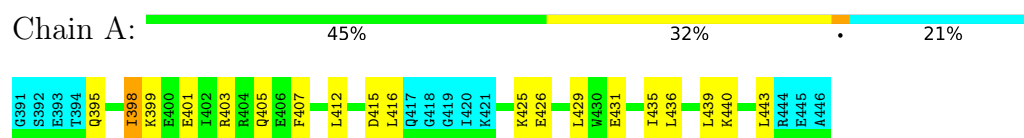
4.2.39 Score per residue for model 39

- Molecule 1: RalA-binding protein 1



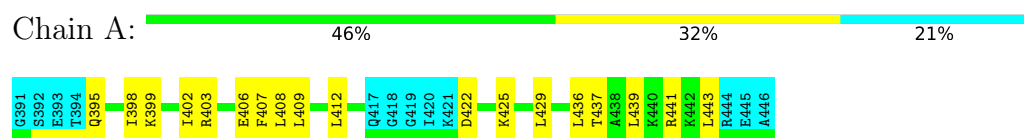
4.2.40 Score per residue for model 40

- Molecule 1: RalA-binding protein 1



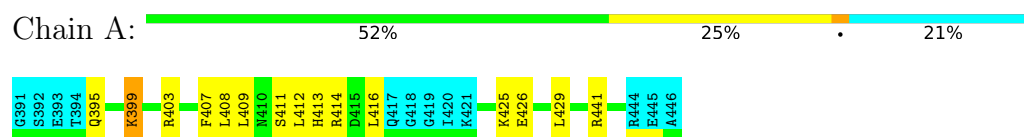
4.2.41 Score per residue for model 41

- Molecule 1: RalA-binding protein 1



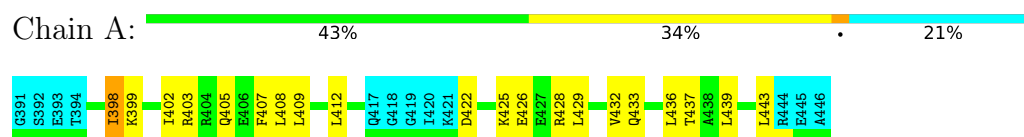
4.2.42 Score per residue for model 42

- Molecule 1: RalA-binding protein 1



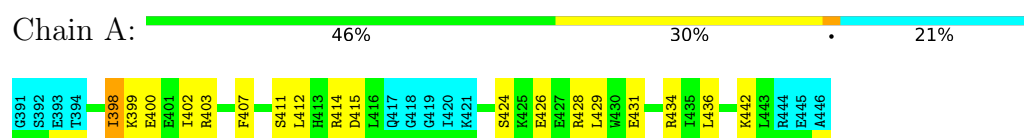
4.2.43 Score per residue for model 43

- Molecule 1: RalA-binding protein 1



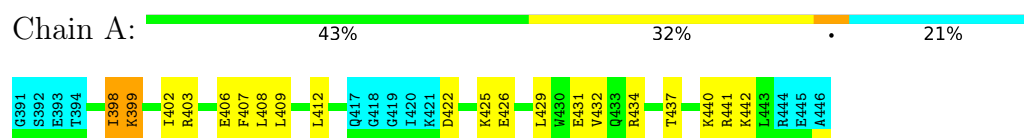
4.2.44 Score per residue for model 44

- Molecule 1: RalA-binding protein 1



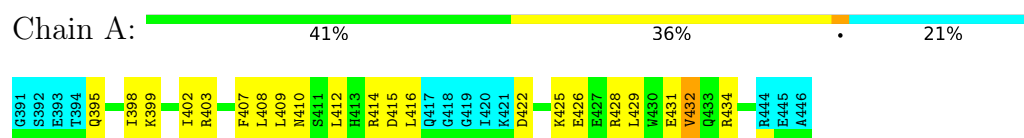
4.2.45 Score per residue for model 45

- Molecule 1: RalA-binding protein 1



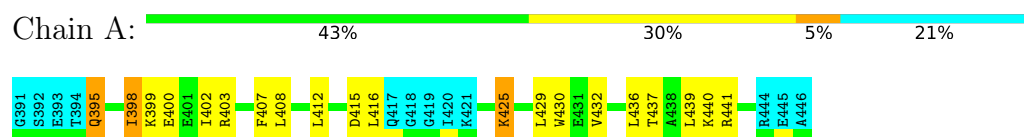
4.2.46 Score per residue for model 46

- Molecule 1: RalA-binding protein 1



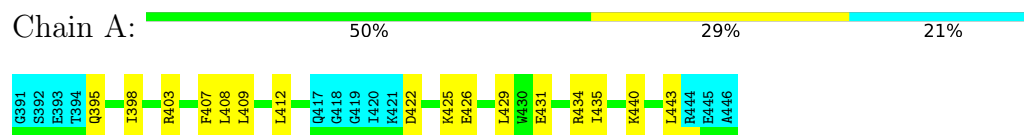
4.2.47 Score per residue for model 47

- Molecule 1: RalA-binding protein 1



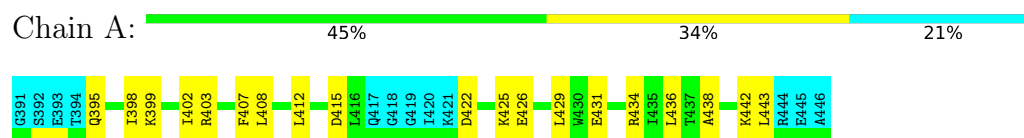
4.2.48 Score per residue for model 48

- Molecule 1: RalA-binding protein 1



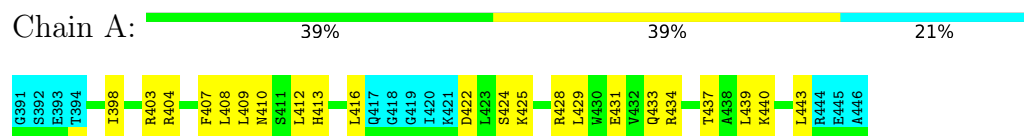
4.2.49 Score per residue for model 49

- Molecule 1: RalA-binding protein 1



4.2.50 Score per residue for model 50

- Molecule 1: RalA-binding protein 1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 50 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
CNS	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	479
Number of shifts mapped to atoms	479
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	58%

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	378	402	401	12±3
All	All	18900	20100	20050	620

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:437:THR:HA	1:A:440:LYS:HE2	0.87	1.46	17	18
1:A:412:LEU:HD11	1:A:429:LEU:HB3	0.77	1.54	15	26
1:A:412:LEU:HB2	1:A:425:LYS:HB3	0.76	1.58	18	5
1:A:398:ILE:HD11	1:A:402:ILE:HD12	0.72	1.61	32	10
1:A:399:LYS:HA	1:A:399:LYS:HE3	0.71	1.61	10	5
1:A:399:LYS:HE2	1:A:399:LYS:HA	0.70	1.63	4	7
1:A:416:LEU:HD21	1:A:425:LYS:HB2	0.68	1.63	17	16
1:A:412:LEU:HB2	1:A:425:LYS:HG2	0.68	1.65	7	2
1:A:408:LEU:O	1:A:412:LEU:HG	0.68	1.88	35	37
1:A:411:SER:O	1:A:414:ARG:HG2	0.66	1.90	44	8
1:A:412:LEU:HB2	1:A:425:LYS:HG3	0.66	1.66	22	11
1:A:422:ASP:HB3	1:A:425:LYS:HD2	0.65	1.68	3	1
1:A:426:GLU:O	1:A:429:LEU:HG	0.64	1.93	11	45
1:A:412:LEU:CD1	1:A:429:LEU:HB3	0.63	2.23	4	36

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:402:ILE:HG13	1:A:436:LEU:HD13	0.63	1.70	26	4
1:A:398:ILE:O	1:A:402:ILE:HB	0.61	1.95	27	6
1:A:395:GLN:O	1:A:399:LYS:HG2	0.61	1.96	41	9
1:A:431:GLU:O	1:A:434:ARG:HG2	0.60	1.97	5	30
1:A:409:LEU:O	1:A:413:HIS:HB2	0.59	1.98	19	8
1:A:399:LYS:O	1:A:402:ILE:HG22	0.58	1.97	43	15
1:A:439:LEU:O	1:A:443:LEU:HG	0.58	1.99	29	10
1:A:437:THR:O	1:A:441:ARG:HG2	0.58	1.99	41	13
1:A:437:THR:HA	1:A:440:LYS:HE3	0.58	1.76	47	1
1:A:412:LEU:HD13	1:A:429:LEU:HB3	0.57	1.75	11	5
1:A:403:ARG:O	1:A:407:PHE:HB2	0.57	1.99	36	49
1:A:398:ILE:HD13	1:A:439:LEU:HD23	0.57	1.76	28	2
1:A:422:ASP:OD1	1:A:425:LYS:HD3	0.57	2.00	38	9
1:A:399:LYS:O	1:A:403:ARG:HG3	0.56	2.01	8	19
1:A:422:ASP:OD1	1:A:425:LYS:HG2	0.56	1.99	49	8
1:A:422:ASP:HB3	1:A:425:LYS:HB2	0.55	1.78	23	1
1:A:412:LEU:HB2	1:A:425:LYS:HE3	0.55	1.76	26	1
1:A:395:GLN:HA	1:A:443:LEU:HD21	0.55	1.78	4	2
1:A:412:LEU:HB2	1:A:425:LYS:CG	0.55	2.32	7	3
1:A:402:ILE:HG13	1:A:436:LEU:HD22	0.55	1.79	49	5
1:A:408:LEU:HD11	1:A:432:VAL:HG11	0.54	1.77	38	6
1:A:405:GLN:NE2	1:A:436:LEU:HB3	0.54	2.18	10	6
1:A:405:GLN:O	1:A:409:LEU:HB2	0.54	2.03	43	7
1:A:422:ASP:CG	1:A:425:LYS:HD3	0.53	2.28	48	8
1:A:429:LEU:O	1:A:433:GLN:HB2	0.53	2.02	50	6
1:A:412:LEU:HB2	1:A:425:LYS:HD2	0.53	1.81	17	1
1:A:401:GLU:O	1:A:405:GLN:HG3	0.53	2.03	31	7
1:A:395:GLN:O	1:A:399:LYS:HD3	0.53	2.03	26	2
1:A:406:GLU:HA	1:A:409:LEU:HB3	0.52	1.81	41	3
1:A:424:SER:O	1:A:428:ARG:HG2	0.52	2.05	50	4
1:A:439:LEU:O	1:A:443:LEU:HB2	0.52	2.05	27	3
1:A:404:ARG:O	1:A:408:LEU:HG	0.51	2.06	28	8
1:A:409:LEU:HD12	1:A:432:VAL:HG23	0.51	1.83	34	2
1:A:402:ILE:HG13	1:A:436:LEU:HB2	0.51	1.83	32	2
1:A:412:LEU:O	1:A:415:ASP:HB2	0.51	2.05	24	1
1:A:428:ARG:O	1:A:432:VAL:HG12	0.51	2.04	19	2
1:A:412:LEU:O	1:A:416:LEU:HG	0.51	2.06	12	6
1:A:431:GLU:OE1	1:A:434:ARG:HD3	0.51	2.06	5	2
1:A:411:SER:O	1:A:414:ARG:HG3	0.50	2.06	20	1
1:A:437:THR:HA	1:A:440:LYS:NZ	0.50	2.22	37	2
1:A:408:LEU:HD11	1:A:432:VAL:HG21	0.50	1.84	45	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:412:LEU:HA	1:A:415:ASP:OD1	0.49	2.07	37	1
1:A:408:LEU:HD12	1:A:409:LEU:N	0.49	2.22	19	14
1:A:436:LEU:HD12	1:A:437:THR:N	0.49	2.23	20	2
1:A:415:ASP:OD2	1:A:425:LYS:HE3	0.49	2.07	40	1
1:A:438:ALA:O	1:A:442:LYS:HD3	0.49	2.07	26	1
1:A:396:ALA:HA	1:A:399:LYS:HB2	0.49	1.83	16	3
1:A:437:THR:O	1:A:441:ARG:HG3	0.48	2.07	14	1
1:A:412:LEU:HA	1:A:415:ASP:OD2	0.48	2.08	21	5
1:A:405:GLN:O	1:A:408:LEU:HD23	0.48	2.09	34	2
1:A:395:GLN:HE21	1:A:443:LEU:HD12	0.48	1.68	38	1
1:A:438:ALA:O	1:A:442:LYS:HG2	0.48	2.07	14	1
1:A:431:GLU:HA	1:A:434:ARG:HG2	0.48	1.85	26	2
1:A:412:LEU:HD12	1:A:413:HIS:N	0.48	2.24	39	3
1:A:426:GLU:HA	1:A:429:LEU:HD23	0.47	1.85	12	1
1:A:409:LEU:HD12	1:A:429:LEU:HB2	0.47	1.86	41	2
1:A:410:ASN:C	1:A:410:ASN:HD22	0.47	2.17	34	2
1:A:422:ASP:OD2	1:A:425:LYS:HG2	0.47	2.09	19	2
1:A:412:LEU:CB	1:A:425:LYS:HE3	0.47	2.39	26	1
1:A:422:ASP:CG	1:A:425:LYS:HG2	0.47	2.34	46	3
1:A:424:SER:O	1:A:428:ARG:HB2	0.46	2.11	44	3
1:A:416:LEU:CD2	1:A:425:LYS:HB2	0.46	2.40	40	2
1:A:412:LEU:HD22	1:A:428:ARG:HB3	0.46	1.87	50	2
1:A:426:GLU:HA	1:A:429:LEU:CD2	0.46	2.40	42	3
1:A:400:GLU:HG3	1:A:403:ARG:HH21	0.46	1.70	34	3
1:A:442:LYS:HD2	1:A:442:LYS:N	0.45	2.27	18	1
1:A:431:GLU:O	1:A:435:ILE:HG13	0.45	2.11	6	7
1:A:398:ILE:HB	1:A:439:LEU:HD23	0.45	1.87	23	2
1:A:438:ALA:O	1:A:442:LYS:HB2	0.45	2.11	49	1
1:A:432:VAL:O	1:A:436:LEU:HG	0.45	2.11	43	2
1:A:410:ASN:O	1:A:414:ARG:HG3	0.45	2.11	46	2
1:A:412:LEU:C	1:A:412:LEU:HD12	0.45	2.36	17	2
1:A:436:LEU:O	1:A:440:LYS:HG2	0.44	2.12	28	2
1:A:406:GLU:HA	1:A:409:LEU:CB	0.44	2.41	41	1
1:A:438:ALA:O	1:A:442:LYS:HD2	0.44	2.13	22	2
1:A:428:ARG:O	1:A:432:VAL:HG23	0.43	2.13	37	3
1:A:429:LEU:HD12	1:A:430:TRP:N	0.43	2.29	4	2
1:A:396:ALA:HA	1:A:399:LYS:HB3	0.43	1.91	19	1
1:A:412:LEU:HA	1:A:415:ASP:HB2	0.42	1.91	19	1
1:A:415:ASP:HB2	1:A:425:LYS:HG2	0.42	1.89	20	1
1:A:425:LYS:HA	1:A:428:ARG:HB3	0.42	1.92	7	1
1:A:395:GLN:NE2	1:A:395:GLN:HA	0.42	2.30	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:408:LEU:HD21	1:A:432:VAL:HG11	0.42	1.91	18	1
1:A:402:ILE:CD1	1:A:436:LEU:HB2	0.42	2.44	43	1
1:A:405:GLN:OE1	1:A:436:LEU:HB3	0.42	2.14	40	1
1:A:405:GLN:NE2	1:A:432:VAL:HG23	0.42	2.30	32	1
1:A:416:LEU:HD21	1:A:425:LYS:HB3	0.42	1.92	42	1
1:A:395:GLN:O	1:A:399:LYS:HB2	0.42	2.15	35	1
1:A:424:SER:O	1:A:428:ARG:HG3	0.42	2.15	33	1
1:A:400:GLU:OE1	1:A:403:ARG:HD2	0.41	2.15	10	1
1:A:414:ARG:NE	1:A:414:ARG:HA	0.41	2.30	27	1
1:A:408:LEU:HA	1:A:411:SER:OG	0.41	2.15	19	2
1:A:428:ARG:O	1:A:432:VAL:HG22	0.41	2.15	39	1
1:A:439:LEU:O	1:A:443:LEU:HD23	0.41	2.15	2	1
1:A:431:GLU:CD	1:A:434:ARG:HD3	0.41	2.41	12	1
1:A:398:ILE:CD1	1:A:440:LYS:HB3	0.41	2.46	40	2
1:A:409:LEU:HA	1:A:412:LEU:HD12	0.41	1.93	29	1
1:A:412:LEU:HB2	1:A:429:LEU:HB3	0.41	1.92	27	1
1:A:396:ALA:HA	1:A:399:LYS:CB	0.40	2.46	16	1
1:A:412:LEU:HD12	1:A:412:LEU:C	0.40	2.41	39	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	44/56 (79%)	44±1 (99±2%)	0±1 (1±2%)	0±0 (0±0%)	100	100
All	All	2200/2800 (79%)	2180 (99%)	20 (1%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	41/49 (84%)	39±1 (95±2%)	2±1 (5±2%)	23 73
All	All	2050/2450 (84%)	1945 (95%)	105 (5%)	23 73

All 16 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	398	ILE	46
1	A	399	LYS	15
1	A	395	GLN	6
1	A	415	ASP	6
1	A	410	ASN	6
1	A	425	LYS	5
1	A	443	LEU	4
1	A	442	LYS	4
1	A	426	GLU	3
1	A	402	ILE	3
1	A	400	GLU	2
1	A	413	HIS	1
1	A	428	ARG	1
1	A	441	ARG	1
1	A	416	LEU	1
1	A	432	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 58% for the well-defined parts and 57% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

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

Total number of shifts	479
Number of shifts mapped to atoms	479
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	54	-0.36 ± 0.18	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 58%, i.e. 402 atoms were assigned a chemical shift out of a possible 693. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	133/221 (60%)	89/89 (100%)	0/88 (0%)	44/44 (100%)
Sidechain	256/442 (58%)	252/283 (89%)	0/133 (0%)	4/26 (15%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	13/30 (43%)	12/15 (80%)	0/12 (0%)	1/3 (33%)
Overall	402/693 (58%)	353/387 (91%)	0/233 (0%)	49/73 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 57%, i.e. 479 atoms were assigned a chemical shift out of a possible 837. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	165/284 (58%)	111/116 (96%)	0/112 (0%)	54/56 (96%)
Sidechain	301/523 (58%)	296/334 (89%)	0/158 (0%)	5/31 (16%)
Aromatic	13/30 (43%)	12/15 (80%)	0/12 (0%)	1/3 (33%)
Overall	479/837 (57%)	419/465 (90%)	0/282 (0%)	60/90 (67%)

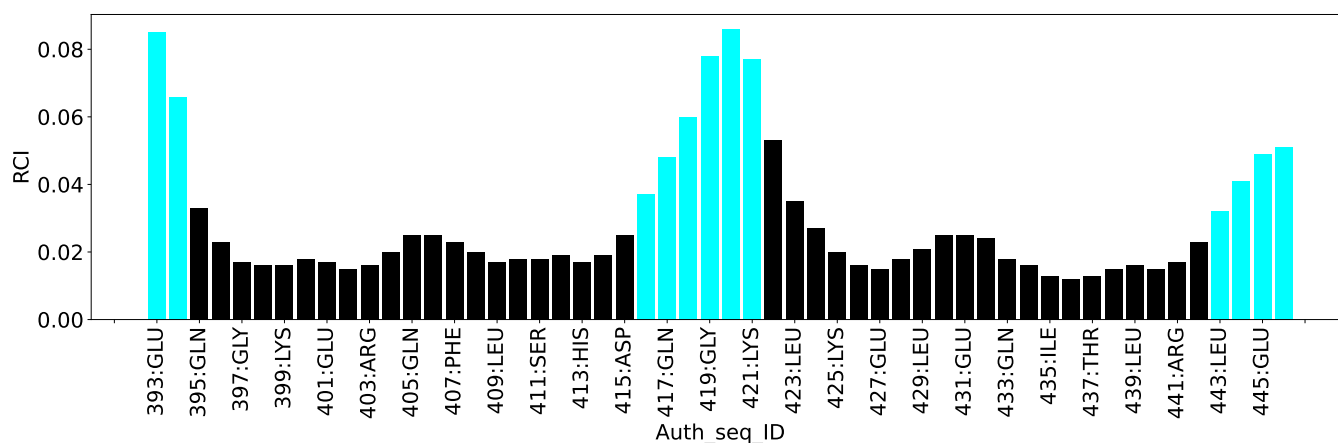
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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	1297
Intra-residue ($ i-j =0$)	606
Sequential ($ i-j =1$)	272
Medium range ($ i-j >1$ and $ i-j <5$)	314
Long range ($ i-j \geq 5$)	105
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	23.2
Number of long range restraints per residue ¹	1.9

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)	24.8	0.2
0.2-0.5 (Medium)	37.3	0.5
>0.5 (Large)	30.4	5.28

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 ⓘ

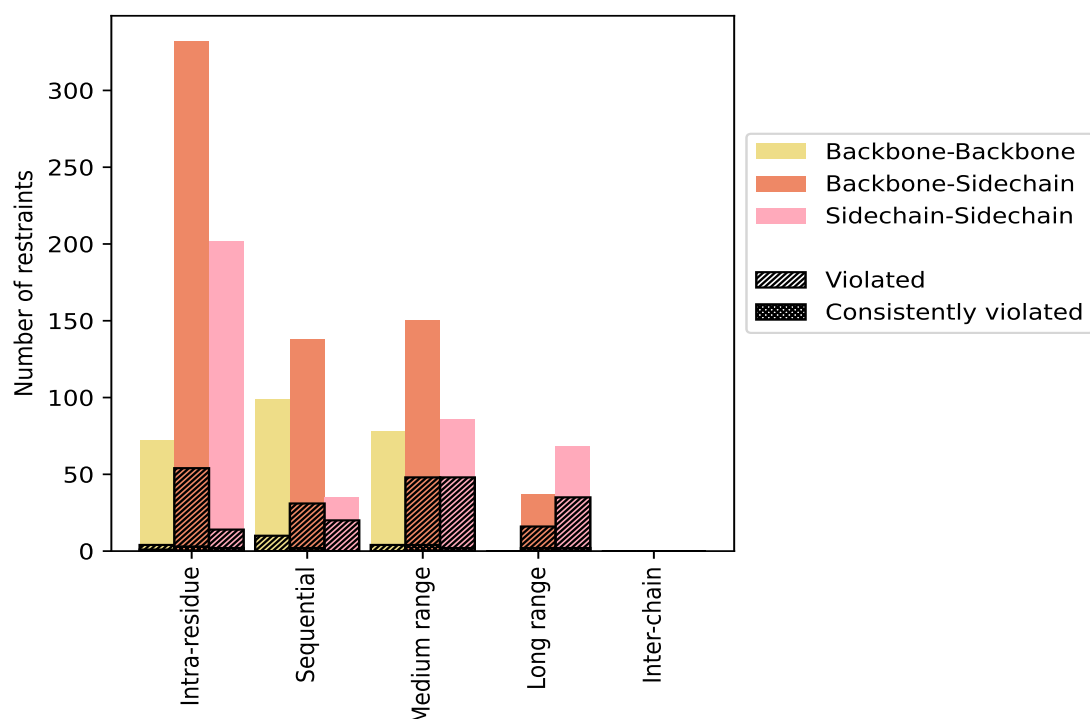
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	606	46.7	72	11.9	5.6	6	1.0	0.5
Backbone-Backbone	72	5.6	4	5.6	0.3	1	1.4	0.1
Backbone-Sidechain	332	25.6	54	16.3	4.2	3	0.9	0.2
Sidechain-Sidechain	202	15.6	14	6.9	1.1	2	1.0	0.2
Sequential ($i-j =1$)	272	21.0	61	22.4	4.7	2	0.7	0.2
Backbone-Backbone	99	7.6	10	10.1	0.8	0	0.0	0.0
Backbone-Sidechain	138	10.6	31	22.5	2.4	2	1.4	0.2
Sidechain-Sidechain	35	2.7	20	57.1	1.5	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	314	24.2	100	31.8	7.7	6	1.9	0.5
Backbone-Backbone	78	6.0	4	5.1	0.3	0	0.0	0.0
Backbone-Sidechain	150	11.6	48	32.0	3.7	4	2.7	0.3
Sidechain-Sidechain	86	6.6	48	55.8	3.7	2	2.3	0.2
Long range ($i-j \geq 5$)	105	8.1	51	48.6	3.9	4	3.8	0.3
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	37	2.9	16	43.2	1.2	2	5.4	0.2
Sidechain-Sidechain	68	5.2	35	51.5	2.7	2	2.9	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	1297	100.0	284	21.9	21.9	18	1.4	1.4
Backbone-Backbone	249	19.2	18	7.2	1.4	1	0.4	0.1
Backbone-Sidechain	657	50.7	149	22.7	11.5	11	1.7	0.8
Sidechain-Sidechain	391	30.1	117	29.9	9.0	6	1.5	0.5

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	15	19	44	19	0	97	0.48	2.38	0.42	0.31
2	22	18	31	25	0	96	0.49	2.45	0.46	0.31
3	15	19	39	18	0	91	0.49	2.41	0.44	0.32
4	18	16	37	23	0	94	0.49	1.65	0.38	0.32
5	16	15	37	22	0	90	0.56	2.31	0.49	0.33
6	19	14	34	18	0	85	0.55	2.38	0.51	0.33
7	23	16	40	21	0	100	0.47	1.71	0.41	0.3
8	17	14	40	23	0	94	0.55	2.43	0.49	0.34
9	18	18	40	18	0	94	0.49	2.31	0.44	0.31
10	19	14	40	18	0	91	0.49	2.43	0.48	0.28

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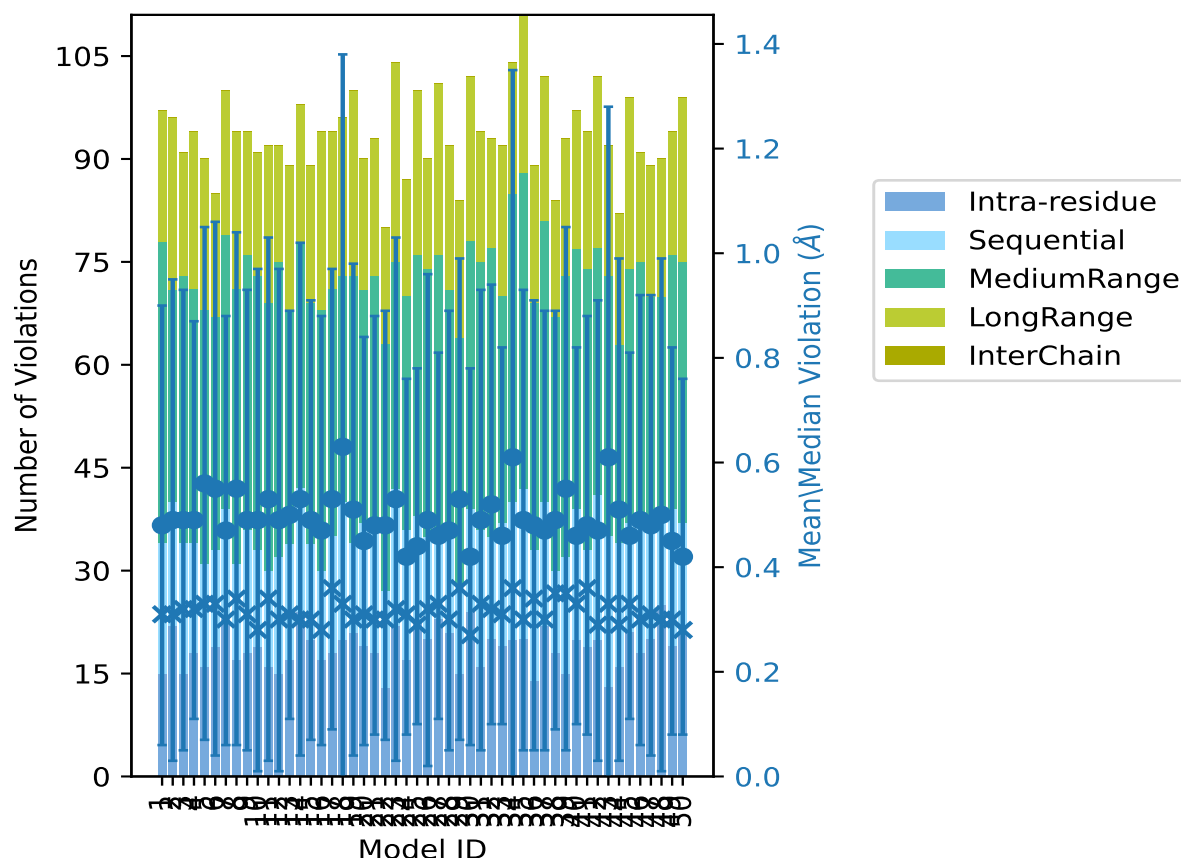
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	16	14	39	23	0	92	0.53	2.37	0.5	0.34
12	15	17	43	17	0	92	0.49	2.44	0.48	0.3
13	17	17	34	21	0	89	0.5	1.68	0.39	0.31
14	24	18	36	20	0	98	0.53	2.4	0.49	0.3
15	20	14	35	20	0	89	0.49	1.86	0.42	0.3
16	17	13	38	26	0	94	0.47	1.7	0.41	0.28
17	18	17	36	23	0	94	0.53	2.22	0.44	0.36
18	20	20	33	23	0	96	0.63	5.1	0.75	0.33
19	21	13	39	27	0	100	0.51	2.45	0.47	0.3
20	19	18	34	19	0	90	0.45	1.68	0.39	0.31
21	18	18	37	20	0	93	0.48	1.76	0.4	0.3
22	13	14	36	17	0	80	0.48	1.82	0.41	0.3
23	22	20	33	29	0	104	0.53	2.32	0.5	0.32
24	17	19	34	17	0	87	0.42	1.86	0.34	0.31
25	23	15	38	24	0	100	0.44	1.89	0.34	0.29
26	20	15	39	16	0	90	0.49	2.35	0.47	0.32
27	23	13	40	25	0	101	0.46	1.72	0.35	0.33
28	21	14	36	21	0	92	0.47	1.96	0.42	0.3
29	15	13	36	20	0	84	0.53	2.3	0.46	0.36
30	24	15	39	24	0	102	0.42	1.73	0.36	0.27
31	16	20	39	19	0	94	0.49	2.43	0.44	0.33
32	20	15	42	16	0	93	0.52	1.84	0.42	0.32
33	19	18	33	22	0	92	0.46	1.61	0.36	0.31
34	20	20	45	19	0	104	0.61	5.28	0.74	0.36
35	20	22	46	23	0	111	0.49	2.13	0.44	0.3
36	14	19	36	20	0	89	0.48	2.33	0.43	0.34
37	22	18	41	21	0	102	0.47	2.32	0.42	0.3
38	18	12	37	17	0	84	0.49	1.69	0.4	0.35
39	15	17	41	20	0	93	0.55	2.39	0.5	0.35
40	20	19	38	20	0	97	0.46	1.97	0.36	0.33
41	19	14	41	20	0	94	0.48	1.82	0.4	0.36
42	20	21	36	25	0	102	0.47	2.44	0.44	0.29
43	13	22	38	19	0	92	0.61	3.75	0.67	0.33
44	16	18	29	19	0	82	0.51	2.42	0.48	0.29
45	21	16	37	25	0	99	0.46	1.8	0.35	0.33
46	18	20	37	16	0	91	0.49	2.5	0.43	0.3
47	20	16	34	19	0	89	0.48	2.27	0.44	0.31
48	25	13	32	20	0	90	0.5	2.5	0.49	0.3
49	19	20	37	18	0	94	0.45	1.7	0.37	0.3
50	21	16	38	24	0	99	0.42	1.75	0.34	0.28

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1013(IR:534, SQ:211, MR:214, LR:54, 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	%
18	10	8	6	0	42	1	2.0
5	6	9	5	0	25	2	4.0
4	6	12	1	0	23	3	6.0
3	3	5	0	0	11	4	8.0

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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	%
5	5	6	2	0	18	5	10.0
5	1	2	3	0	11	6	12.0
0	2	3	1	0	6	7	14.0
1	2	2	1	0	6	8	16.0
2	2	3	1	0	8	9	18.0
2	0	3	0	0	5	10	20.0
1	1	4	1	0	7	11	22.0
1	2	1	0	0	4	12	24.0
1	2	3	1	0	7	13	26.0
1	0	1	0	0	2	14	28.0
0	2	1	1	0	4	15	30.0
1	0	1	2	0	4	16	32.0
0	0	1	3	0	4	17	34.0
0	0	1	2	0	3	18	36.0
1	0	0	2	0	3	19	38.0
2	1	1	0	0	4	20	40.0
1	0	0	1	0	2	21	42.0
0	1	1	1	0	3	22	44.0
0	2	2	0	0	4	23	46.0
1	0	1	0	0	2	24	48.0
0	0	1	1	0	2	25	50.0
0	0	2	0	0	2	26	52.0
0	1	0	0	0	1	27	54.0
0	0	1	1	0	2	28	56.0
0	0	0	0	0	0	29	58.0
1	0	0	0	0	1	30	60.0
0	1	0	2	0	3	31	62.0
0	0	1	1	0	2	32	64.0
0	0	0	1	0	1	33	66.0
0	0	0	0	0	0	34	68.0
0	0	0	2	0	2	35	70.0
0	1	1	0	0	2	36	72.0
0	0	0	0	0	0	37	74.0
1	0	2	0	0	3	38	76.0
0	0	1	0	0	1	39	78.0
0	0	0	0	0	0	40	80.0
0	2	2	0	0	4	41	82.0
2	0	1	0	0	3	42	84.0
1	0	3	0	0	4	43	86.0
1	0	0	1	0	2	44	88.0
2	2	1	0	0	5	45	90.0

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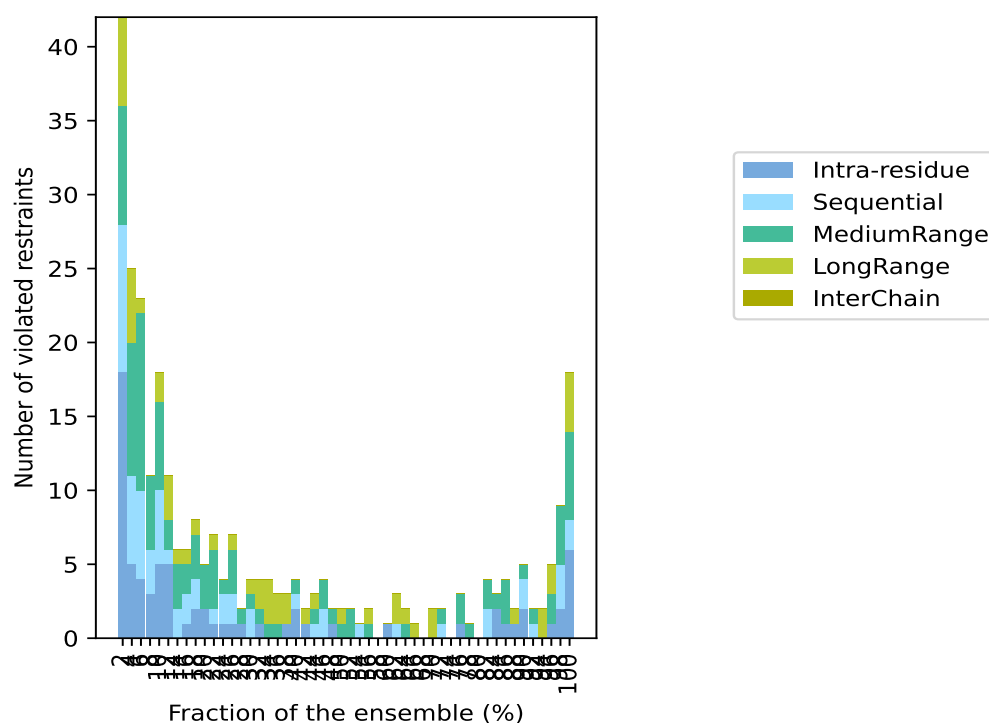
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	1	1	0	0	2	46	92.0
0	0	0	2	0	2	47	94.0
1	0	2	2	0	5	48	96.0
2	3	4	0	0	9	49	98.0
6	2	6	4	0	18	50	100.0

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

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

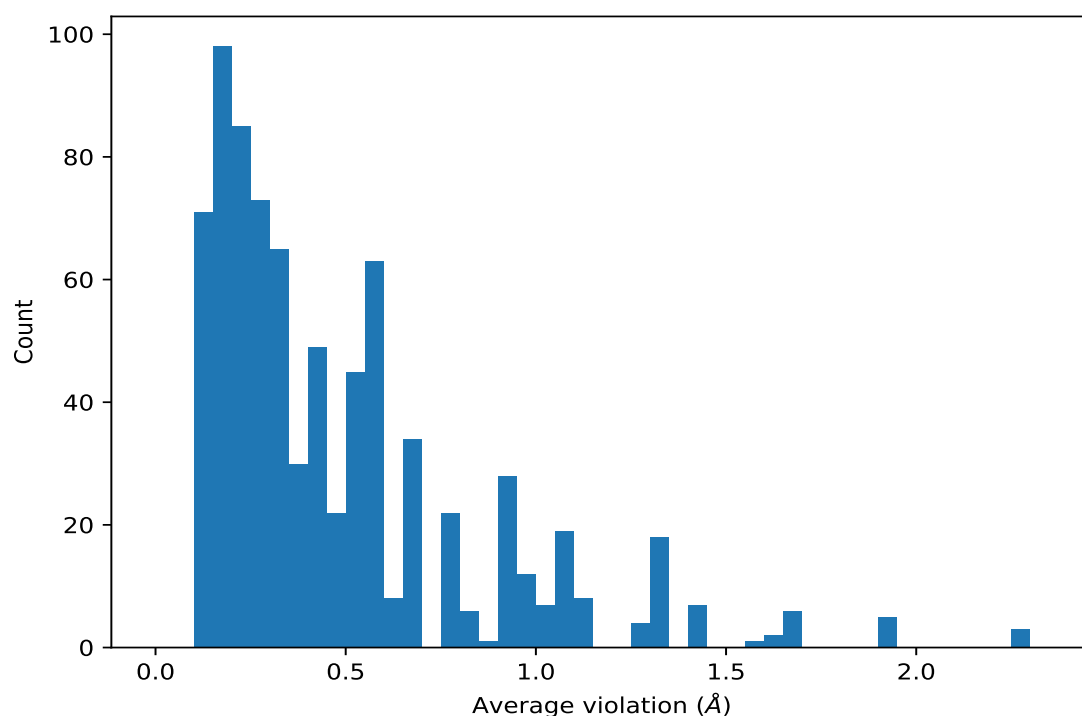
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1142)	1:408:A:LEU:HD11	1:406:A:GLU:HG3	50	1.93	0.96	2.26
(1,1142)	1:408:A:LEU:HD12	1:406:A:GLU:HG3	50	1.93	0.96	2.26
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	50	1.93	0.96	2.26
(1,1142)	1:408:A:LEU:HD11	1:433:A:GLN:HG3	50	1.93	0.96	2.26
(1,1142)	1:408:A:LEU:HD13	1:433:A:GLN:HG3	50	1.93	0.96	2.26
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG23	50	1.7	0.16	1.67
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG11	50	1.7	0.16	1.67
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG12	50	1.7	0.16	1.67
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG21	50	1.7	0.16	1.67
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG13	50	1.7	0.16	1.67
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG22	50	1.7	0.16	1.67
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD23	50	1.08	0.16	1.08
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD11	50	1.08	0.16	1.08
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD13	50	1.08	0.16	1.08
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD21	50	1.08	0.16	1.08
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD12	50	1.08	0.16	1.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD22	50	1.08	0.16	1.08
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	50	1.03	0.68	0.86
(1,1082)	1:408:A:LEU:HD13	1:402:A:ILE:HA	50	1.03	0.68	0.86
(1,1082)	1:408:A:LEU:HD11	1:402:A:ILE:HA	50	1.03	0.68	0.86
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	50	1.02	0.43	1.26
(1,115)	1:398:A:ILE:HG13	1:406:A:GLU:HG3	50	1.02	0.43	1.26
(1,1130)	1:408:A:LEU:HD12	1:405:A:GLN:HG3	50	0.94	0.4	0.82
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	50	0.94	0.4	0.82
(1,1130)	1:408:A:LEU:HD23	1:405:A:GLN:HG3	50	0.94	0.4	0.82
(1,1130)	1:408:A:LEU:HD22	1:405:A:GLN:HG3	50	0.94	0.4	0.82
(1,1130)	1:408:A:LEU:HD11	1:405:A:GLN:HG3	50	0.94	0.4	0.82
(1,1130)	1:408:A:LEU:HD13	1:405:A:GLN:HG3	50	0.94	0.4	0.82
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	50	0.83	0.21	0.78
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	50	0.83	0.21	0.78
(1,811)	1:435:A:ILE:HA	1:434:A:ARG:HB2	50	0.83	0.21	0.78
(1,811)	1:426:A:GLU:HA	1:428:A:ARG:HB2	50	0.83	0.21	0.78
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	50	0.6	0.13	0.61
(1,1213)	1:431:A:GLU:H	1:434:A:ARG:HB3	50	0.6	0.13	0.61
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	50	0.41	0.13	0.38
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG12	50	0.41	0.13	0.38
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	50	0.37	0.15	0.3
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	50	0.37	0.15	0.3
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB3	50	0.31	0.04	0.31
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	50	0.31	0.04	0.31
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	50	0.31	0.01	0.31
(1,756)	1:442:A:LYS:H	1:442:A:LYS:HA	50	0.31	0.01	0.31
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	50	0.29	0.02	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	50	0.29	0.02	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	50	0.29	0.02	0.3
(1,92)	1:408:A:LEU:HD21	1:408:A:LEU:HA	50	0.29	0.02	0.3
(1,92)	1:408:A:LEU:HD22	1:408:A:LEU:HA	50	0.29	0.02	0.3
(1,92)	1:408:A:LEU:HD23	1:408:A:LEU:HA	50	0.29	0.02	0.3
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	50	0.28	0.07	0.26
(1,1207)	1:412:A:LEU:H	1:429:A:LEU:HB3	50	0.28	0.07	0.26
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	50	0.23	0.02	0.23
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG3	50	0.23	0.02	0.23
(1,1099)	1:408:A:LEU:HD12	1:408:A:LEU:HG	50	0.21	0.01	0.21
(1,1099)	1:408:A:LEU:HD13	1:408:A:LEU:HG	50	0.21	0.01	0.21
(1,1099)	1:408:A:LEU:HD23	1:408:A:LEU:HG	50	0.21	0.01	0.21
(1,1099)	1:408:A:LEU:HD11	1:408:A:LEU:HG	50	0.21	0.01	0.21
(1,1099)	1:408:A:LEU:HD22	1:408:A:LEU:HG	50	0.21	0.01	0.21
(1,1099)	1:408:A:LEU:HD21	1:408:A:LEU:HG	50	0.21	0.01	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1100)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	50	0.17	0.03	0.16
(1,1100)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	50	0.17	0.03	0.16
(1,1100)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	50	0.17	0.03	0.16
(1,1100)	1:435:A:ILE:HD11	1:435:A:ILE:HG12	50	0.17	0.03	0.16
(1,1100)	1:435:A:ILE:HD12	1:435:A:ILE:HG12	50	0.17	0.03	0.16
(1,1100)	1:443:A:LEU:HD22	1:443:A:LEU:HB3	50	0.17	0.03	0.16
(1,1100)	1:443:A:LEU:HD23	1:443:A:LEU:HG	50	0.17	0.03	0.16
(1,1100)	1:443:A:LEU:HD23	1:443:A:LEU:HB3	50	0.17	0.03	0.16
(1,1100)	1:435:A:ILE:HD13	1:435:A:ILE:HG12	50	0.17	0.03	0.16
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	50	0.12	0.0	0.12
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	49	1.06	0.28	1.12
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	49	1.06	0.28	1.12
(1,948)	1:410:A:ASN:HB3	1:408:A:LEU:HD11	49	1.06	0.28	1.12
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	49	1.06	0.28	1.12
(1,1124)	1:429:A:LEU:HD23	1:425:A:LYS:HB2	49	0.98	0.48	0.87
(1,1124)	1:429:A:LEU:HD23	1:428:A:ARG:HB3	49	0.98	0.48	0.87
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	49	0.98	0.48	0.87
(1,1124)	1:429:A:LEU:HD22	1:425:A:LYS:HB2	49	0.98	0.48	0.87
(1,1124)	1:429:A:LEU:HD22	1:428:A:ARG:HB3	49	0.98	0.48	0.87
(1,1124)	1:429:A:LEU:HD22	1:428:A:ARG:HB2	49	0.98	0.48	0.87
(1,1124)	1:429:A:LEU:HD23	1:428:A:ARG:HB2	49	0.98	0.48	0.87
(1,1124)	1:429:A:LEU:HD21	1:428:A:ARG:HB3	49	0.98	0.48	0.87
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	49	0.96	0.28	1.02
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	49	0.96	0.28	1.02
(1,947)	1:410:A:ASN:HB3	1:408:A:LEU:HD11	49	0.96	0.28	1.02
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	49	0.96	0.28	1.02
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	49	0.59	0.14	0.59
(1,1033)	1:402:A:ILE:HG22	1:400:A:GLU:HA	49	0.59	0.14	0.59
(1,1033)	1:416:A:LEU:HD21	1:413:A:HIS:HA	49	0.59	0.14	0.59
(1,1033)	1:402:A:ILE:HG21	1:400:A:GLU:HA	49	0.59	0.14	0.59
(1,1033)	1:416:A:LEU:HD22	1:413:A:HIS:HA	49	0.59	0.14	0.59
(1,1033)	1:416:A:LEU:HD23	1:413:A:HIS:HA	49	0.59	0.14	0.59
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	49	0.47	0.33	0.4
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	49	0.47	0.33	0.4
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	49	0.47	0.33	0.4
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	49	0.41	0.2	0.33
(1,781)	1:413:A:HIS:HD2	1:412:A:LEU:HA	49	0.41	0.2	0.33
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	49	0.41	0.14	0.41
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	49	0.41	0.14	0.41
(1,1097)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	49	0.16	0.03	0.16
(1,1097)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	49	0.16	0.03	0.16
(1,1097)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	49	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1097)	1:423:A:LEU:HD23	1:423:A:LEU:HB3	49	0.16	0.03	0.16
(1,1097)	1:416:A:LEU:HD13	1:416:A:LEU:HB3	49	0.16	0.03	0.16
(1,1097)	1:416:A:LEU:HD12	1:416:A:LEU:HB2	49	0.16	0.03	0.16
(1,1097)	1:416:A:LEU:HD11	1:416:A:LEU:HB3	49	0.16	0.03	0.16
(1,1097)	1:416:A:LEU:HD12	1:416:A:LEU:HB3	49	0.16	0.03	0.16
(1,1097)	1:436:A:LEU:HD22	1:436:A:LEU:HG	49	0.16	0.03	0.16
(1,1097)	1:423:A:LEU:HD22	1:423:A:LEU:HB3	49	0.16	0.03	0.16
(1,1097)	1:416:A:LEU:HD12	1:416:A:LEU:HG	49	0.16	0.03	0.16
(1,1097)	1:443:A:LEU:HD12	1:443:A:LEU:HB2	49	0.16	0.03	0.16
(1,1097)	1:423:A:LEU:HD21	1:423:A:LEU:HB3	49	0.16	0.03	0.16
(1,1097)	1:443:A:LEU:HD11	1:443:A:LEU:HG	49	0.16	0.03	0.16
(1,1097)	1:436:A:LEU:HD13	1:436:A:LEU:HG	49	0.16	0.03	0.16
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	49	0.13	0.01	0.13
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG13	48	1.41	0.7	1.55
(1,931)	1:406:A:GLU:HG3	1:398:A:ILE:HG12	48	1.41	0.7	1.55
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG11	48	1.41	0.7	1.55
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG21	48	1.41	0.7	1.55
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG22	48	1.41	0.7	1.55
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG12	48	1.41	0.7	1.55
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG23	48	1.41	0.7	1.55
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	48	1.31	0.35	1.35
(1,1096)	1:402:A:ILE:HG22	1:440:A:LYS:HE3	48	1.31	0.35	1.35
(1,1096)	1:412:A:LEU:HD11	1:425:A:LYS:HE2	48	1.31	0.35	1.35
(1,1096)	1:420:A:ILE:HG21	1:421:A:LYS:HE2	48	1.31	0.35	1.35
(1,1096)	1:412:A:LEU:HD13	1:425:A:LYS:HE3	48	1.31	0.35	1.35
(1,1096)	1:402:A:ILE:HG23	1:440:A:LYS:HE3	48	1.31	0.35	1.35
(1,1096)	1:412:A:LEU:HD13	1:425:A:LYS:HE2	48	1.31	0.35	1.35
(1,1096)	1:412:A:LEU:HD11	1:425:A:LYS:HE3	48	1.31	0.35	1.35
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE3	48	1.31	0.35	1.35
(1,1096)	1:402:A:ILE:HG12	1:440:A:LYS:HE2	48	1.31	0.35	1.35
(1,1096)	1:402:A:ILE:HG21	1:440:A:LYS:HE3	48	1.31	0.35	1.35
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD11	48	0.93	0.44	0.87
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG22	48	0.93	0.44	0.87
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD13	48	0.93	0.44	0.87
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD12	48	0.93	0.44	0.87
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG23	48	0.93	0.44	0.87
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG21	48	0.93	0.44	0.87
(1,906)	1:404:A:ARG:HG3	1:436:A:LEU:HD22	48	0.93	0.44	0.87
(1,906)	1:414:A:ARG:HG3	1:416:A:LEU:HD13	48	0.93	0.44	0.87
(1,1002)	1:420:A:ILE:HG22	1:416:A:LEU:HA	48	0.91	0.19	0.91
(1,1002)	1:420:A:ILE:HG23	1:421:A:LYS:HA	48	0.91	0.19	0.91
(1,1002)	1:420:A:ILE:HG21	1:421:A:LYS:HA	48	0.91	0.19	0.91

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1002)	1:420:A:ILE:HG22	1:421:A:LYS:HA	48	0.91	0.19	0.91
(1,1002)	1:420:A:ILE:HG23	1:416:A:LEU:HA	48	0.91	0.19	0.91
(1,1002)	1:420:A:ILE:HG21	1:416:A:LEU:HA	48	0.91	0.19	0.91
(1,1002)	1:436:A:LEU:HD11	1:437:A:THR:HB	48	0.91	0.19	0.91
(1,1002)	1:436:A:LEU:HD12	1:437:A:THR:HB	48	0.91	0.19	0.91
(1,1002)	1:436:A:LEU:HD13	1:437:A:THR:HB	48	0.91	0.19	0.91
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	48	0.26	0.04	0.26
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB2	48	0.26	0.04	0.26
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG13	47	0.33	0.07	0.33
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	47	0.33	0.07	0.33
(1,1017)	1:398:A:ILE:HG13	1:436:A:LEU:HA	47	0.33	0.07	0.33
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	47	0.33	0.07	0.33
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	46	0.8	0.39	0.78
(1,783)	1:407:A:PHE:HD1	1:404:A:ARG:HG3	46	0.8	0.39	0.78
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	46	0.26	0.04	0.27
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	45	0.7	0.28	0.68
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD22	45	0.7	0.28	0.68
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD21	45	0.7	0.28	0.68
(1,875)	1:417:A:GLN:HA	1:420:A:ILE:HD11	45	0.7	0.28	0.68
(1,875)	1:417:A:GLN:HA	1:420:A:ILE:HD12	45	0.7	0.28	0.68
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	45	0.22	0.04	0.23
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB3	45	0.22	0.04	0.23
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	45	0.2	0.05	0.19
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	45	0.2	0.05	0.19
(1,1159)	1:440:A:LYS:HG2	1:440:A:LYS:HD3	45	0.18	0.04	0.19
(1,1159)	1:399:A:LYS:HG2	1:399:A:LYS:HD3	45	0.18	0.04	0.19
(1,1159)	1:421:A:LYS:HG2	1:421:A:LYS:HD3	45	0.18	0.04	0.19
(1,1159)	1:440:A:LYS:HG3	1:440:A:LYS:HD2	45	0.18	0.04	0.19
(1,1159)	1:421:A:LYS:HG3	1:421:A:LYS:HD2	45	0.18	0.04	0.19
(1,1159)	1:399:A:LYS:HG3	1:399:A:LYS:HD2	45	0.18	0.04	0.19
(1,1160)	1:414:A:ARG:HG2	1:414:A:ARG:HB3	45	0.17	0.03	0.18
(1,1160)	1:428:A:ARG:HG3	1:428:A:ARG:HB2	45	0.17	0.03	0.18
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	45	0.17	0.03	0.18
(1,1160)	1:403:A:ARG:HG2	1:403:A:ARG:HB3	45	0.17	0.03	0.18
(1,1160)	1:428:A:ARG:HG3	1:428:A:ARG:HB3	45	0.17	0.03	0.18
(1,1160)	1:403:A:ARG:HG3	1:403:A:ARG:HB2	45	0.17	0.03	0.18
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	44	0.44	0.34	0.3
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD21	44	0.44	0.34	0.3
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD22	44	0.44	0.34	0.3
(1,1199)	1:414:A:ARG:HB3	1:414:A:ARG:HG2	44	0.17	0.03	0.17
(1,1199)	1:428:A:ARG:HB2	1:428:A:ARG:HG3	44	0.17	0.03	0.17
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	44	0.17	0.03	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1199)	1:428:A:ARG:HB3	1:428:A:ARG:HG2	44	0.17	0.03	0.17
(1,1199)	1:428:A:ARG:HB2	1:428:A:ARG:HG2	44	0.17	0.03	0.17
(1,1199)	1:403:A:ARG:HB2	1:403:A:ARG:HG3	44	0.17	0.03	0.17
(1,1199)	1:403:A:ARG:HB3	1:403:A:ARG:HG2	44	0.17	0.03	0.17
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	43	0.54	0.15	0.56
(1,1227)	1:413:A:HIS:H	1:413:A:HIS:HE1	43	0.54	0.15	0.56
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	43	0.46	0.15	0.48
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	43	0.46	0.15	0.48
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	43	0.23	0.1	0.2
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG13	43	0.23	0.1	0.2
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	43	0.21	0.09	0.2
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	43	0.21	0.09	0.2
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB3	43	0.21	0.09	0.2
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG22	42	0.39	0.16	0.36
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG21	42	0.39	0.16	0.36
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG23	42	0.39	0.16	0.36
(1,868)	1:421:A:LYS:HA	1:423:A:LEU:HD22	42	0.39	0.16	0.36
(1,868)	1:416:A:LEU:HA	1:416:A:LEU:HD11	42	0.39	0.16	0.36
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HD12	42	0.39	0.16	0.36
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG23	42	0.21	0.07	0.21
(1,739)	1:439:A:LEU:H	1:439:A:LEU:HD11	42	0.21	0.07	0.21
(1,739)	1:439:A:LEU:H	1:439:A:LEU:HD12	42	0.21	0.07	0.21
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG22	42	0.21	0.07	0.21
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG21	42	0.21	0.07	0.21
(1,739)	1:439:A:LEU:H	1:439:A:LEU:HD13	42	0.21	0.07	0.21
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	42	0.19	0.05	0.18
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG12	41	1.29	0.34	1.34
(1,762)	1:436:A:LEU:H	1:398:A:ILE:HG12	41	1.29	0.34	1.34
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG11	41	1.29	0.34	1.34
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG13	41	1.29	0.34	1.34
(1,1162)	1:394:A:THR:HG22	1:393:A:GLU:HB3	41	1.07	0.52	1.05
(1,1162)	1:394:A:THR:HG23	1:393:A:GLU:HB3	41	1.07	0.52	1.05
(1,1162)	1:394:A:THR:HG23	1:395:A:GLN:HB2	41	1.07	0.52	1.05
(1,1162)	1:394:A:THR:HG21	1:395:A:GLN:HB2	41	1.07	0.52	1.05
(1,1162)	1:394:A:THR:HG22	1:395:A:GLN:HB3	41	1.07	0.52	1.05
(1,1162)	1:394:A:THR:HG21	1:395:A:GLN:HB3	41	1.07	0.52	1.05
(1,1162)	1:394:A:THR:HG22	1:395:A:GLN:HB2	41	1.07	0.52	1.05
(1,1162)	1:394:A:THR:HG21	1:393:A:GLU:HB3	41	1.07	0.52	1.05
(1,1162)	1:394:A:THR:HG23	1:395:A:GLN:HB3	41	1.07	0.52	1.05
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	41	0.35	0.08	0.37
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD2	41	0.35	0.08	0.37
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	41	0.17	0.03	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	39	0.29	0.09	0.3
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD11	38	1.32	0.45	1.49
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD13	38	1.32	0.45	1.49
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD12	38	1.32	0.45	1.49
(1,796)	1:395:A:GLN:HE21	1:439:A:LEU:HD23	38	1.32	0.45	1.49
(1,796)	1:395:A:GLN:HE21	1:402:A:ILE:HD11	38	1.32	0.45	1.49
(1,796)	1:395:A:GLN:HE21	1:439:A:LEU:HD22	38	1.32	0.45	1.49
(1,796)	1:395:A:GLN:HE21	1:439:A:LEU:HD21	38	1.32	0.45	1.49
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB2	38	0.79	0.17	0.78
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB1	38	0.79	0.17	0.78
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB3	38	0.79	0.17	0.78
(1,731)	1:441:A:ARG:H	1:442:A:LYS:HG3	38	0.79	0.17	0.78
(1,825)	1:439:A:LEU:HA	1:443:A:LEU:HG	38	0.47	0.16	0.59
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	38	0.47	0.16	0.59
(1,825)	1:439:A:LEU:HA	1:442:A:LYS:HD2	38	0.47	0.16	0.59
(1,825)	1:439:A:LEU:HA	1:442:A:LYS:HD3	38	0.47	0.16	0.59
(1,825)	1:434:A:ARG:HA	1:434:A:ARG:HG3	38	0.47	0.16	0.59
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	36	0.53	0.22	0.59
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	36	0.52	0.11	0.5
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	36	0.52	0.11	0.5
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD12	35	0.55	0.28	0.5
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD13	35	0.55	0.28	0.5
(1,937)	1:440:A:LYS:HE3	1:402:A:ILE:HD11	35	0.55	0.28	0.5
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD11	35	0.55	0.28	0.5
(1,937)	1:440:A:LYS:HE2	1:398:A:ILE:HD13	35	0.55	0.28	0.5
(1,937)	1:440:A:LYS:HE2	1:398:A:ILE:HD12	35	0.55	0.28	0.5
(1,937)	1:425:A:LYS:HE3	1:412:A:LEU:HD23	35	0.55	0.28	0.5
(1,937)	1:440:A:LYS:HE3	1:402:A:ILE:HD13	35	0.55	0.28	0.5
(1,937)	1:440:A:LYS:HE3	1:402:A:ILE:HD12	35	0.55	0.28	0.5
(1,937)	1:425:A:LYS:HE3	1:412:A:LEU:HD21	35	0.55	0.28	0.5
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	35	0.24	0.2	0.17
(1,1206)	1:398:A:ILE:H	1:399:A:LYS:HD3	33	0.76	0.28	0.86
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HG	33	0.76	0.28	0.86
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HB3	33	0.76	0.28	0.86
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HB2	33	0.76	0.28	0.86
(1,1206)	1:398:A:ILE:H	1:399:A:LYS:HD2	33	0.76	0.28	0.86
(1,1131)	1:416:A:LEU:HD23	1:425:A:LYS:HD3	32	0.79	0.31	0.92
(1,1131)	1:416:A:LEU:HD22	1:425:A:LYS:HD3	32	0.79	0.31	0.92
(1,1131)	1:416:A:LEU:HD23	1:425:A:LYS:HD2	32	0.79	0.31	0.92
(1,1131)	1:416:A:LEU:HD21	1:425:A:LYS:HD2	32	0.79	0.31	0.92
(1,1131)	1:416:A:LEU:HD22	1:429:A:LEU:HG	32	0.79	0.31	0.92
(1,1131)	1:416:A:LEU:HD21	1:429:A:LEU:HG	32	0.79	0.31	0.92

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1131)	1:416:A:LEU:HD21	1:425:A:LYS:HD3	32	0.79	0.31	0.92
(1,1131)	1:416:A:LEU:HD22	1:425:A:LYS:HD2	32	0.79	0.31	0.92
(1,1131)	1:416:A:LEU:HD23	1:429:A:LEU:HG	32	0.79	0.31	0.92
(1,1137)	1:412:A:LEU:HD23	1:432:A:VAL:HB	32	0.63	0.24	0.7
(1,1137)	1:412:A:LEU:HD22	1:432:A:VAL:HB	32	0.63	0.24	0.7
(1,1137)	1:398:A:ILE:HD11	1:401:A:GLU:HB2	32	0.63	0.24	0.7
(1,1137)	1:398:A:ILE:HD13	1:401:A:GLU:HB2	32	0.63	0.24	0.7
(1,1137)	1:412:A:LEU:HD21	1:432:A:VAL:HB	32	0.63	0.24	0.7
(1,1137)	1:398:A:ILE:HD12	1:401:A:GLU:HB2	32	0.63	0.24	0.7
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB2	31	0.58	0.34	0.5
(1,786)	1:407:A:PHE:HE2	1:403:A:ARG:HB3	31	0.58	0.34	0.5
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB3	31	0.58	0.34	0.5
(1,786)	1:405:A:GLN:HE22	1:402:A:ILE:HB	31	0.58	0.34	0.5
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	31	0.37	0.1	0.39
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB2	31	0.37	0.1	0.39
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	31	0.25	0.07	0.27
(1,1101)	1:436:A:LEU:HD21	1:436:A:LEU:HB3	30	0.13	0.02	0.13
(1,1101)	1:436:A:LEU:HD11	1:436:A:LEU:HB2	30	0.13	0.02	0.13
(1,1101)	1:436:A:LEU:HD23	1:436:A:LEU:HB3	30	0.13	0.02	0.13
(1,1101)	1:436:A:LEU:HD12	1:436:A:LEU:HB2	30	0.13	0.02	0.13
(1,1101)	1:436:A:LEU:HD22	1:436:A:LEU:HB3	30	0.13	0.02	0.13
(1,1101)	1:398:A:ILE:HG22	1:440:A:LYS:HB3	30	0.13	0.02	0.13
(1,1101)	1:398:A:ILE:HG21	1:440:A:LYS:HB3	30	0.13	0.02	0.13
(1,1101)	1:398:A:ILE:HG22	1:398:A:ILE:HB	30	0.13	0.02	0.13
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	28	0.49	0.32	0.4
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	28	0.28	0.11	0.25
(1,1109)	1:409:A:LEU:HD11	1:432:A:VAL:HB	28	0.28	0.11	0.25
(1,1109)	1:439:A:LEU:HD22	1:401:A:GLU:HB2	28	0.28	0.11	0.25
(1,1109)	1:439:A:LEU:HD21	1:401:A:GLU:HB2	28	0.28	0.11	0.25
(1,1109)	1:409:A:LEU:HD23	1:406:A:GLU:HB3	28	0.28	0.11	0.25
(1,1109)	1:402:A:ILE:HG21	1:406:A:GLU:HB2	28	0.28	0.11	0.25
(1,1109)	1:402:A:ILE:HG13	1:406:A:GLU:HB2	28	0.28	0.11	0.25
(1,1109)	1:439:A:LEU:HD23	1:401:A:GLU:HB2	28	0.28	0.11	0.25
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	27	0.91	0.41	1.08
(1,793)	1:413:A:HIS:HD2	1:412:A:LEU:HB2	27	0.91	0.41	1.08
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD3	26	0.23	0.09	0.22
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD2	26	0.23	0.09	0.22
(1,794)	1:430:A:TRP:HD1	1:433:A:GLN:HA	26	0.2	0.06	0.2
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	26	0.2	0.06	0.2
(1,794)	1:430:A:TRP:HD1	1:427:A:GLU:HA	26	0.2	0.06	0.2
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD23	25	1.1	0.47	1.22
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD22	25	1.1	0.47	1.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD21	25	1.1	0.47	1.22
(1,920)	1:395:A:GLN:HB3	1:398:A:ILE:HD13	25	1.1	0.47	1.22
(1,920)	1:417:A:GLN:HB2	1:420:A:ILE:HD12	25	1.1	0.47	1.22
(1,920)	1:400:A:GLU:HB2	1:402:A:ILE:HG21	25	1.1	0.47	1.22
(1,920)	1:432:A:VAL:HB	1:402:A:ILE:HG13	25	1.1	0.47	1.22
(1,920)	1:395:A:GLN:HB3	1:398:A:ILE:HD11	25	1.1	0.47	1.22
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	25	0.56	0.6	0.29
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	25	0.56	0.6	0.29
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	25	0.56	0.6	0.29
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	25	0.56	0.6	0.29
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	25	0.56	0.6	0.29
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	25	0.56	0.6	0.29
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	25	0.56	0.6	0.29
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	25	0.56	0.6	0.29
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	25	0.56	0.6	0.29
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD21	25	0.56	0.6	0.29
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD22	25	0.56	0.6	0.29
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD23	25	0.56	0.6	0.29
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD21	25	0.56	0.6	0.29
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD22	25	0.56	0.6	0.29
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD23	25	0.56	0.6	0.29
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD21	25	0.56	0.6	0.29
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD22	25	0.56	0.6	0.29
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD23	25	0.56	0.6	0.29
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB2	24	0.27	0.12	0.24
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB1	24	0.27	0.12	0.24
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB3	24	0.27	0.12	0.24
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	24	0.19	0.01	0.19
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD3	23	0.42	0.13	0.46
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD3	23	0.42	0.13	0.46
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD3	23	0.42	0.13	0.46
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD2	23	0.42	0.13	0.46
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD2	23	0.42	0.13	0.46
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD2	23	0.42	0.13	0.46
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD21	23	0.27	0.13	0.26
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD22	23	0.27	0.13	0.26
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD23	23	0.27	0.13	0.26
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD11	23	0.27	0.13	0.26
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD12	23	0.27	0.13	0.26
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD13	23	0.27	0.13	0.26
(1,924)	1:428:A:ARG:HB3	1:429:A:LEU:HD23	23	0.26	0.11	0.23
(1,924)	1:412:A:LEU:HB2	1:429:A:LEU:HD23	23	0.26	0.11	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,924)	1:412:A:LEU:HB2	1:429:A:LEU:HD22	23	0.26	0.11	0.23
(1,924)	1:428:A:ARG:HB3	1:429:A:LEU:HD22	23	0.26	0.11	0.23
(1,924)	1:428:A:ARG:HB2	1:429:A:LEU:HD21	23	0.26	0.11	0.23
(1,924)	1:412:A:LEU:HB2	1:429:A:LEU:HD21	23	0.26	0.11	0.23
(1,924)	1:428:A:ARG:HB3	1:429:A:LEU:HD21	23	0.26	0.11	0.23
(1,842)	1:437:A:THR:HB	1:434:A:ARG:HB2	23	0.25	0.06	0.26
(1,842)	1:413:A:HIS:HA	1:412:A:LEU:HB2	23	0.25	0.06	0.26
(1,842)	1:405:A:GLN:HA	1:408:A:LEU:HB3	23	0.25	0.06	0.26
(1,842)	1:413:A:HIS:HA	1:425:A:LYS:HB2	23	0.25	0.06	0.26
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	22	0.63	0.24	0.58
(1,1089)	1:432:A:VAL:HB	1:405:A:GLN:HG2	22	0.63	0.24	0.58
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	22	0.29	0.07	0.3
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	22	0.18	0.04	0.18
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	22	0.18	0.04	0.18
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	22	0.18	0.04	0.18
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD11	22	0.18	0.04	0.18
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD12	22	0.18	0.04	0.18
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD13	22	0.18	0.04	0.18
(1,907)	1:405:A:GLN:HG3	1:408:A:LEU:HD12	21	0.36	0.17	0.33
(1,907)	1:405:A:GLN:HG3	1:436:A:LEU:HD21	21	0.36	0.17	0.33
(1,907)	1:405:A:GLN:HG3	1:408:A:LEU:HD21	21	0.36	0.17	0.33
(1,907)	1:405:A:GLN:HG3	1:408:A:LEU:HD23	21	0.36	0.17	0.33
(1,907)	1:405:A:GLN:HG3	1:408:A:LEU:HD22	21	0.36	0.17	0.33
(1,907)	1:405:A:GLN:HG3	1:436:A:LEU:HD23	21	0.36	0.17	0.33
(1,907)	1:406:A:GLU:HB2	1:436:A:LEU:HD22	21	0.36	0.17	0.33
(1,907)	1:406:A:GLU:HB2	1:436:A:LEU:HD23	21	0.36	0.17	0.33
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	21	0.12	0.01	0.13
(1,258)	1:394:A:THR:H	1:394:A:THR:HB	21	0.12	0.01	0.13
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD23	20	0.27	0.13	0.24
(1,919)	1:415:A:ASP:HB2	1:412:A:LEU:HD11	20	0.27	0.13	0.24
(1,919)	1:415:A:ASP:HB2	1:412:A:LEU:HD13	20	0.27	0.13	0.24
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD21	20	0.27	0.13	0.24
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD22	20	0.27	0.13	0.24
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	20	0.27	0.08	0.28
(1,733)	1:440:A:LYS:H	1:440:A:LYS:HB3	20	0.27	0.08	0.28
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	20	0.22	0.09	0.21
(1,89)	1:394:A:THR:HG23	1:394:A:THR:HB	20	0.11	0.01	0.11
(1,89)	1:394:A:THR:HG23	1:394:A:THR:HA	20	0.11	0.01	0.11
(1,89)	1:394:A:THR:HG21	1:394:A:THR:HA	20	0.11	0.01	0.11
(1,89)	1:394:A:THR:HG22	1:394:A:THR:HA	20	0.11	0.01	0.11
(1,89)	1:394:A:THR:HG21	1:394:A:THR:HB	20	0.11	0.01	0.11
(1,1113)	1:409:A:LEU:HD11	1:433:A:GLN:HB3	19	0.56	0.37	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1113)	1:436:A:LEU:HD23	1:432:A:VAL:HB	19	0.56	0.37	0.4
(1,1113)	1:409:A:LEU:HD13	1:433:A:GLN:HB3	19	0.56	0.37	0.4
(1,1113)	1:436:A:LEU:HD21	1:432:A:VAL:HB	19	0.56	0.37	0.4
(1,1113)	1:443:A:LEU:HD13	1:393:A:GLU:HB3	19	0.56	0.37	0.4
(1,1113)	1:443:A:LEU:HD12	1:393:A:GLU:HB3	19	0.56	0.37	0.4
(1,1113)	1:436:A:LEU:HD22	1:432:A:VAL:HB	19	0.56	0.37	0.4
(1,1196)	1:398:A:ILE:HD13	1:440:A:LYS:HG2	19	0.33	0.18	0.25
(1,1196)	1:398:A:ILE:HD11	1:440:A:LYS:HG2	19	0.33	0.18	0.25
(1,1196)	1:398:A:ILE:HD12	1:440:A:LYS:HG2	19	0.33	0.18	0.25
(1,1196)	1:398:A:ILE:HD13	1:399:A:LYS:HG2	19	0.33	0.18	0.25
(1,1196)	1:402:A:ILE:HD12	1:440:A:LYS:HG2	19	0.33	0.18	0.25
(1,1196)	1:402:A:ILE:HD13	1:440:A:LYS:HG2	19	0.33	0.18	0.25
(1,1196)	1:398:A:ILE:HD12	1:399:A:LYS:HG2	19	0.33	0.18	0.25
(1,1196)	1:398:A:ILE:HD13	1:399:A:LYS:HG3	19	0.33	0.18	0.25
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	19	0.17	0.04	0.17
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG2	19	0.17	0.04	0.17
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	18	0.89	0.29	0.95
(1,1112)	1:443:A:LEU:HD12	1:393:A:GLU:HB3	18	0.54	0.36	0.4
(1,1112)	1:436:A:LEU:HD22	1:432:A:VAL:HB	18	0.54	0.36	0.4
(1,1112)	1:409:A:LEU:HD11	1:433:A:GLN:HB3	18	0.54	0.36	0.4
(1,1112)	1:436:A:LEU:HD21	1:432:A:VAL:HB	18	0.54	0.36	0.4
(1,1112)	1:436:A:LEU:HD23	1:432:A:VAL:HB	18	0.54	0.36	0.4
(1,1112)	1:443:A:LEU:HD13	1:393:A:GLU:HB3	18	0.54	0.36	0.4
(1,1112)	1:409:A:LEU:HD13	1:433:A:GLN:HB3	18	0.54	0.36	0.4
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB2	18	0.25	0.1	0.22
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB3	18	0.25	0.1	0.22
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	17	0.65	0.26	0.71
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	17	0.65	0.26	0.71
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	17	0.65	0.26	0.71
(1,909)	1:440:A:LYS:HE3	1:436:A:LEU:HD13	17	0.65	0.37	0.55
(1,909)	1:440:A:LYS:HE2	1:436:A:LEU:HD12	17	0.65	0.37	0.55
(1,909)	1:440:A:LYS:HE2	1:436:A:LEU:HD13	17	0.65	0.37	0.55
(1,909)	1:440:A:LYS:HE3	1:398:A:ILE:HG22	17	0.65	0.37	0.55
(1,909)	1:440:A:LYS:HE3	1:436:A:LEU:HD12	17	0.65	0.37	0.55
(1,909)	1:440:A:LYS:HE3	1:436:A:LEU:HD11	17	0.65	0.37	0.55
(1,909)	1:440:A:LYS:HE3	1:398:A:ILE:HG23	17	0.65	0.37	0.55
(1,909)	1:425:A:LYS:HE2	1:412:A:LEU:HD11	17	0.65	0.37	0.55
(1,909)	1:425:A:LYS:HE3	1:412:A:LEU:HD11	17	0.65	0.37	0.55
(1,909)	1:440:A:LYS:HE3	1:398:A:ILE:HG21	17	0.65	0.37	0.55
(1,1107)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	17	0.26	0.12	0.23
(1,1107)	1:398:A:ILE:HG12	1:440:A:LYS:HD3	17	0.26	0.12	0.23
(1,1107)	1:398:A:ILE:HG13	1:440:A:LYS:HD2	17	0.26	0.12	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	17	0.13	0.01	0.13
(1,1128)	1:408:A:LEU:HD11	1:432:A:VAL:HB	16	0.68	0.24	0.71
(1,1128)	1:408:A:LEU:HD12	1:432:A:VAL:HB	16	0.68	0.24	0.71
(1,1128)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	16	0.68	0.24	0.71
(1,1128)	1:408:A:LEU:HD13	1:432:A:VAL:HB	16	0.68	0.24	0.71
(1,1128)	1:408:A:LEU:HD22	1:405:A:GLN:HG3	16	0.68	0.24	0.71
(1,1128)	1:408:A:LEU:HD23	1:405:A:GLN:HG3	16	0.68	0.24	0.71
(1,961)	1:422:A:ASP:HB2	1:425:A:LYS:HB2	16	0.53	0.16	0.54
(1,961)	1:406:A:GLU:HG3	1:402:A:ILE:HB	16	0.53	0.16	0.54
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD2	16	0.24	0.07	0.23
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD3	16	0.24	0.07	0.23
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD21	16	0.18	0.05	0.18
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD22	16	0.18	0.05	0.18
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD23	16	0.18	0.05	0.18
(1,1161)	1:441:A:ARG:HG2	1:445:A:GLU:HG2	15	0.42	0.48	0.22
(1,1161)	1:404:A:ARG:HG3	1:405:A:GLN:HG3	15	0.42	0.48	0.22
(1,1157)	1:396:A:ALA:HB1	1:395:A:GLN:HB3	15	0.36	0.23	0.25
(1,1157)	1:396:A:ALA:HB3	1:400:A:GLU:HB2	15	0.36	0.23	0.25
(1,1157)	1:396:A:ALA:HB1	1:400:A:GLU:HB2	15	0.36	0.23	0.25
(1,1157)	1:396:A:ALA:HB2	1:395:A:GLN:HB3	15	0.36	0.23	0.25
(1,1157)	1:396:A:ALA:HB3	1:395:A:GLN:HB3	15	0.36	0.23	0.25
(1,1157)	1:396:A:ALA:HB2	1:400:A:GLU:HB2	15	0.36	0.23	0.25
(1,860)	1:429:A:LEU:HA	1:429:A:LEU:HG	15	0.28	0.02	0.28
(2,3)	1:406:A:GLU:HB3	1:410:A:ASN:HA	15	0.13	0.03	0.13
(1,1141)	1:416:A:LEU:HD21	1:415:A:ASP:HB3	14	0.34	0.13	0.31
(1,1141)	1:402:A:ILE:HG23	1:399:A:LYS:HE2	14	0.34	0.13	0.31
(1,1141)	1:409:A:LEU:HD22	1:410:A:ASN:HB2	14	0.34	0.13	0.31
(1,1141)	1:416:A:LEU:HD22	1:415:A:ASP:HB3	14	0.34	0.13	0.31
(1,1141)	1:402:A:ILE:HG21	1:399:A:LYS:HE2	14	0.34	0.13	0.31
(1,1141)	1:416:A:LEU:HD23	1:415:A:ASP:HB3	14	0.34	0.13	0.31
(1,1141)	1:409:A:LEU:HD21	1:410:A:ASN:HB2	14	0.34	0.13	0.31
(1,253)	1:442:A:LYS:H	1:442:A:LYS:HD2	14	0.25	0.05	0.26
(1,253)	1:442:A:LYS:H	1:442:A:LYS:HD3	14	0.25	0.05	0.26
(1,517)	1:416:A:LEU:HG	1:415:A:ASP:HB2	13	0.51	0.15	0.48
(1,923)	1:441:A:ARG:HD3	1:437:A:THR:HG23	13	0.49	0.28	0.37
(1,923)	1:413:A:HIS:HB2	1:412:A:LEU:HG	13	0.49	0.28	0.37
(1,923)	1:441:A:ARG:HD2	1:437:A:THR:HG22	13	0.49	0.28	0.37
(1,923)	1:441:A:ARG:HD2	1:437:A:THR:HG23	13	0.49	0.28	0.37
(1,923)	1:441:A:ARG:HD3	1:437:A:THR:HG21	13	0.49	0.28	0.37
(1,923)	1:441:A:ARG:HD3	1:437:A:THR:HG22	13	0.49	0.28	0.37
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG11	13	0.44	0.18	0.46
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG13	13	0.44	0.18	0.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG23	13	0.44	0.18	0.46
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG12	13	0.44	0.18	0.46
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG22	13	0.44	0.18	0.46
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG21	13	0.44	0.18	0.46
(1,1122)	1:416:A:LEU:HD11	1:426:A:GLU:HG3	13	0.41	0.19	0.35
(1,1122)	1:436:A:LEU:HD11	1:433:A:GLN:HG2	13	0.41	0.19	0.35
(1,1122)	1:416:A:LEU:HD13	1:426:A:GLU:HG3	13	0.41	0.19	0.35
(1,1122)	1:416:A:LEU:HD11	1:426:A:GLU:HG2	13	0.41	0.19	0.35
(1,1122)	1:436:A:LEU:HD12	1:433:A:GLN:HG2	13	0.41	0.19	0.35
(1,967)	1:405:A:GLN:HG2	1:408:A:LEU:HG	13	0.36	0.17	0.33
(1,967)	1:415:A:ASP:HB2	1:425:A:LYS:HB3	13	0.36	0.17	0.33
(1,967)	1:415:A:ASP:HB2	1:416:A:LEU:HG	13	0.36	0.17	0.33
(1,1045)	1:435:A:ILE:HG13	1:431:A:GLU:HA	13	0.18	0.05	0.19
(1,758)	1:442:A:LYS:H	1:442:A:LYS:HB2	13	0.15	0.05	0.13
(1,758)	1:442:A:LYS:H	1:441:A:ARG:HB2	13	0.15	0.05	0.13
(1,758)	1:428:A:ARG:H	1:428:A:ARG:HB2	13	0.15	0.05	0.13
(1,1132)	1:408:A:LEU:HD23	1:404:A:ARG:HB3	12	0.43	0.63	0.18
(1,1132)	1:408:A:LEU:HD12	1:405:A:GLN:HB3	12	0.43	0.63	0.18
(1,1132)	1:408:A:LEU:HD11	1:405:A:GLN:HB3	12	0.43	0.63	0.18
(1,1132)	1:408:A:LEU:HD22	1:404:A:ARG:HB3	12	0.43	0.63	0.18
(1,1132)	1:408:A:LEU:HD13	1:405:A:GLN:HB3	12	0.43	0.63	0.18
(1,117)	1:398:A:ILE:HG13	1:399:A:LYS:HE3	12	0.26	0.19	0.24
(1,117)	1:398:A:ILE:HG12	1:399:A:LYS:HE3	12	0.26	0.19	0.24
(1,117)	1:398:A:ILE:HG12	1:399:A:LYS:HE2	12	0.26	0.19	0.24
(1,866)	1:423:A:LEU:HA	1:423:A:LEU:HD11	12	0.22	0.09	0.18
(1,866)	1:423:A:LEU:HA	1:423:A:LEU:HD12	12	0.22	0.09	0.18
(1,866)	1:423:A:LEU:HA	1:423:A:LEU:HD13	12	0.22	0.09	0.18
(1,342)	1:422:A:ASP:H	1:421:A:LYS:HB3	12	0.14	0.02	0.15
(1,342)	1:422:A:ASP:H	1:421:A:LYS:HB2	12	0.14	0.02	0.15
(1,192)	1:400:A:GLU:H	1:400:A:GLU:HB3	11	0.7	0.15	0.76
(1,435)	1:405:A:GLN:HE22	1:401:A:GLU:HG2	11	0.66	0.37	0.47
(1,435)	1:405:A:GLN:HE22	1:401:A:GLU:HG3	11	0.66	0.37	0.47
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD11	11	0.53	0.08	0.52
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD12	11	0.53	0.08	0.52
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD13	11	0.53	0.08	0.52
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD11	11	0.53	0.08	0.52
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD12	11	0.53	0.08	0.52
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD13	11	0.53	0.08	0.52
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD11	11	0.53	0.08	0.52
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD12	11	0.53	0.08	0.52
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD13	11	0.53	0.08	0.52
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG21	11	0.23	0.08	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG22	11	0.23	0.08	0.22
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG23	11	0.23	0.08	0.22
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG21	11	0.23	0.08	0.22
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG22	11	0.23	0.08	0.22
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG23	11	0.23	0.08	0.22
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG21	11	0.23	0.08	0.22
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG22	11	0.23	0.08	0.22
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG23	11	0.23	0.08	0.22
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD21	11	0.2	0.04	0.19
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD22	11	0.2	0.04	0.19
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD23	11	0.2	0.04	0.19
(1,769)	1:429:A:LEU:H	1:428:A:ARG:HA	11	0.16	0.01	0.16
(1,769)	1:426:A:GLU:H	1:423:A:LEU:HA	11	0.16	0.01	0.16
(1,769)	1:407:A:PHE:H	1:404:A:ARG:HA	11	0.16	0.01	0.16
(1,726)	1:446:A:ALA:H	1:445:A:GLU:HA	11	0.15	0.02	0.15
(1,921)	1:409:A:LEU:HG	1:412:A:LEU:HD21	10	0.55	0.26	0.49
(1,921)	1:425:A:LYS:HD2	1:416:A:LEU:HD23	10	0.55	0.26	0.49
(1,921)	1:429:A:LEU:HG	1:416:A:LEU:HD23	10	0.55	0.26	0.49
(1,921)	1:409:A:LEU:HG	1:412:A:LEU:HD23	10	0.55	0.26	0.49
(1,921)	1:425:A:LYS:HD3	1:416:A:LEU:HD22	10	0.55	0.26	0.49
(1,921)	1:425:A:LYS:HD3	1:416:A:LEU:HD23	10	0.55	0.26	0.49
(1,921)	1:429:A:LEU:HG	1:416:A:LEU:HD21	10	0.55	0.26	0.49
(1,1133)	1:412:A:LEU:HD21	1:409:A:LEU:HG	10	0.51	0.26	0.46
(1,1133)	1:412:A:LEU:HD22	1:409:A:LEU:HG	10	0.51	0.26	0.46
(1,1133)	1:412:A:LEU:HD23	1:429:A:LEU:HG	10	0.51	0.26	0.46
(1,1133)	1:412:A:LEU:HD23	1:409:A:LEU:HG	10	0.51	0.26	0.46
(1,1133)	1:412:A:LEU:HD22	1:429:A:LEU:HG	10	0.51	0.26	0.46
(1,362)	1:414:A:ARG:H	1:414:A:ARG:HG2	10	0.28	0.11	0.24
(1,642)	1:416:A:LEU:H	1:412:A:LEU:HB3	10	0.25	0.1	0.24
(1,642)	1:416:A:LEU:H	1:412:A:LEU:HB2	10	0.25	0.1	0.24
(1,249)	1:401:A:GLU:HA	1:401:A:GLU:HB2	10	0.16	0.05	0.16
(1,249)	1:401:A:GLU:HA	1:401:A:GLU:HB3	10	0.16	0.05	0.16
(1,1127)	1:420:A:ILE:HG23	1:422:A:ASP:HB3	9	0.56	0.37	0.58
(1,1127)	1:420:A:ILE:HG22	1:422:A:ASP:HB3	9	0.56	0.37	0.58
(1,1127)	1:420:A:ILE:HG21	1:422:A:ASP:HB3	9	0.56	0.37	0.58
(1,1127)	1:436:A:LEU:HD21	1:405:A:GLN:HG2	9	0.56	0.37	0.58
(1,1127)	1:409:A:LEU:HD21	1:410:A:ASN:HB2	9	0.56	0.37	0.58
(1,390)	1:445:A:GLU:H	1:445:A:GLU:HB2	9	0.37	0.05	0.36
(1,1119)	1:432:A:VAL:HG13	1:431:A:GLU:HB3	9	0.35	0.17	0.28
(1,1119)	1:432:A:VAL:HG11	1:431:A:GLU:HB3	9	0.35	0.17	0.28
(1,1119)	1:432:A:VAL:HG12	1:431:A:GLU:HB3	9	0.35	0.17	0.28
(1,360)	1:414:A:ARG:H	1:414:A:ARG:HD2	9	0.32	0.1	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,360)	1:414:A:ARG:H	1:414:A:ARG:HD3	9	0.32	0.1	0.36
(1,911)	1:405:A:GLN:HG3	1:408:A:LEU:HD12	9	0.31	0.15	0.35
(1,911)	1:405:A:GLN:HG3	1:436:A:LEU:HD21	9	0.31	0.15	0.35
(1,911)	1:405:A:GLN:HG3	1:408:A:LEU:HD21	9	0.31	0.15	0.35
(1,911)	1:405:A:GLN:HG3	1:408:A:LEU:HD22	9	0.31	0.15	0.35
(1,911)	1:406:A:GLU:HB3	1:409:A:LEU:HD22	9	0.31	0.15	0.35
(1,911)	1:405:A:GLN:HG3	1:436:A:LEU:HD23	9	0.31	0.15	0.35
(1,911)	1:406:A:GLU:HB3	1:409:A:LEU:HD11	9	0.31	0.15	0.35
(1,114)	1:398:A:ILE:HG12	1:401:A:GLU:HB2	9	0.24	0.06	0.25
(1,114)	1:398:A:ILE:HG13	1:401:A:GLU:HB2	9	0.24	0.06	0.25
(1,472)	1:410:A:ASN:HD22	1:414:A:ARG:HB2	9	0.2	0.09	0.19
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD11	9	0.12	0.01	0.12
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD12	9	0.12	0.01	0.12
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD13	9	0.12	0.01	0.12
(1,1095)	1:398:A:ILE:HG22	1:440:A:LYS:HE3	8	0.48	0.24	0.5
(1,1095)	1:436:A:LEU:HD12	1:440:A:LYS:HE3	8	0.48	0.24	0.5
(1,1095)	1:436:A:LEU:HD11	1:440:A:LYS:HE3	8	0.48	0.24	0.5
(1,1095)	1:412:A:LEU:HD11	1:425:A:LYS:HE2	8	0.48	0.24	0.5
(1,1095)	1:398:A:ILE:HG21	1:440:A:LYS:HE3	8	0.48	0.24	0.5
(1,753)	1:434:A:ARG:H	1:433:A:GLN:HG2	8	0.26	0.23	0.14
(1,753)	1:400:A:GLU:H	1:400:A:GLU:HG3	8	0.26	0.23	0.14
(1,776)	1:444:A:ARG:H	1:443:A:LEU:HB2	8	0.26	0.11	0.22
(1,776)	1:444:A:ARG:H	1:443:A:LEU:HB3	8	0.26	0.11	0.22
(1,808)	1:424:A:SER:HA	1:427:A:GLU:HG2	8	0.24	0.09	0.25
(1,808)	1:416:A:LEU:HA	1:417:A:GLN:HG2	8	0.24	0.09	0.25
(1,808)	1:416:A:LEU:HA	1:417:A:GLN:HG3	8	0.24	0.09	0.25
(1,910)	1:440:A:LYS:HG2	1:398:A:ILE:HD13	8	0.17	0.08	0.15
(1,910)	1:399:A:LYS:HG3	1:402:A:ILE:HG23	8	0.17	0.08	0.15
(1,910)	1:440:A:LYS:HG2	1:436:A:LEU:HD11	8	0.17	0.08	0.15
(1,910)	1:399:A:LYS:HG3	1:402:A:ILE:HG22	8	0.17	0.08	0.15
(1,910)	1:399:A:LYS:HG2	1:398:A:ILE:HD13	8	0.17	0.08	0.15
(1,910)	1:399:A:LYS:HG3	1:402:A:ILE:HG21	8	0.17	0.08	0.15
(1,910)	1:399:A:LYS:HG2	1:398:A:ILE:HD12	8	0.17	0.08	0.15
(1,1000)	1:420:A:ILE:HG22	1:420:A:ILE:HA	8	0.15	0.02	0.15
(1,1000)	1:420:A:ILE:HG21	1:420:A:ILE:HA	8	0.15	0.02	0.15
(1,1000)	1:420:A:ILE:HG23	1:420:A:ILE:HA	8	0.15	0.02	0.15
(1,1201)	1:405:A:GLN:HE22	1:401:A:GLU:HG3	7	0.34	0.09	0.33
(1,1201)	1:405:A:GLN:HE22	1:401:A:GLU:HG2	7	0.34	0.09	0.33
(1,1201)	1:405:A:GLN:HE22	1:431:A:GLU:HG3	7	0.34	0.09	0.33
(1,974)	1:403:A:ARG:HD3	1:400:A:GLU:HG3	7	0.33	0.19	0.36
(1,974)	1:403:A:ARG:HD2	1:400:A:GLU:HG3	7	0.33	0.19	0.36
(1,974)	1:403:A:ARG:HD3	1:400:A:GLU:HG2	7	0.33	0.19	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,974)	1:403:A:ARG:HD2	1:400:A:GLU:HG2	7	0.33	0.19	0.36
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD11	7	0.23	0.04	0.23
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD12	7	0.23	0.04	0.23
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD13	7	0.23	0.04	0.23
(1,229)	1:396:A:ALA:H	1:394:A:THR:HA	7	0.21	0.09	0.19
(1,229)	1:396:A:ALA:H	1:394:A:THR:HB	7	0.21	0.09	0.19
(1,72)	1:440:A:LYS:HE2	1:441:A:ARG:HG2	7	0.2	0.06	0.19
(1,72)	1:440:A:LYS:HE3	1:441:A:ARG:HG2	7	0.2	0.06	0.19
(1,1117)	1:412:A:LEU:HD22	1:408:A:LEU:HB2	7	0.19	0.07	0.16
(1,1117)	1:412:A:LEU:HD23	1:408:A:LEU:HB2	7	0.19	0.07	0.16
(1,1117)	1:398:A:ILE:HD12	1:436:A:LEU:HB2	7	0.19	0.07	0.16
(2,2)	1:415:A:ASP:HB3	1:420:A:ILE:HG13	6	0.78	0.6	0.63
(1,929)	1:425:A:LYS:HD2	1:416:A:LEU:HD23	6	0.55	0.19	0.6
(1,929)	1:425:A:LYS:HD3	1:416:A:LEU:HD23	6	0.55	0.19	0.6
(1,929)	1:425:A:LYS:HD3	1:416:A:LEU:HD22	6	0.55	0.19	0.6
(1,929)	1:425:A:LYS:HD2	1:416:A:LEU:HD22	6	0.55	0.19	0.6
(1,1143)	1:398:A:ILE:HG23	1:399:A:LYS:HE3	6	0.54	0.32	0.5
(1,1143)	1:398:A:ILE:HG23	1:399:A:LYS:HE2	6	0.54	0.32	0.5
(1,1143)	1:398:A:ILE:HG21	1:399:A:LYS:HE3	6	0.54	0.32	0.5
(1,1143)	1:398:A:ILE:HG22	1:399:A:LYS:HE3	6	0.54	0.32	0.5
(1,1143)	1:398:A:ILE:HG22	1:399:A:LYS:HE2	6	0.54	0.32	0.5
(1,1066)	1:398:A:ILE:HD12	1:440:A:LYS:HA	6	0.4	0.17	0.37
(1,1066)	1:398:A:ILE:HD11	1:440:A:LYS:HA	6	0.4	0.17	0.37
(1,1066)	1:416:A:LEU:HD23	1:426:A:GLU:HA	6	0.4	0.17	0.37
(1,55)	1:417:A:GLN:HE21	1:414:A:ARG:HB3	6	0.32	0.11	0.36
(1,55)	1:417:A:GLN:HE21	1:414:A:ARG:HB2	6	0.32	0.11	0.36
(1,856)	1:409:A:LEU:HA	1:409:A:LEU:HG	6	0.27	0.22	0.18
(1,856)	1:429:A:LEU:HA	1:429:A:LEU:HG	6	0.27	0.22	0.18
(1,1200)	1:442:A:LYS:H	1:442:A:LYS:HB3	6	0.24	0.04	0.26
(1,1225)	1:427:A:GLU:H	1:412:A:LEU:HD13	6	0.22	0.09	0.24
(1,1225)	1:427:A:GLU:H	1:416:A:LEU:HD12	6	0.22	0.09	0.24
(1,1225)	1:427:A:GLU:H	1:416:A:LEU:HD13	6	0.22	0.09	0.24
(1,1225)	1:427:A:GLU:H	1:416:A:LEU:HD11	6	0.22	0.09	0.24
(1,735)	1:440:A:LYS:H	1:440:A:LYS:HG2	6	0.17	0.03	0.17
(1,38)	1:425:A:LYS:HA	1:425:A:LYS:HG2	6	0.15	0.04	0.15
(1,999)	1:412:A:LEU:HB2	1:412:A:LEU:HA	6	0.11	0.01	0.12
(1,999)	1:412:A:LEU:HB3	1:412:A:LEU:HA	6	0.11	0.01	0.12
(1,999)	1:442:A:LYS:HB2	1:442:A:LYS:HA	6	0.11	0.01	0.12
(1,43)	1:417:A:GLN:HA	1:420:A:ILE:HG12	5	1.56	0.29	1.72
(1,1006)	1:412:A:LEU:HD11	1:413:A:HIS:HA	5	0.51	0.54	0.21
(1,1006)	1:443:A:LEU:HD21	1:443:A:LEU:HA	5	0.51	0.54	0.21
(1,1006)	1:412:A:LEU:HD13	1:413:A:HIS:HA	5	0.51	0.54	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1006)	1:412:A:LEU:HD12	1:413:A:HIS:HA	5	0.51	0.54	0.21
(1,544)	1:444:A:ARG:H	1:395:A:GLN:HE21	5	0.5	0.31	0.55
(1,15)	1:420:A:ILE:H	1:420:A:ILE:HG23	5	0.44	0.14	0.47
(1,15)	1:420:A:ILE:H	1:420:A:ILE:HD13	5	0.44	0.14	0.47
(1,15)	1:420:A:ILE:H	1:420:A:ILE:HG21	5	0.44	0.14	0.47
(1,15)	1:420:A:ILE:H	1:420:A:ILE:HD11	5	0.44	0.14	0.47
(1,15)	1:420:A:ILE:H	1:420:A:ILE:HD12	5	0.44	0.14	0.47
(1,754)	1:411:A:SER:H	1:412:A:LEU:HD12	5	0.42	0.09	0.43
(1,754)	1:411:A:SER:H	1:408:A:LEU:HD12	5	0.42	0.09	0.43
(1,754)	1:411:A:SER:H	1:409:A:LEU:HD22	5	0.42	0.09	0.43
(1,754)	1:411:A:SER:H	1:408:A:LEU:HD13	5	0.42	0.09	0.43
(1,331)	1:413:A:HIS:H	1:412:A:LEU:HG	5	0.33	0.04	0.33
(1,1192)	1:420:A:ILE:HG21	1:420:A:ILE:HG13	5	0.31	0.01	0.31
(1,1192)	1:420:A:ILE:HG22	1:420:A:ILE:HG13	5	0.31	0.01	0.31
(1,1192)	1:420:A:ILE:HG23	1:420:A:ILE:HG13	5	0.31	0.01	0.31
(1,320)	1:405:A:GLN:H	1:405:A:GLN:HG3	5	0.3	0.15	0.32
(1,1111)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	5	0.23	0.1	0.19
(1,1111)	1:398:A:ILE:HG12	1:440:A:LYS:HD3	5	0.23	0.1	0.19
(1,344)	1:412:A:LEU:H	1:411:A:SER:HB2	5	0.2	0.05	0.22
(1,1165)	1:446:A:ALA:HB2	1:445:A:GLU:HB2	5	0.19	0.05	0.2
(1,1165)	1:446:A:ALA:HB1	1:445:A:GLU:HB2	5	0.19	0.05	0.2
(1,391)	1:417:A:GLN:H	1:417:A:GLN:HB3	5	0.18	0.03	0.19
(1,391)	1:417:A:GLN:H	1:417:A:GLN:HB2	5	0.18	0.03	0.19
(1,963)	1:410:A:ASN:HB2	1:409:A:LEU:HB3	5	0.16	0.08	0.13
(1,963)	1:422:A:ASP:HB3	1:425:A:LYS:HB2	5	0.16	0.08	0.13
(1,988)	1:406:A:GLU:HB2	1:403:A:ARG:HA	5	0.15	0.03	0.14
(1,813)	1:397:A:GLY:HA2	1:400:A:GLU:HB2	5	0.14	0.02	0.13
(1,813)	1:406:A:GLU:HA	1:405:A:GLN:HB3	5	0.14	0.02	0.13
(1,813)	1:406:A:GLU:HA	1:405:A:GLN:HB2	5	0.14	0.02	0.13
(1,1049)	1:435:A:ILE:HG13	1:431:A:GLU:HA	5	0.13	0.02	0.13
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD21	5	0.11	0.01	0.11
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD22	5	0.11	0.01	0.11
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD23	5	0.11	0.01	0.11
(1,1150)	1:442:A:LYS:HD3	1:442:A:LYS:HB3	5	0.11	0.0	0.11
(1,1150)	1:442:A:LYS:HD2	1:442:A:LYS:HB3	5	0.11	0.0	0.11
(1,939)	1:413:A:HIS:HB2	1:412:A:LEU:HD12	4	0.7	0.36	0.55
(1,939)	1:413:A:HIS:HB2	1:409:A:LEU:HD23	4	0.7	0.36	0.55
(1,939)	1:413:A:HIS:HB2	1:416:A:LEU:HD11	4	0.7	0.36	0.55
(1,939)	1:413:A:HIS:HB2	1:409:A:LEU:HD22	4	0.7	0.36	0.55
(1,83)	1:408:A:LEU:HD11	1:412:A:LEU:HD21	4	0.34	0.22	0.24
(1,83)	1:408:A:LEU:HD11	1:412:A:LEU:HD22	4	0.34	0.22	0.24
(1,83)	1:408:A:LEU:HD11	1:412:A:LEU:HD23	4	0.34	0.22	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,83)	1:408:A:LEU:HD12	1:412:A:LEU:HD21	4	0.34	0.22	0.24
(1,83)	1:408:A:LEU:HD12	1:412:A:LEU:HD22	4	0.34	0.22	0.24
(1,83)	1:408:A:LEU:HD12	1:412:A:LEU:HD23	4	0.34	0.22	0.24
(1,83)	1:408:A:LEU:HD13	1:412:A:LEU:HD21	4	0.34	0.22	0.24
(1,83)	1:408:A:LEU:HD13	1:412:A:LEU:HD22	4	0.34	0.22	0.24
(1,83)	1:408:A:LEU:HD13	1:412:A:LEU:HD23	4	0.34	0.22	0.24
(1,722)	1:403:A:ARG:H	1:404:A:ARG:HG3	4	0.24	0.04	0.24
(1,1236)	1:430:A:TRP:HE1	1:434:A:ARG:HA	4	0.24	0.09	0.26
(1,341)	1:422:A:ASP:H	1:421:A:LYS:HA	4	0.22	0.06	0.22
(1,1209)	1:429:A:LEU:H	1:427:A:GLU:HB3	4	0.21	0.04	0.2
(1,500)	1:413:A:HIS:HB2	1:410:A:ASN:HA	4	0.19	0.05	0.19
(1,370)	1:419:A:GLY:H	1:419:A:GLY:HA2	4	0.14	0.02	0.15
(1,238)	1:411:A:SER:H	1:411:A:SER:HB3	4	0.12	0.02	0.12
(1,303)	1:430:A:TRP:HE1	1:433:A:GLN:HB2	4	0.12	0.0	0.12
(1,957)	1:445:A:GLU:HG2	1:445:A:GLU:HB3	4	0.11	0.0	0.11
(1,957)	1:406:A:GLU:HB3	1:406:A:GLU:HG2	4	0.11	0.0	0.11
(1,112)	1:408:A:LEU:HD11	1:409:A:LEU:HB2	3	2.28	0.0	2.28
(1,112)	1:408:A:LEU:HD12	1:409:A:LEU:HB2	3	2.28	0.0	2.28
(1,112)	1:408:A:LEU:HD13	1:409:A:LEU:HB2	3	2.28	0.0	2.28
(1,1063)	1:408:A:LEU:HD11	1:429:A:LEU:HA	3	0.91	0.64	0.71
(1,1063)	1:408:A:LEU:HD13	1:429:A:LEU:HA	3	0.91	0.64	0.71
(1,1063)	1:408:A:LEU:HD12	1:411:A:SER:HB2	3	0.91	0.64	0.71
(2,4)	1:408:A:LEU:HD11	1:406:A:GLU:HA	3	0.78	0.09	0.82
(2,4)	1:408:A:LEU:HD12	1:406:A:GLU:HA	3	0.78	0.09	0.82
(2,4)	1:408:A:LEU:HD13	1:406:A:GLU:HA	3	0.78	0.09	0.82
(1,119)	1:408:A:LEU:HD11	1:409:A:LEU:HG	3	0.69	0.09	0.7
(1,119)	1:408:A:LEU:HD12	1:409:A:LEU:HG	3	0.69	0.09	0.7
(1,119)	1:408:A:LEU:HD13	1:409:A:LEU:HG	3	0.69	0.09	0.7
(1,797)	1:395:A:GLN:HE21	1:398:A:ILE:HG23	3	0.54	0.31	0.59
(1,1068)	1:441:A:ARG:HG2	1:437:A:THR:HB	3	0.52	0.41	0.27
(1,1068)	1:404:A:ARG:HG3	1:405:A:GLN:HA	3	0.52	0.41	0.27
(1,425)	1:413:A:HIS:HD2	1:416:A:LEU:HD21	3	0.51	0.02	0.5
(1,425)	1:413:A:HIS:HD2	1:416:A:LEU:HD22	3	0.51	0.02	0.5
(1,425)	1:413:A:HIS:HD2	1:416:A:LEU:HD23	3	0.51	0.02	0.5
(1,413)	1:420:A:ILE:H	1:420:A:ILE:HG12	3	0.41	0.06	0.4
(1,616)	1:439:A:LEU:H	1:442:A:LYS:HD3	3	0.4	0.2	0.32
(1,899)	1:433:A:GLN:HB3	1:409:A:LEU:HD11	3	0.36	0.08	0.42
(1,899)	1:433:A:GLN:HB3	1:409:A:LEU:HD13	3	0.36	0.08	0.42
(1,294)	1:409:A:LEU:H	1:408:A:LEU:HD11	3	0.31	0.02	0.31
(1,294)	1:409:A:LEU:H	1:408:A:LEU:HD12	3	0.31	0.02	0.31
(1,294)	1:409:A:LEU:H	1:408:A:LEU:HD13	3	0.31	0.02	0.31
(1,724)	1:405:A:GLN:H	1:405:A:GLN:HE22	3	0.22	0.07	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,765)	1:405:A:GLN:H	1:405:A:GLN:HG3	3	0.2	0.09	0.16
(1,738)	1:440:A:LYS:HA	1:443:A:LEU:HB3	3	0.18	0.06	0.21
(1,738)	1:440:A:LYS:HA	1:443:A:LEU:HB2	3	0.18	0.06	0.21
(1,730)	1:438:A:ALA:H	1:435:A:ILE:HG22	3	0.18	0.05	0.21
(1,730)	1:438:A:ALA:H	1:435:A:ILE:HG23	3	0.18	0.05	0.21
(1,730)	1:441:A:ARG:H	1:398:A:ILE:HG21	3	0.18	0.05	0.21
(1,5)	1:394:A:THR:H	1:393:A:GLU:HB3	3	0.17	0.04	0.19
(1,121)	1:429:A:LEU:HD11	1:433:A:GLN:HG3	3	0.17	0.03	0.18
(1,121)	1:429:A:LEU:HD12	1:433:A:GLN:HG3	3	0.17	0.03	0.18
(1,121)	1:429:A:LEU:HD13	1:433:A:GLN:HG3	3	0.17	0.03	0.18
(1,79)	1:430:A:TRP:HB3	1:427:A:GLU:HA	3	0.16	0.05	0.15
(1,471)	1:433:A:GLN:HE22	1:429:A:LEU:HD11	3	0.16	0.0	0.16
(1,471)	1:433:A:GLN:HE22	1:429:A:LEU:HD12	3	0.16	0.0	0.16
(1,471)	1:433:A:GLN:HE22	1:429:A:LEU:HD13	3	0.16	0.0	0.16
(1,1116)	1:435:A:ILE:HD11	1:431:A:GLU:HG2	3	0.12	0.01	0.11
(1,1116)	1:435:A:ILE:HD12	1:431:A:GLU:HG2	3	0.12	0.01	0.11
(1,1116)	1:435:A:ILE:HD13	1:431:A:GLU:HG2	3	0.12	0.01	0.11
(1,193)	1:434:A:ARG:H	1:433:A:GLN:H	3	0.11	0.01	0.11
(1,143)	1:441:A:ARG:H	1:440:A:LYS:HA	3	0.11	0.01	0.1
(1,1104)	1:435:A:ILE:HG22	1:435:A:ILE:HB	3	0.11	0.01	0.1
(1,1104)	1:398:A:ILE:HG21	1:440:A:LYS:HB3	3	0.11	0.01	0.1
(1,1104)	1:412:A:LEU:HD11	1:412:A:LEU:HB2	3	0.11	0.01	0.1
(1,1062)	1:408:A:LEU:HD13	1:411:A:SER:HB2	2	1.6	0.07	1.6
(1,1062)	1:408:A:LEU:HD12	1:411:A:SER:HB2	2	1.6	0.07	1.6
(1,787)	1:405:A:GLN:HE22	1:436:A:LEU:HD23	2	1.01	0.34	1.01
(1,787)	1:405:A:GLN:HE22	1:436:A:LEU:HD22	2	1.01	0.34	1.01
(1,1234)	1:433:A:GLN:HE22	1:409:A:LEU:HD12	2	0.43	0.18	0.43
(1,1234)	1:433:A:GLN:HE22	1:409:A:LEU:HD11	2	0.43	0.18	0.43
(1,22)	1:395:A:GLN:HE21	1:398:A:ILE:HG21	2	0.34	0.1	0.34
(1,22)	1:395:A:GLN:HE21	1:398:A:ILE:HG22	2	0.34	0.1	0.34
(1,22)	1:395:A:GLN:HE21	1:398:A:ILE:HG23	2	0.34	0.1	0.34
(1,1071)	1:443:A:LEU:HD23	1:393:A:GLU:HA	2	0.29	0.12	0.29
(1,1071)	1:409:A:LEU:HD22	1:410:A:ASN:HA	2	0.29	0.12	0.29
(1,415)	1:420:A:ILE:H	1:420:A:ILE:HB	2	0.27	0.02	0.27
(1,465)	1:395:A:GLN:HE21	1:443:A:LEU:HB3	2	0.24	0.15	0.24
(1,734)	1:399:A:LYS:H	1:399:A:LYS:HD3	2	0.24	0.1	0.24
(1,1134)	1:416:A:LEU:HD21	1:415:A:ASP:HB2	2	0.24	0.04	0.24
(1,1134)	1:416:A:LEU:HD23	1:422:A:ASP:HB3	2	0.24	0.04	0.24
(1,1091)	1:425:A:LYS:HB2	1:422:A:ASP:HB3	2	0.24	0.08	0.24
(1,848)	1:424:A:SER:HA	1:427:A:GLU:HB3	2	0.24	0.05	0.24
(1,751)	1:398:A:ILE:HA	1:439:A:LEU:HD21	2	0.22	0.11	0.22
(1,751)	1:398:A:ILE:HA	1:439:A:LEU:HD22	2	0.22	0.11	0.22

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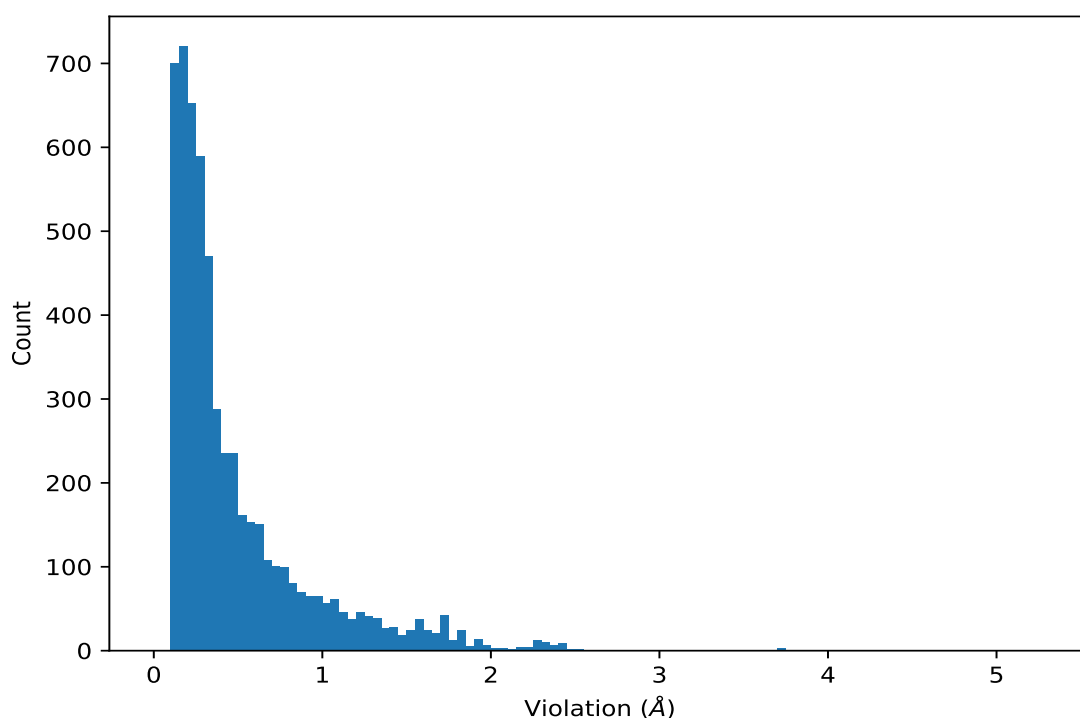
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1125)	1:409:A:LEU:HD12	1:433:A:GLN:HB2	2	0.22	0.1	0.22
(1,2)	1:445:A:GLU:H	1:444:A:ARG:HG2	2	0.22	0.02	0.22
(1,873)	1:425:A:LYS:HA	1:412:A:LEU:HD23	2	0.2	0.09	0.2
(1,1282)	1:446:A:ALA:H	1:444:A:ARG:HG2	2	0.16	0.04	0.16
(1,1282)	1:446:A:ALA:H	1:444:A:ARG:HG3	2	0.16	0.04	0.16
(1,986)	1:410:A:ASN:HB2	1:407:A:PHE:HA	2	0.16	0.02	0.16
(1,986)	1:422:A:ASP:HB3	1:416:A:LEU:HA	2	0.16	0.02	0.16
(1,361)	1:414:A:ARG:H	1:414:A:ARG:HB3	2	0.15	0.0	0.15
(1,737)	1:440:A:LYS:H	1:398:A:ILE:HD13	2	0.15	0.02	0.15
(1,737)	1:440:A:LYS:H	1:398:A:ILE:HD12	2	0.15	0.02	0.15
(1,1008)	1:412:A:LEU:HD13	1:413:A:HIS:HA	2	0.14	0.03	0.14
(1,1008)	1:412:A:LEU:HD12	1:413:A:HIS:HA	2	0.14	0.03	0.14
(1,938)	1:409:A:LEU:HG	1:408:A:LEU:HD13	2	0.14	0.04	0.14
(1,211)	1:430:A:TRP:H	1:427:A:GLU:HA	2	0.12	0.01	0.12
(1,469)	1:394:A:THR:HA	1:396:A:ALA:HB1	2	0.12	0.02	0.12
(1,469)	1:394:A:THR:HA	1:396:A:ALA:HB2	2	0.12	0.02	0.12
(1,469)	1:394:A:THR:HA	1:396:A:ALA:HB3	2	0.12	0.02	0.12
(1,555)	1:395:A:GLN:HE21	1:395:A:GLN:HA	2	0.11	0.0	0.11
(1,805)	1:428:A:ARG:HA	1:428:A:ARG:HD2	2	0.11	0.01	0.11
(1,805)	1:428:A:ARG:HA	1:428:A:ARG:HD3	2	0.11	0.01	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	34	5.28
(1,1142)	1:408:A:LEU:HD11	1:433:A:GLN:HG3	18	5.1
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	43	3.75
(1,1082)	1:408:A:LEU:HD13	1:402:A:ILE:HA	43	3.73
(1,1082)	1:408:A:LEU:HD13	1:402:A:ILE:HA	34	3.71
(1,1082)	1:408:A:LEU:HD11	1:402:A:ILE:HA	18	3.7
(1,1142)	1:408:A:LEU:HD11	1:406:A:GLU:HG3	46	2.5
(1,931)	1:406:A:GLU:HG3	1:398:A:ILE:HG12	48	2.5
(1,1142)	1:408:A:LEU:HD11	1:406:A:GLU:HG3	2	2.45
(1,1142)	1:408:A:LEU:HD11	1:406:A:GLU:HG3	19	2.45
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	12	2.44
(1,1142)	1:408:A:LEU:HD11	1:406:A:GLU:HG3	42	2.44
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	8	2.43
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	10	2.43
(1,1142)	1:408:A:LEU:HD11	1:406:A:GLU:HG3	31	2.43
(1,1142)	1:408:A:LEU:HD12	1:406:A:GLU:HG3	44	2.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1142)	1:408:A:LEU:HD11	1:406:A:GLU:HG3	3	2.41
(1,1132)	1:408:A:LEU:HD11	1:405:A:GLN:HB3	18	2.41
(1,1142)	1:408:A:LEU:HD11	1:406:A:GLU:HG3	14	2.4
(1,931)	1:406:A:GLU:HG3	1:398:A:ILE:HG12	39	2.39
(1,1142)	1:408:A:LEU:HD11	1:406:A:GLU:HG3	1	2.38
(1,1142)	1:408:A:LEU:HD12	1:406:A:GLU:HG3	6	2.38
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD13	19	2.38
(1,1142)	1:408:A:LEU:HD12	1:406:A:GLU:HG3	11	2.37
(1,1142)	1:408:A:LEU:HD11	1:406:A:GLU:HG3	26	2.35
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	36	2.33
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	23	2.32
(1,1142)	1:408:A:LEU:HD11	1:406:A:GLU:HG3	37	2.32
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	48	2.32
(1,1142)	1:408:A:LEU:HD11	1:406:A:GLU:HG3	5	2.31
(1,1142)	1:408:A:LEU:HD11	1:406:A:GLU:HG3	9	2.31
(1,931)	1:406:A:GLU:HG3	1:398:A:ILE:HG12	11	2.31
(1,194)	1:433:A:GLN:H	1:409:A:LEU:HD11	29	2.3
(1,194)	1:433:A:GLN:H	1:409:A:LEU:HD12	29	2.3
(1,194)	1:433:A:GLN:H	1:409:A:LEU:HD13	29	2.3
(1,112)	1:408:A:LEU:HD11	1:409:A:LEU:HB2	34	2.29
(1,112)	1:408:A:LEU:HD12	1:409:A:LEU:HB2	34	2.29
(1,112)	1:408:A:LEU:HD13	1:409:A:LEU:HB2	34	2.29
(1,112)	1:408:A:LEU:HD11	1:409:A:LEU:HB2	18	2.28
(1,112)	1:408:A:LEU:HD12	1:409:A:LEU:HB2	18	2.28
(1,112)	1:408:A:LEU:HD13	1:409:A:LEU:HB2	18	2.28
(1,112)	1:408:A:LEU:HD11	1:409:A:LEU:HB2	43	2.28
(1,112)	1:408:A:LEU:HD12	1:409:A:LEU:HB2	43	2.28
(1,112)	1:408:A:LEU:HD13	1:409:A:LEU:HB2	43	2.28
(1,1142)	1:408:A:LEU:HD12	1:406:A:GLU:HG3	47	2.27
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG21	34	2.27
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	39	2.25
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	17	2.22
(1,931)	1:406:A:GLU:HG3	1:398:A:ILE:HG12	10	2.21
(1,931)	1:406:A:GLU:HG3	1:398:A:ILE:HG12	2	2.2
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG22	23	2.2
(1,931)	1:406:A:GLU:HG3	1:398:A:ILE:HG12	6	2.19
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG21	8	2.18
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG22	47	2.17
(1,931)	1:406:A:GLU:HG3	1:398:A:ILE:HG12	14	2.15
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG12	12	2.14
(1,931)	1:406:A:GLU:HG3	1:398:A:ILE:HG12	35	2.13
(1,1142)	1:408:A:LEU:HD13	1:433:A:GLN:HG3	35	2.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,931)	1:406:A:GLU:HG3	1:398:A:ILE:HG12	18	2.09
(1,931)	1:406:A:GLU:HG3	1:398:A:ILE:HG12	5	2.07
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG23	31	2.02
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG22	5	2.02
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG13	8	2.02
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG23	43	1.99
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG11	2	1.98
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG11	40	1.97
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG23	28	1.96
(1,1162)	1:394:A:THR:HG23	1:393:A:GLU:HB3	6	1.95
(1,920)	1:400:A:GLU:HB2	1:402:A:ILE:HG21	35	1.95
(1,1162)	1:394:A:THR:HG22	1:393:A:GLU:HB3	2	1.94
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD13	8	1.92
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG12	9	1.92
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG11	9	1.91
(1,796)	1:395:A:GLN:HE21	1:439:A:LEU:HD23	23	1.91
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	29	1.91
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	29	1.91
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	29	1.91
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	29	1.91
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	29	1.91
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	29	1.91
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	29	1.91
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	29	1.91
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	29	1.91
(1,1162)	1:394:A:THR:HG21	1:393:A:GLU:HB3	25	1.89
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG22	44	1.89
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG11	10	1.88
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG11	24	1.86
(1,43)	1:417:A:GLN:HA	1:420:A:ILE:HG12	15	1.86
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	35	1.84
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG11	42	1.84
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG22	32	1.84
(1,1162)	1:394:A:THR:HG21	1:395:A:GLN:HB2	22	1.82
(1,1162)	1:394:A:THR:HG22	1:393:A:GLU:HB3	34	1.82
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG12	23	1.82
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG12	25	1.82
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD21	41	1.82
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD22	41	1.82
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD23	41	1.82
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD21	41	1.82
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD22	41	1.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD23	41	1.82
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD21	41	1.82
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD22	41	1.82
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD23	41	1.82
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	41	1.81
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG11	36	1.81
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	34	1.81
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	34	1.81
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	34	1.81
(1,1130)	1:408:A:LEU:HD22	1:405:A:GLN:HG3	32	1.8
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD23	45	1.8
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG12	31	1.8
(1,1063)	1:408:A:LEU:HD13	1:429:A:LEU:HA	43	1.78
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG23	1	1.77
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG21	11	1.77
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG22	17	1.77
(1,1124)	1:429:A:LEU:HD22	1:428:A:ARG:HB2	42	1.76
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	10	1.76
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG21	39	1.76
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD11	21	1.76
(1,1130)	1:408:A:LEU:HD12	1:405:A:GLN:HG3	5	1.75
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG21	50	1.75
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD12	34	1.75
(1,43)	1:417:A:GLN:HA	1:420:A:ILE:HG12	34	1.75
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG22	14	1.74
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD12	12	1.74
(1,1161)	1:441:A:ARG:HG2	1:445:A:GLU:HG2	32	1.73
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	15	1.73
(1,1096)	1:412:A:LEU:HD11	1:425:A:LYS:HE2	30	1.73
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD13	3	1.73
(1,796)	1:395:A:GLN:HE21	1:439:A:LEU:HD23	28	1.73
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD11	39	1.73
(1,1162)	1:394:A:THR:HG23	1:393:A:GLU:HB3	26	1.72
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG21	19	1.72
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG21	15	1.72
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD12	26	1.72
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD21	27	1.72
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD22	27	1.72
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD23	27	1.72
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD21	27	1.72
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD22	27	1.72
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD23	27	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD21	27	1.72
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD22	27	1.72
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD23	27	1.72
(1,43)	1:417:A:GLN:HA	1:420:A:ILE:HG12	48	1.72
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG23	7	1.71
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD11	14	1.71
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	43	1.71
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	43	1.71
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	43	1.71
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD21	35	1.71
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD22	35	1.71
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD23	35	1.71
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD21	35	1.71
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD22	35	1.71
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD23	35	1.71
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD21	35	1.71
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD22	35	1.71
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD23	35	1.71
(1,1162)	1:394:A:THR:HG22	1:393:A:GLU:HB3	11	1.7
(1,1162)	1:394:A:THR:HG23	1:393:A:GLU:HB3	15	1.7
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	16	1.7
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	42	1.7
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG22	49	1.7
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	48	1.7
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	28	1.69
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG23	38	1.69
(1,762)	1:436:A:LEU:H	1:398:A:ILE:HG12	48	1.69
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	1	1.68
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	20	1.68
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG22	13	1.68
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG22	20	1.68
(1,762)	1:436:A:LEU:H	1:398:A:ILE:HG12	20	1.68
(1,1162)	1:394:A:THR:HG23	1:393:A:GLU:HB3	23	1.67
(1,1062)	1:408:A:LEU:HD12	1:411:A:SER:HB2	43	1.67
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG12	21	1.67
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG22	30	1.67
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG23	34	1.67
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG23	42	1.67
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG21	16	1.66
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG21	47	1.66
(1,762)	1:436:A:LEU:H	1:398:A:ILE:HG12	7	1.66
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG23	4	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG21	6	1.65
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG13	12	1.65
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD13	50	1.65
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	29	1.64
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD11	6	1.64
(1,762)	1:436:A:LEU:H	1:398:A:ILE:HG12	18	1.64
(1,1096)	1:412:A:LEU:HD13	1:425:A:LYS:HE2	24	1.63
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD12	31	1.63
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG11	14	1.63
(1,762)	1:436:A:LEU:H	1:398:A:ILE:HG12	30	1.63
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG21	17	1.62
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG11	44	1.62
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG22	46	1.62
(1,920)	1:395:A:GLN:HB3	1:398:A:ILE:HD11	41	1.62
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD11	43	1.62
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	16	1.62
(2,2)	1:415:A:ASP:HB3	1:420:A:ILE:HG13	3	1.61
(1,1162)	1:394:A:THR:HG21	1:393:A:GLU:HB3	40	1.61
(1,1124)	1:429:A:LEU:HD23	1:428:A:ARG:HB2	43	1.61
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG21	18	1.61
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG23	41	1.61
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG11	46	1.61
(1,762)	1:436:A:LEU:H	1:398:A:ILE:HG12	33	1.61
(1,1162)	1:394:A:THR:HG23	1:395:A:GLN:HB2	38	1.6
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG22	27	1.6
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG21	33	1.6
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD13	32	1.6
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG12	16	1.6
(1,1124)	1:429:A:LEU:HD22	1:425:A:LYS:HB2	8	1.59
(1,1096)	1:412:A:LEU:HD11	1:425:A:LYS:HE2	6	1.59
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG12	3	1.59
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG23	48	1.59
(1,762)	1:436:A:LEU:H	1:398:A:ILE:HG12	13	1.59
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG13	19	1.59
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	39	1.59
(1,1130)	1:408:A:LEU:HD12	1:405:A:GLN:HG3	26	1.58
(1,1130)	1:408:A:LEU:HD13	1:405:A:GLN:HG3	44	1.58
(1,1096)	1:402:A:ILE:HG22	1:440:A:LYS:HE3	9	1.58
(1,1006)	1:443:A:LEU:HD21	1:443:A:LEU:HA	35	1.58
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD21	45	1.58
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD22	45	1.58
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD23	45	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD21	45	1.58
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD22	45	1.58
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD23	45	1.58
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD21	45	1.58
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD22	45	1.58
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD23	45	1.58
(1,1130)	1:408:A:LEU:HD13	1:405:A:GLN:HG3	28	1.57
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG11	37	1.57
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG21	37	1.57
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD12	36	1.57
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	13	1.56
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG13	36	1.56
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG12	19	1.56
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG23	22	1.56
(1,796)	1:395:A:GLN:HE21	1:402:A:ILE:HD11	27	1.56
(1,762)	1:436:A:LEU:H	1:398:A:ILE:HG12	41	1.56
(1,1124)	1:429:A:LEU:HD22	1:425:A:LYS:HB2	6	1.55
(1,1124)	1:429:A:LEU:HD22	1:428:A:ARG:HB3	7	1.55
(1,1124)	1:429:A:LEU:HD22	1:425:A:LYS:HB2	12	1.55
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	45	1.55
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	18	1.55
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	18	1.55
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	18	1.55
(1,1130)	1:408:A:LEU:HD22	1:405:A:GLN:HG3	21	1.54
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE3	39	1.54
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG12	26	1.54
(1,920)	1:395:A:GLN:HB3	1:398:A:ILE:HD13	29	1.54
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD12	37	1.54
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	38	1.54
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	34	1.54
(1,1161)	1:441:A:ARG:HG2	1:445:A:GLU:HG2	28	1.53
(1,1124)	1:429:A:LEU:HD23	1:428:A:ARG:HB3	21	1.53
(1,1124)	1:429:A:LEU:HD22	1:428:A:ARG:HB2	23	1.53
(1,1096)	1:402:A:ILE:HG23	1:440:A:LYS:HE3	37	1.53
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG13	26	1.53
(1,793)	1:413:A:HIS:HD2	1:412:A:LEU:HB2	8	1.53
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	7	1.53
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG12	46	1.53
(1,1162)	1:394:A:THR:HG21	1:393:A:GLU:HB3	39	1.52
(1,1096)	1:412:A:LEU:HD11	1:425:A:LYS:HE2	36	1.52
(1,1062)	1:408:A:LEU:HD13	1:411:A:SER:HB2	18	1.52
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	18	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	11	1.51
(2,2)	1:415:A:ASP:HB3	1:420:A:ILE:HG13	23	1.5
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG13	1	1.5
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD13	20	1.5
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD13	29	1.5
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	9	1.5
(1,1124)	1:429:A:LEU:HD22	1:425:A:LYS:HB2	22	1.49
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	11	1.49
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD13	16	1.49
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG12	11	1.49
(1,762)	1:436:A:LEU:H	1:398:A:ILE:HG12	49	1.49
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	26	1.49
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD11	7	1.48
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD12	24	1.48
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	38	1.47
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	49	1.47
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD11	41	1.47
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG13	17	1.47
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	37	1.47
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	3	1.46
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD13	32	1.46
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG21	29	1.46
(1,1124)	1:429:A:LEU:HD22	1:425:A:LYS:HB2	20	1.45
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	19	1.45
(1,1096)	1:402:A:ILE:HG22	1:440:A:LYS:HE3	4	1.44
(1,1096)	1:412:A:LEU:HD13	1:425:A:LYS:HE3	14	1.44
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG21	7	1.44
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD13	15	1.44
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG11	15	1.44
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	12	1.44
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	17	1.44
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	44	1.44
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	47	1.43
(1,793)	1:413:A:HIS:HD2	1:412:A:LEU:HB2	21	1.43
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG12	29	1.43
(1,1113)	1:443:A:LEU:HD13	1:393:A:GLU:HB3	23	1.42
(1,1112)	1:443:A:LEU:HD13	1:393:A:GLU:HB3	23	1.42
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	33	1.42
(1,948)	1:410:A:ASN:HB3	1:408:A:LEU:HD11	5	1.42
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG11	3	1.42
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD22	17	1.41
(1,1130)	1:408:A:LEU:HD12	1:405:A:GLN:HG3	1	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1124)	1:429:A:LEU:HD22	1:425:A:LYS:HB2	30	1.41
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	18	1.41
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG21	5	1.41
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	8	1.41
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	10	1.41
(1,793)	1:413:A:HIS:HD2	1:412:A:LEU:HB2	20	1.4
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	12	1.4
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	2	1.4
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	47	1.4
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	5	1.4
(1,1130)	1:408:A:LEU:HD11	1:405:A:GLN:HG3	23	1.39
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	13	1.39
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	34	1.39
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	11	1.39
(1,931)	1:406:A:GLU:HG3	1:398:A:ILE:HG12	43	1.39
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	6	1.39
(1,1124)	1:429:A:LEU:HD23	1:428:A:ARG:HB3	4	1.38
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG11	27	1.38
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG13	22	1.38
(1,1130)	1:408:A:LEU:HD22	1:405:A:GLN:HG3	31	1.37
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	46	1.37
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	49	1.37
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG12	35	1.37
(1,887)	1:408:A:LEU:HA	1:432:A:VAL:HG13	45	1.37
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD22	29	1.37
(1,793)	1:413:A:HIS:HD2	1:412:A:LEU:HB2	7	1.37
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	46	1.37
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	22	1.36
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	44	1.36
(1,906)	1:404:A:ARG:HG3	1:436:A:LEU:HD22	33	1.36
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	1	1.36
(1,1124)	1:429:A:LEU:HD22	1:425:A:LYS:HB2	11	1.35
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	39	1.35
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	14	1.35
(1,787)	1:405:A:GLN:HE22	1:436:A:LEU:HD23	17	1.35
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	14	1.35
(1,43)	1:417:A:GLN:HA	1:420:A:ILE:HG12	14	1.35
(1,1130)	1:408:A:LEU:HD11	1:405:A:GLN:HG3	36	1.34
(1,1124)	1:429:A:LEU:HD23	1:425:A:LYS:HB2	14	1.34
(1,1124)	1:429:A:LEU:HD21	1:428:A:ARG:HB3	44	1.34
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD22	18	1.34
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD21	22	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:432:A:VAL:HB	1:402:A:ILE:HG13	38	1.34
(1,909)	1:440:A:LYS:HE3	1:436:A:LEU:HD11	19	1.34
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD22	11	1.34
(1,793)	1:413:A:HIS:HD2	1:412:A:LEU:HB2	43	1.34
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG13	21	1.34
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG11	32	1.34
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG13	50	1.34
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	3	1.34
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	31	1.34
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD23	6	1.33
(1,1127)	1:436:A:LEU:HD21	1:405:A:GLN:HG2	40	1.33
(1,1124)	1:429:A:LEU:HD23	1:425:A:LYS:HB2	1	1.33
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	21	1.33
(1,1002)	1:420:A:ILE:HG22	1:416:A:LEU:HA	17	1.33
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD23	39	1.33
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	15	1.33
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	35	1.33
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD23	27	1.32
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD22	48	1.32
(1,1162)	1:394:A:THR:HG22	1:393:A:GLU:HB3	13	1.32
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	40	1.32
(1,1124)	1:429:A:LEU:HD23	1:425:A:LYS:HB2	3	1.32
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	48	1.32
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	19	1.32
(1,947)	1:410:A:ASN:HB3	1:408:A:LEU:HD11	5	1.32
(1,793)	1:413:A:HIS:HD2	1:412:A:LEU:HB2	30	1.32
(1,1124)	1:429:A:LEU:HD22	1:425:A:LYS:HB2	10	1.31
(1,939)	1:413:A:HIS:HB2	1:416:A:LEU:HD11	35	1.31
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	36	1.31
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD11	7	1.3
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD23	34	1.3
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	11	1.3
(1,1096)	1:402:A:ILE:HG23	1:440:A:LYS:HE3	19	1.3
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD13	12	1.3
(1,1162)	1:394:A:THR:HG22	1:393:A:GLU:HB3	8	1.29
(1,1096)	1:412:A:LEU:HD11	1:425:A:LYS:HE2	23	1.29
(1,1002)	1:436:A:LEU:HD11	1:437:A:THR:HB	15	1.29
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	10	1.29
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	13	1.29
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	34	1.29
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD21	17	1.29
(1,811)	1:435:A:ILE:HA	1:434:A:ARG:HB2	6	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	6	1.29
(1,435)	1:405:A:GLN:HE22	1:401:A:GLU:HG2	26	1.29
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	18	1.29
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	11	1.28
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD22	38	1.28
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD22	50	1.28
(1,786)	1:407:A:PHE:HE2	1:403:A:ARG:HB3	32	1.28
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	46	1.28
(1,762)	1:436:A:LEU:H	1:398:A:ILE:HG12	38	1.28
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD13	15	1.27
(1,1124)	1:429:A:LEU:HD22	1:425:A:LYS:HB2	9	1.27
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	46	1.27
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD21	4	1.27
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	4	1.27
(1,811)	1:426:A:GLU:HA	1:428:A:ARG:HB2	23	1.27
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG12	2	1.27
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	5	1.27
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	7	1.26
(1,1162)	1:394:A:THR:HG22	1:393:A:GLU:HB3	12	1.26
(1,1130)	1:408:A:LEU:HD22	1:405:A:GLN:HG3	42	1.26
(1,1002)	1:436:A:LEU:HD13	1:437:A:THR:HB	40	1.26
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	44	1.26
(1,762)	1:436:A:LEU:H	1:398:A:ILE:HG12	4	1.26
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG13	23	1.26
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG12	24	1.26
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD13	29	1.25
(1,1162)	1:394:A:THR:HG23	1:393:A:GLU:HB3	42	1.25
(1,1131)	1:416:A:LEU:HD23	1:425:A:LYS:HD3	23	1.25
(1,1130)	1:408:A:LEU:HD23	1:405:A:GLN:HG3	4	1.25
(1,1130)	1:408:A:LEU:HD22	1:405:A:GLN:HG3	27	1.25
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	39	1.25
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG13	31	1.25
(1,115)	1:398:A:ILE:HG13	1:406:A:GLU:HG3	42	1.25
(1,1142)	1:408:A:LEU:HD12	1:406:A:GLU:HG3	45	1.24
(1,1130)	1:408:A:LEU:HD11	1:405:A:GLN:HG3	17	1.24
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD21	16	1.24
(1,909)	1:440:A:LYS:HE3	1:398:A:ILE:HG22	4	1.24
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD22	39	1.24
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD12	38	1.24
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	5	1.24
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	14	1.24
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD23	42	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1096)	1:420:A:ILE:HG21	1:421:A:LYS:HE2	8	1.23
(1,1002)	1:420:A:ILE:HG23	1:416:A:LEU:HA	39	1.23
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	3	1.23
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD23	49	1.23
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD11	45	1.23
(1,796)	1:395:A:GLN:HE21	1:439:A:LEU:HD22	49	1.23
(1,786)	1:407:A:PHE:HE2	1:403:A:ARG:HB3	5	1.23
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	10	1.23
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG13	25	1.23
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD22	10	1.22
(1,1162)	1:394:A:THR:HG22	1:395:A:GLN:HB3	9	1.22
(1,1142)	1:408:A:LEU:HD12	1:406:A:GLU:HG3	22	1.22
(1,1130)	1:408:A:LEU:HD22	1:405:A:GLN:HG3	37	1.22
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	33	1.22
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	47	1.22
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	19	1.22
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD21	14	1.22
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	28	1.22
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	49	1.22
(1,435)	1:405:A:GLN:HE22	1:401:A:GLU:HG3	17	1.22
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD21	20	1.21
(1,1124)	1:429:A:LEU:HD23	1:425:A:LYS:HB2	13	1.21
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	12	1.21
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	40	1.21
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	25	1.21
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	36	1.21
(1,937)	1:440:A:LYS:HE2	1:398:A:ILE:HD13	34	1.21
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD21	5	1.21
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD21	33	1.21
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	44	1.21
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	16	1.2
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD12	8	1.2
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD21	11	1.2
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	14	1.2
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD11	22	1.2
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG11	8	1.2
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	26	1.2
(1,1002)	1:420:A:ILE:HG21	1:416:A:LEU:HA	38	1.19
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	37	1.19
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	10	1.19
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	21	1.19
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	47	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,793)	1:413:A:HIS:HD2	1:412:A:LEU:HB2	23	1.19
(1,762)	1:436:A:LEU:H	1:398:A:ILE:HG12	47	1.19
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD12	37	1.18
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	7	1.18
(1,1131)	1:416:A:LEU:HD23	1:425:A:LYS:HD2	26	1.18
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	2	1.18
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	46	1.18
(1,786)	1:407:A:PHE:HE2	1:403:A:ARG:HB3	44	1.18
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG12	10	1.18
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD11	5	1.17
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD21	46	1.17
(1,1162)	1:394:A:THR:HG23	1:393:A:GLU:HB3	5	1.17
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	5	1.17
(1,1096)	1:402:A:ILE:HG12	1:440:A:LYS:HE2	43	1.17
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	29	1.17
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	22	1.17
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	19	1.17
(1,1130)	1:408:A:LEU:HD22	1:405:A:GLN:HG3	8	1.16
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	43	1.16
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD23	6	1.16
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD12	10	1.16
(1,793)	1:413:A:HIS:HD2	1:412:A:LEU:HB2	3	1.16
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG12	27	1.16
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	9	1.15
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD23	28	1.15
(1,1142)	1:408:A:LEU:HD12	1:406:A:GLU:HG3	28	1.15
(1,1133)	1:412:A:LEU:HD21	1:409:A:LEU:HG	32	1.15
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	3	1.15
(1,1124)	1:429:A:LEU:HD22	1:425:A:LYS:HB2	32	1.15
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	9	1.15
(1,786)	1:407:A:PHE:HE2	1:403:A:ARG:HB3	26	1.15
(1,115)	1:398:A:ILE:HG13	1:406:A:GLU:HG3	23	1.15
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD21	22	1.14
(1,1162)	1:394:A:THR:HG23	1:393:A:GLU:HB3	33	1.14
(1,1131)	1:416:A:LEU:HD23	1:425:A:LYS:HD2	41	1.14
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	31	1.14
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	26	1.14
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD21	13	1.14
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG22	39	1.14
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD13	3	1.13
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD21	16	1.13
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD21	36	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1131)	1:416:A:LEU:HD22	1:425:A:LYS:HD3	45	1.13
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	14	1.13
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	30	1.13
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	32	1.13
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	3	1.13
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	16	1.13
(1,793)	1:413:A:HIS:HD2	1:412:A:LEU:HB2	42	1.13
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	25	1.13
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	4	1.12
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	30	1.12
(1,1130)	1:408:A:LEU:HD23	1:405:A:GLN:HG3	12	1.12
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	18	1.12
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	31	1.12
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	48	1.12
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	33	1.12
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	47	1.12
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	10	1.12
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	42	1.12
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD12	4	1.12
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HB2	50	1.11
(1,1142)	1:408:A:LEU:HD12	1:406:A:GLU:HG3	38	1.11
(1,1002)	1:420:A:ILE:HG23	1:416:A:LEU:HA	22	1.11
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	17	1.11
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	36	1.11
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD21	38	1.11
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	9	1.11
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD11	2	1.11
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG11	39	1.11
(1,1206)	1:398:A:ILE:H	1:399:A:LYS:HD3	32	1.1
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HB3	33	1.1
(1,1131)	1:416:A:LEU:HD22	1:429:A:LEU:HG	37	1.1
(1,1068)	1:404:A:ARG:HG3	1:405:A:GLN:HA	14	1.1
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	35	1.1
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	6	1.1
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB3	42	1.1
(1,43)	1:417:A:GLN:HA	1:420:A:ILE:HG12	40	1.1
(1,1131)	1:416:A:LEU:HD21	1:425:A:LYS:HD2	33	1.09
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	37	1.09
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD21	7	1.09
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB2	44	1.09
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD23	1	1.08
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD11	2	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD23	13	1.08
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD13	30	1.08
(1,1206)	1:398:A:ILE:H	1:399:A:LYS:HD3	18	1.08
(1,1142)	1:408:A:LEU:HD12	1:406:A:GLU:HG3	27	1.08
(1,1142)	1:408:A:LEU:HD11	1:406:A:GLU:HG3	29	1.08
(1,1130)	1:408:A:LEU:HD22	1:405:A:GLN:HG3	45	1.08
(1,1113)	1:443:A:LEU:HD13	1:393:A:GLU:HB3	21	1.08
(1,1112)	1:443:A:LEU:HD13	1:393:A:GLU:HB3	21	1.08
(1,1002)	1:420:A:ILE:HG22	1:416:A:LEU:HA	16	1.08
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	1	1.08
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	13	1.08
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB2	39	1.08
(1,762)	1:436:A:LEU:H	1:398:A:ILE:HG12	34	1.08
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD21	18	1.07
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD23	41	1.07
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD21	43	1.07
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HG	21	1.07
(1,1142)	1:408:A:LEU:HD12	1:406:A:GLU:HG3	24	1.07
(1,1142)	1:408:A:LEU:HD11	1:406:A:GLU:HG3	33	1.07
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	49	1.07
(1,1131)	1:416:A:LEU:HD21	1:425:A:LYS:HD3	50	1.07
(1,1128)	1:408:A:LEU:HD12	1:432:A:VAL:HB	40	1.07
(1,1096)	1:402:A:ILE:HG21	1:440:A:LYS:HE3	44	1.07
(1,1002)	1:420:A:ILE:HG23	1:416:A:LEU:HA	34	1.07
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	40	1.07
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	29	1.07
(1,909)	1:440:A:LYS:HE3	1:436:A:LEU:HD12	8	1.07
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	24	1.07
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	24	1.07
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	24	1.07
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	48	1.06
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD22	33	1.06
(1,1162)	1:394:A:THR:HG21	1:395:A:GLN:HB3	10	1.06
(1,1142)	1:408:A:LEU:HD12	1:406:A:GLU:HG3	15	1.06
(1,1142)	1:408:A:LEU:HD12	1:406:A:GLU:HG3	21	1.06
(1,1096)	1:402:A:ILE:HG12	1:440:A:LYS:HE2	48	1.06
(1,1002)	1:420:A:ILE:HG23	1:416:A:LEU:HA	6	1.06
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	43	1.06
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD22	4	1.06
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	48	1.06
(1,783)	1:407:A:PHE:HD1	1:404:A:ARG:HG3	26	1.06
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	17	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	17	1.06
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	17	1.06
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HB3	19	1.05
(1,1162)	1:394:A:THR:HG21	1:395:A:GLN:HB3	46	1.05
(1,1137)	1:398:A:ILE:HD11	1:401:A:GLU:HB2	4	1.05
(1,1131)	1:416:A:LEU:HD22	1:425:A:LYS:HD2	40	1.05
(1,1002)	1:420:A:ILE:HG23	1:416:A:LEU:HA	9	1.05
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	24	1.05
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	9	1.05
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD13	21	1.05
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	12	1.05
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	16	1.05
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG11	6	1.05
(1,1143)	1:398:A:ILE:HG23	1:399:A:LYS:HE3	5	1.04
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	32	1.04
(1,1137)	1:398:A:ILE:HD11	1:401:A:GLU:HB2	49	1.04
(1,1096)	1:412:A:LEU:HD11	1:425:A:LYS:HE3	34	1.04
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	1	1.04
(1,1002)	1:420:A:ILE:HG23	1:416:A:LEU:HA	12	1.04
(1,1002)	1:420:A:ILE:HG23	1:421:A:LYS:HA	48	1.04
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	2	1.04
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	26	1.04
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG21	4	1.04
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG21	35	1.04
(1,786)	1:407:A:PHE:HE2	1:403:A:ARG:HB3	28	1.04
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	44	1.04
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD11	21	1.03
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD23	32	1.03
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD13	50	1.03
(1,1206)	1:398:A:ILE:H	1:399:A:LYS:HD3	13	1.03
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	16	1.03
(1,1128)	1:408:A:LEU:HD12	1:432:A:VAL:HB	28	1.03
(1,1002)	1:420:A:ILE:HG22	1:421:A:LYS:HA	32	1.03
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	8	1.03
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	14	1.03
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	30	1.03
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	32	1.03
(1,814)	1:397:A:GLY:HA2	1:401:A:GLU:HG3	32	1.03
(1,796)	1:395:A:GLN:HE21	1:439:A:LEU:HD22	42	1.03
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB2	23	1.03
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB2	26	1.03
(1,1162)	1:394:A:THR:HG22	1:395:A:GLN:HB2	14	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	37	1.02
(1,1002)	1:420:A:ILE:HG23	1:416:A:LEU:HA	49	1.02
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	7	1.02
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	31	1.02
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	48	1.02
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD23	20	1.02
(1,909)	1:440:A:LYS:HE3	1:436:A:LEU:HD12	37	1.02
(1,1142)	1:408:A:LEU:HD11	1:406:A:GLU:HG3	13	1.01
(1,1142)	1:408:A:LEU:HD12	1:406:A:GLU:HG3	40	1.01
(1,1131)	1:416:A:LEU:HD23	1:425:A:LYS:HD2	5	1.01
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	50	1.01
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	17	1.01
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD11	14	1.01
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG22	23	1.01
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	39	1.01
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB1	2	1.01
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD23	12	1.0
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HB2	11	1.0
(1,1142)	1:408:A:LEU:HD12	1:406:A:GLU:HG3	4	1.0
(1,1131)	1:416:A:LEU:HD21	1:425:A:LYS:HD2	46	1.0
(1,1002)	1:436:A:LEU:HD13	1:437:A:THR:HB	43	1.0
(1,1002)	1:420:A:ILE:HG23	1:421:A:LYS:HA	46	1.0
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	22	1.0
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD13	13	1.0
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD22	49	1.0
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	47	1.0
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	32	1.0
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB2	9	1.0
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	19	0.99
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD23	9	0.99
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD21	24	0.99
(1,1131)	1:416:A:LEU:HD22	1:425:A:LYS:HD3	49	0.99
(1,1113)	1:409:A:LEU:HD13	1:433:A:GLN:HB3	17	0.99
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	47	0.99
(1,1002)	1:420:A:ILE:HG22	1:416:A:LEU:HA	1	0.99
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG22	16	0.99
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	20	0.99
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	8	0.99
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	43	0.99
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB3	39	0.99
(1,435)	1:405:A:GLN:HE22	1:401:A:GLU:HG2	44	0.99
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD21	4	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD23	49	0.98
(1,1162)	1:394:A:THR:HG23	1:395:A:GLN:HB2	31	0.98
(1,1142)	1:408:A:LEU:HD11	1:406:A:GLU:HG3	20	0.98
(1,1142)	1:408:A:LEU:HD12	1:406:A:GLU:HG3	25	0.98
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	12	0.98
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	28	0.98
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	1	0.98
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	13	0.98
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	44	0.98
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	13	0.98
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB1	49	0.98
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD21	44	0.97
(1,1082)	1:408:A:LEU:HD11	1:402:A:ILE:HA	13	0.97
(1,1082)	1:408:A:LEU:HD11	1:402:A:ILE:HA	41	0.97
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	23	0.97
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	40	0.97
(1,909)	1:425:A:LYS:HE2	1:412:A:LEU:HD11	17	0.97
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD11	1	0.97
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD21	11	0.97
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	38	0.97
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	28	0.97
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG12	5	0.97
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	17	0.96
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HG	7	0.96
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	50	0.96
(1,1128)	1:408:A:LEU:HD12	1:432:A:VAL:HB	44	0.96
(1,1082)	1:408:A:LEU:HD11	1:402:A:ILE:HA	48	0.96
(1,1002)	1:420:A:ILE:HG23	1:421:A:LYS:HA	2	0.96
(1,1002)	1:420:A:ILE:HG22	1:416:A:LEU:HA	31	0.96
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	41	0.96
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG21	41	0.96
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD22	43	0.96
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	37	0.96
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG13	35	0.96
(1,435)	1:405:A:GLN:HE22	1:401:A:GLU:HG2	28	0.96
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	18	0.95
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	35	0.95
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD23	19	0.95
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD23	31	0.95
(1,1131)	1:416:A:LEU:HD21	1:429:A:LEU:HG	27	0.95
(1,1131)	1:416:A:LEU:HD22	1:425:A:LYS:HD3	34	0.95
(1,1082)	1:408:A:LEU:HD11	1:402:A:ILE:HA	29	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	32	0.95
(1,1002)	1:420:A:ILE:HG23	1:416:A:LEU:HA	19	0.95
(1,1002)	1:420:A:ILE:HG21	1:416:A:LEU:HA	37	0.95
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	15	0.95
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	24	0.95
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD13	4	0.95
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	9	0.95
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	11	0.95
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG11	45	0.95
(1,1131)	1:416:A:LEU:HD23	1:425:A:LYS:HD3	18	0.94
(1,1131)	1:416:A:LEU:HD22	1:425:A:LYS:HD3	19	0.94
(1,1130)	1:408:A:LEU:HD23	1:405:A:GLN:HG3	25	0.94
(1,1082)	1:408:A:LEU:HD13	1:402:A:ILE:HA	47	0.94
(1,1002)	1:420:A:ILE:HG21	1:416:A:LEU:HA	13	0.94
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	25	0.94
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	2	0.94
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG22	15	0.94
(1,921)	1:425:A:LYS:HD2	1:416:A:LEU:HD23	41	0.94
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG21	28	0.94
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG23	47	0.94
(1,544)	1:444:A:ARG:H	1:395:A:GLN:HE21	7	0.94
(1,1206)	1:398:A:ILE:H	1:399:A:LYS:HD3	1	0.93
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HB3	4	0.93
(1,1162)	1:394:A:THR:HG23	1:393:A:GLU:HB3	43	0.93
(1,1082)	1:408:A:LEU:HD13	1:402:A:ILE:HA	7	0.93
(1,1033)	1:402:A:ILE:HG21	1:400:A:GLU:HA	28	0.93
(1,1002)	1:420:A:ILE:HG21	1:416:A:LEU:HA	11	0.93
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	8	0.93
(1,921)	1:425:A:LYS:HD3	1:416:A:LEU:HD22	45	0.93
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	35	0.93
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD11	14	0.92
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD22	47	0.92
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HB2	16	0.92
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HB2	48	0.92
(1,1131)	1:416:A:LEU:HD23	1:425:A:LYS:HD3	8	0.92
(1,1130)	1:408:A:LEU:HD22	1:405:A:GLN:HG3	9	0.92
(1,1113)	1:409:A:LEU:HD11	1:433:A:GLN:HB3	19	0.92
(1,1113)	1:409:A:LEU:HD13	1:433:A:GLN:HB3	31	0.92
(1,1112)	1:409:A:LEU:HD11	1:433:A:GLN:HB3	19	0.92
(1,1112)	1:409:A:LEU:HD13	1:433:A:GLN:HB3	31	0.92
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	45	0.92
(1,1082)	1:408:A:LEU:HD11	1:402:A:ILE:HA	17	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	27	0.92
(1,1082)	1:408:A:LEU:HD11	1:402:A:ILE:HA	39	0.92
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	11	0.92
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	7	0.92
(1,909)	1:440:A:LYS:HE3	1:436:A:LEU:HD11	39	0.92
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD11	14	0.92
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	32	0.92
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	43	0.92
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	22	0.92
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	32	0.92
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	32	0.92
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	32	0.92
(1,1131)	1:416:A:LEU:HD23	1:425:A:LYS:HD2	29	0.91
(1,1127)	1:409:A:LEU:HD21	1:410:A:ASN:HB2	20	0.91
(1,1082)	1:408:A:LEU:HD13	1:402:A:ILE:HA	4	0.91
(1,1002)	1:420:A:ILE:HG22	1:416:A:LEU:HA	4	0.91
(1,1002)	1:420:A:ILE:HG23	1:416:A:LEU:HA	18	0.91
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	50	0.91
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD21	37	0.91
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	41	0.91
(2,2)	1:415:A:ASP:HB3	1:420:A:ILE:HG13	40	0.9
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HB3	34	0.9
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HG	42	0.9
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	22	0.9
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	22	0.9
(1,923)	1:441:A:ARG:HD2	1:437:A:THR:HG23	45	0.9
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD12	6	0.9
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	41	0.9
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	22	0.9
(1,786)	1:405:A:GLN:HE22	1:402:A:ILE:HB	49	0.9
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB2	31	0.9
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB1	38	0.9
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HG	5	0.89
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	2	0.89
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	21	0.89
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	23	0.89
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	9	0.89
(1,1082)	1:408:A:LEU:HD13	1:402:A:ILE:HA	21	0.89
(1,1082)	1:408:A:LEU:HD11	1:402:A:ILE:HA	23	0.89
(1,1082)	1:408:A:LEU:HD11	1:402:A:ILE:HA	33	0.89
(1,1082)	1:408:A:LEU:HD13	1:402:A:ILE:HA	45	0.89
(1,1082)	1:408:A:LEU:HD13	1:402:A:ILE:HA	49	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	6	0.89
(1,937)	1:440:A:LYS:HE2	1:398:A:ILE:HD13	11	0.89
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG22	7	0.89
(1,923)	1:441:A:ARG:HD3	1:437:A:THR:HG22	29	0.89
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD13	15	0.89
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG23	50	0.89
(1,797)	1:395:A:GLN:HE21	1:398:A:ILE:HG23	7	0.89
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB3	29	0.89
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD22	23	0.88
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	15	0.88
(1,1082)	1:408:A:LEU:HD11	1:402:A:ILE:HA	16	0.88
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	38	0.88
(1,1002)	1:420:A:ILE:HG22	1:416:A:LEU:HA	41	0.88
(1,1002)	1:420:A:ILE:HG22	1:416:A:LEU:HA	50	0.88
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	12	0.88
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	28	0.88
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG21	38	0.88
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	47	0.88
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	30	0.88
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	46	0.88
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	8	0.87
(2,4)	1:408:A:LEU:HD11	1:406:A:GLU:HA	34	0.87
(2,4)	1:408:A:LEU:HD12	1:406:A:GLU:HA	34	0.87
(2,4)	1:408:A:LEU:HD13	1:406:A:GLU:HA	34	0.87
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD11	45	0.87
(1,1124)	1:429:A:LEU:HD23	1:425:A:LYS:HB2	33	0.87
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	25	0.87
(1,1002)	1:420:A:ILE:HG23	1:416:A:LEU:HA	27	0.87
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	23	0.87
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD13	29	0.87
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG23	13	0.87
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG23	31	0.87
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	14	0.87
(1,517)	1:416:A:LEU:HG	1:415:A:ASP:HB2	42	0.87
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD13	25	0.86
(1,1213)	1:431:A:GLU:H	1:434:A:ARG:HB3	9	0.86
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HB2	20	0.86
(1,1142)	1:408:A:LEU:HD13	1:406:A:GLU:HG3	41	0.86
(1,1137)	1:398:A:ILE:HD11	1:401:A:GLU:HB2	16	0.86
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	25	0.86
(1,1082)	1:408:A:LEU:HD11	1:402:A:ILE:HA	35	0.86
(1,1082)	1:408:A:LEU:HD13	1:402:A:ILE:HA	50	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:420:A:ILE:HG23	1:416:A:LEU:HA	7	0.86
(1,1002)	1:420:A:ILE:HG22	1:416:A:LEU:HA	44	0.86
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	41	0.86
(1,937)	1:440:A:LYS:HE2	1:398:A:ILE:HD12	17	0.86
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD11	36	0.86
(1,1162)	1:394:A:THR:HG22	1:393:A:GLU:HB3	36	0.85
(1,1137)	1:398:A:ILE:HD12	1:401:A:GLU:HB2	20	0.85
(1,1137)	1:398:A:ILE:HD12	1:401:A:GLU:HB2	30	0.85
(1,1113)	1:409:A:LEU:HD11	1:433:A:GLN:HB3	8	0.85
(1,1112)	1:409:A:LEU:HD11	1:433:A:GLN:HB3	8	0.85
(1,1082)	1:408:A:LEU:HD13	1:402:A:ILE:HA	6	0.85
(1,1082)	1:408:A:LEU:HD11	1:402:A:ILE:HA	20	0.85
(1,1082)	1:408:A:LEU:HD11	1:402:A:ILE:HA	36	0.85
(1,1002)	1:420:A:ILE:HG22	1:421:A:LYS:HA	5	0.85
(1,1002)	1:420:A:ILE:HG22	1:416:A:LEU:HA	30	0.85
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	15	0.85
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	17	0.85
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	45	0.85
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	39	0.84
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	40	0.84
(1,1206)	1:398:A:ILE:H	1:399:A:LYS:HD2	35	0.84
(1,1143)	1:398:A:ILE:HG22	1:399:A:LYS:HE3	49	0.84
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	27	0.84
(1,1095)	1:436:A:LEU:HD11	1:440:A:LYS:HE3	19	0.84
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	1	0.84
(1,1082)	1:408:A:LEU:HD13	1:402:A:ILE:HA	32	0.84
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	37	0.84
(1,1002)	1:420:A:ILE:HG22	1:416:A:LEU:HA	36	0.84
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	25	0.84
(1,937)	1:425:A:LYS:HE3	1:412:A:LEU:HD23	35	0.84
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG23	36	0.84
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	1	0.84
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	44	0.84
(1,781)	1:413:A:HIS:HD2	1:412:A:LEU:HA	16	0.84
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB1	18	0.84
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB1	46	0.84
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	16	0.84
(1,1206)	1:398:A:ILE:H	1:399:A:LYS:HD3	31	0.83
(1,1137)	1:398:A:ILE:HD12	1:401:A:GLU:HB2	33	0.83
(1,1122)	1:416:A:LEU:HD11	1:426:A:GLU:HG2	44	0.83
(1,1082)	1:408:A:LEU:HD11	1:402:A:ILE:HA	8	0.83
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	14	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	19	0.83
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	26	0.83
(1,1082)	1:408:A:LEU:HD13	1:402:A:ILE:HA	30	0.83
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG22	3	0.83
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	38	0.83
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB1	37	0.83
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	43	0.83
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	46	0.83
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	46	0.83
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	46	0.83
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	13	0.82
(2,4)	1:408:A:LEU:HD11	1:406:A:GLU:HA	18	0.82
(2,4)	1:408:A:LEU:HD12	1:406:A:GLU:HA	18	0.82
(2,4)	1:408:A:LEU:HD13	1:406:A:GLU:HA	18	0.82
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	34	0.82
(1,1130)	1:408:A:LEU:HD23	1:405:A:GLN:HG3	43	0.82
(1,1128)	1:408:A:LEU:HD13	1:432:A:VAL:HB	36	0.82
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	25	0.82
(1,1082)	1:408:A:LEU:HD11	1:402:A:ILE:HA	12	0.82
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	31	0.82
(1,1002)	1:420:A:ILE:HG22	1:416:A:LEU:HA	8	0.82
(1,1002)	1:420:A:ILE:HG23	1:416:A:LEU:HA	21	0.82
(1,1002)	1:420:A:ILE:HG21	1:416:A:LEU:HA	35	0.82
(1,1002)	1:420:A:ILE:HG23	1:416:A:LEU:HA	42	0.82
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	30	0.82
(1,796)	1:395:A:GLN:HE21	1:439:A:LEU:HD21	47	0.82
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	26	0.81
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	36	0.81
(1,1082)	1:408:A:LEU:HD13	1:402:A:ILE:HA	11	0.81
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD11	10	0.81
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG13	12	0.81
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD12	25	0.81
(1,868)	1:416:A:LEU:HA	1:416:A:LEU:HD11	15	0.81
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	35	0.81
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	48	0.81
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB2	16	0.81
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB2	27	0.81
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	21	0.81
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	21	0.81
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	21	0.81
(1,117)	1:398:A:ILE:HG12	1:399:A:LYS:HE3	5	0.81
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD23	26	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:443:A:LEU:H	1:398:A:ILE:HD11	40	0.8
(1,1137)	1:398:A:ILE:HD12	1:401:A:GLU:HB2	15	0.8
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	18	0.8
(1,1128)	1:408:A:LEU:HD11	1:432:A:VAL:HB	42	0.8
(1,1096)	1:412:A:LEU:HD11	1:425:A:LYS:HE2	28	0.8
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	3	0.8
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	5	0.8
(1,1082)	1:408:A:LEU:HD11	1:402:A:ILE:HA	10	0.8
(1,1082)	1:408:A:LEU:HD13	1:402:A:ILE:HA	28	0.8
(1,1082)	1:408:A:LEU:HD13	1:402:A:ILE:HA	40	0.8
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	42	0.8
(1,1002)	1:420:A:ILE:HG23	1:416:A:LEU:HA	26	0.8
(1,929)	1:425:A:LYS:HD2	1:416:A:LEU:HD22	27	0.8
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG22	42	0.8
(1,781)	1:413:A:HIS:HD2	1:412:A:LEU:HA	18	0.8
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD21	39	0.79
(1,1157)	1:396:A:ALA:HB3	1:400:A:GLU:HB2	39	0.79
(1,1137)	1:398:A:ILE:HD11	1:401:A:GLU:HB2	35	0.79
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	9	0.79
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	2	0.79
(1,1082)	1:408:A:LEU:HD13	1:402:A:ILE:HA	44	0.79
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	46	0.79
(1,961)	1:406:A:GLU:HG3	1:402:A:ILE:HB	2	0.79
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	6	0.79
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD12	48	0.79
(1,923)	1:441:A:ARG:HD3	1:437:A:THR:HG21	27	0.79
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	33	0.79
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB2	38	0.79
(1,783)	1:407:A:PHE:HD1	1:404:A:ARG:HG3	18	0.79
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB1	6	0.79
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	17	0.79
(1,119)	1:408:A:LEU:HD11	1:409:A:LEU:HG	34	0.79
(1,119)	1:408:A:LEU:HD12	1:409:A:LEU:HG	34	0.79
(1,119)	1:408:A:LEU:HD13	1:409:A:LEU:HG	34	0.79
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	1	0.78
(1,1213)	1:431:A:GLU:H	1:434:A:ARG:HB3	25	0.78
(1,1157)	1:396:A:ALA:HB3	1:400:A:GLU:HB2	17	0.78
(1,1137)	1:398:A:ILE:HD11	1:401:A:GLU:HB2	34	0.78
(1,1082)	1:408:A:LEU:HD12	1:402:A:ILE:HA	24	0.78
(1,967)	1:415:A:ASP:HB2	1:416:A:LEU:HG	18	0.78
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG21	45	0.78
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	25	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	7	0.78
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	46	0.78
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB3	6	0.78
(1,781)	1:413:A:HIS:HD2	1:412:A:LEU:HA	11	0.78
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG13	43	0.78
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB1	8	0.78
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB2	13	0.78
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB2	47	0.78
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	34	0.78
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	2	0.78
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	2	0.78
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	2	0.78
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	23	0.77
(1,1222)	1:443:A:LEU:H	1:439:A:LEU:HD22	35	0.77
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	27	0.77
(1,1137)	1:398:A:ILE:HD13	1:401:A:GLU:HB2	14	0.77
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	31	0.77
(1,1002)	1:420:A:ILE:HG21	1:421:A:LYS:HA	14	0.77
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	7	0.77
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	3	0.77
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	5	0.77
(1,781)	1:413:A:HIS:HD2	1:412:A:LEU:HA	25	0.77
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB2	11	0.77
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB1	35	0.77
(1,192)	1:400:A:GLU:H	1:400:A:GLU:HB3	46	0.77
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	19	0.76
(1,1124)	1:429:A:LEU:HD23	1:425:A:LYS:HB2	15	0.76
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	38	0.76
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	50	0.76
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	27	0.76
(1,1033)	1:402:A:ILE:HG22	1:400:A:GLU:HA	27	0.76
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG22	50	0.76
(1,923)	1:441:A:ARG:HD3	1:437:A:THR:HG21	25	0.76
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD21	31	0.76
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD22	32	0.76
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD22	45	0.76
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD13	33	0.76
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	1	0.76
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	50	0.76
(1,781)	1:413:A:HIS:HD2	1:412:A:LEU:HA	48	0.76
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB3	10	0.76
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB1	24	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	7	0.76
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	23	0.76
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	23	0.76
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	23	0.76
(1,192)	1:400:A:GLU:H	1:400:A:GLU:HB3	4	0.76
(1,192)	1:400:A:GLU:H	1:400:A:GLU:HB3	27	0.76
(1,192)	1:400:A:GLU:H	1:400:A:GLU:HB3	28	0.76
(1,192)	1:400:A:GLU:H	1:400:A:GLU:HB3	30	0.76
(1,192)	1:400:A:GLU:H	1:400:A:GLU:HB3	50	0.76
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	30	0.75
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HG	2	0.75
(1,1137)	1:398:A:ILE:HD11	1:401:A:GLU:HB2	38	0.75
(1,1137)	1:398:A:ILE:HD12	1:401:A:GLU:HB2	47	0.75
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	13	0.75
(1,1113)	1:409:A:LEU:HD11	1:433:A:GLN:HB3	2	0.75
(1,1112)	1:409:A:LEU:HD11	1:433:A:GLN:HB3	2	0.75
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	36	0.75
(1,1002)	1:420:A:ILE:HG22	1:416:A:LEU:HA	29	0.75
(1,1002)	1:420:A:ILE:HG22	1:416:A:LEU:HA	45	0.75
(1,1002)	1:420:A:ILE:HG21	1:416:A:LEU:HA	47	0.75
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD12	20	0.75
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG22	29	0.75
(1,921)	1:429:A:LEU:HG	1:416:A:LEU:HD21	27	0.75
(1,856)	1:429:A:LEU:HA	1:429:A:LEU:HG	29	0.75
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	19	0.75
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	25	0.75
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	26	0.75
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	10	0.75
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB1	25	0.75
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	3	0.75
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	2	0.74
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	37	0.74
(1,1196)	1:402:A:ILE:HD13	1:440:A:LYS:HG2	28	0.74
(1,1162)	1:394:A:THR:HG21	1:395:A:GLN:HB3	30	0.74
(1,1133)	1:412:A:LEU:HD22	1:429:A:LEU:HG	25	0.74
(1,1131)	1:416:A:LEU:HD22	1:425:A:LYS:HD3	4	0.74
(1,1131)	1:416:A:LEU:HD22	1:425:A:LYS:HD3	30	0.74
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	26	0.74
(1,1095)	1:398:A:ILE:HG22	1:440:A:LYS:HE3	4	0.74
(1,1033)	1:402:A:ILE:HG22	1:400:A:GLU:HA	5	0.74
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	21	0.74
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG21	22	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,923)	1:441:A:ARG:HD2	1:437:A:THR:HG22	35	0.74
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	1	0.74
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB2	33	0.74
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	35	0.74
(1,192)	1:400:A:GLU:H	1:400:A:GLU:HB3	14	0.74
(1,192)	1:400:A:GLU:H	1:400:A:GLU:HB3	17	0.74
(1,192)	1:400:A:GLU:H	1:400:A:GLU:HB3	21	0.74
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	28	0.73
(1,1196)	1:398:A:ILE:HD11	1:440:A:LYS:HG2	19	0.73
(1,1162)	1:394:A:THR:HG21	1:395:A:GLN:HB3	16	0.73
(1,1162)	1:394:A:THR:HG21	1:395:A:GLN:HB2	17	0.73
(1,1137)	1:398:A:ILE:HD13	1:401:A:GLU:HB2	22	0.73
(1,1137)	1:398:A:ILE:HD12	1:401:A:GLU:HB2	50	0.73
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	27	0.73
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG22	17	0.73
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	18	0.73
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	8	0.73
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	19	0.73
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	19	0.73
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	19	0.73
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	42	0.72
(1,1131)	1:416:A:LEU:HD23	1:425:A:LYS:HD3	2	0.72
(1,1128)	1:408:A:LEU:HD11	1:432:A:VAL:HB	1	0.72
(1,1128)	1:408:A:LEU:HD11	1:432:A:VAL:HB	3	0.72
(1,1128)	1:408:A:LEU:HD22	1:405:A:GLN:HG3	9	0.72
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	7	0.72
(1,1033)	1:402:A:ILE:HG21	1:400:A:GLU:HA	9	0.72
(1,1033)	1:402:A:ILE:HG22	1:400:A:GLU:HA	39	0.72
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG23	30	0.72
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD22	4	0.72
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	34	0.72
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD12	35	0.72
(1,781)	1:413:A:HIS:HD2	1:412:A:LEU:HA	12	0.72
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	38	0.72
(1,192)	1:400:A:GLU:H	1:400:A:GLU:HB3	49	0.72
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	4	0.71
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	32	0.71
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	44	0.71
(1,1131)	1:416:A:LEU:HD23	1:425:A:LYS:HD3	16	0.71
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	12	0.71
(1,1063)	1:408:A:LEU:HD11	1:429:A:LEU:HA	18	0.71
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	8	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:436:A:LEU:HD12	1:437:A:THR:HB	20	0.71
(1,921)	1:425:A:LYS:HD2	1:416:A:LEU:HD23	29	0.71
(1,907)	1:405:A:GLN:HG3	1:408:A:LEU:HD12	1	0.71
(1,781)	1:413:A:HIS:HD2	1:412:A:LEU:HA	38	0.71
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB3	41	0.71
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	10	0.71
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	13	0.71
(1,517)	1:416:A:LEU:HG	1:415:A:ASP:HB2	40	0.71
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	8	0.71
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	8	0.71
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	8	0.71
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	33	0.71
(1,83)	1:408:A:LEU:HD11	1:412:A:LEU:HD21	27	0.71
(1,83)	1:408:A:LEU:HD11	1:412:A:LEU:HD22	27	0.71
(1,83)	1:408:A:LEU:HD11	1:412:A:LEU:HD23	27	0.71
(1,83)	1:408:A:LEU:HD12	1:412:A:LEU:HD21	27	0.71
(1,83)	1:408:A:LEU:HD12	1:412:A:LEU:HD22	27	0.71
(1,83)	1:408:A:LEU:HD12	1:412:A:LEU:HD23	27	0.71
(1,83)	1:408:A:LEU:HD13	1:412:A:LEU:HD21	27	0.71
(1,83)	1:408:A:LEU:HD13	1:412:A:LEU:HD22	27	0.71
(1,83)	1:408:A:LEU:HD13	1:412:A:LEU:HD23	27	0.71
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	25	0.7
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	8	0.7
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	12	0.7
(1,1206)	1:398:A:ILE:H	1:399:A:LYS:HD3	39	0.7
(1,1162)	1:394:A:THR:HG21	1:395:A:GLN:HB2	7	0.7
(1,1137)	1:398:A:ILE:HD11	1:401:A:GLU:HB2	11	0.7
(1,1137)	1:398:A:ILE:HD13	1:401:A:GLU:HB2	43	0.7
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	16	0.7
(1,1128)	1:408:A:LEU:HD11	1:432:A:VAL:HB	37	0.7
(1,1122)	1:436:A:LEU:HD11	1:433:A:GLN:HG2	37	0.7
(1,1002)	1:420:A:ILE:HG23	1:416:A:LEU:HA	33	0.7
(1,961)	1:406:A:GLU:HG3	1:402:A:ILE:HB	39	0.7
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	4	0.7
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD12	46	0.7
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	20	0.7
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG22	5	0.7
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	8	0.7
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	41	0.7
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	7	0.7
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB2	1	0.7
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB1	40	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,544)	1:444:A:ARG:H	1:395:A:GLN:HE21	35	0.7
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	50	0.7
(1,119)	1:408:A:LEU:HD11	1:409:A:LEU:HG	43	0.7
(1,119)	1:408:A:LEU:HD12	1:409:A:LEU:HG	43	0.7
(1,119)	1:408:A:LEU:HD13	1:409:A:LEU:HG	43	0.7
(1,1137)	1:398:A:ILE:HD13	1:401:A:GLU:HB2	7	0.69
(1,1137)	1:398:A:ILE:HD12	1:401:A:GLU:HB2	29	0.69
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	40	0.69
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	1	0.69
(1,1033)	1:416:A:LEU:HD22	1:413:A:HIS:HA	13	0.69
(1,1002)	1:420:A:ILE:HG23	1:416:A:LEU:HA	10	0.69
(1,961)	1:406:A:GLU:HG3	1:402:A:ILE:HB	31	0.69
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD13	18	0.69
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD11	42	0.69
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG23	30	0.69
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	18	0.69
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD22	34	0.69
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	12	0.69
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	16	0.69
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	50	0.69
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	29	0.69
(1,783)	1:407:A:PHE:HD1	1:404:A:ARG:HG3	33	0.69
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	34	0.69
(1,781)	1:413:A:HIS:HD2	1:412:A:LEU:HA	47	0.69
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD11	9	0.69
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD12	9	0.69
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD13	9	0.69
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD11	9	0.69
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD12	9	0.69
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD13	9	0.69
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD11	9	0.69
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD12	9	0.69
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD13	9	0.69
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	37	0.68
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HB2	37	0.68
(1,1132)	1:408:A:LEU:HD23	1:404:A:ARG:HB3	34	0.68
(1,1132)	1:408:A:LEU:HD22	1:404:A:ARG:HB3	43	0.68
(1,1127)	1:436:A:LEU:HD21	1:405:A:GLN:HG2	23	0.68
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD11	24	0.68
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	10	0.68
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD22	19	0.68
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB2	24	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,781)	1:413:A:HIS:HD2	1:412:A:LEU:HA	4	0.68
(1,781)	1:413:A:HIS:HD2	1:412:A:LEU:HA	40	0.68
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB2	34	0.68
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	12	0.68
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	31	0.68
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	31	0.68
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	31	0.68
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	30	0.68
(1,435)	1:405:A:GLN:HE22	1:401:A:GLU:HG2	5	0.68
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	3	0.67
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	7	0.67
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	16	0.67
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	48	0.67
(1,1206)	1:398:A:ILE:H	1:399:A:LYS:HD3	41	0.67
(1,1162)	1:394:A:THR:HG23	1:395:A:GLN:HB2	20	0.67
(1,1137)	1:398:A:ILE:HD13	1:401:A:GLU:HB2	5	0.67
(1,1137)	1:398:A:ILE:HD13	1:401:A:GLU:HB2	6	0.67
(1,1131)	1:416:A:LEU:HD23	1:429:A:LEU:HG	42	0.67
(1,1130)	1:408:A:LEU:HD23	1:405:A:GLN:HG3	10	0.67
(1,1128)	1:408:A:LEU:HD11	1:432:A:VAL:HB	26	0.67
(1,1033)	1:402:A:ILE:HG22	1:400:A:GLU:HA	2	0.67
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	22	0.67
(1,974)	1:403:A:ARG:HD3	1:400:A:GLU:HG3	5	0.67
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG21	24	0.67
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	21	0.67
(1,753)	1:400:A:GLU:H	1:400:A:GLU:HG3	23	0.67
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	16	0.67
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	39	0.67
(1,616)	1:439:A:LEU:H	1:442:A:LYS:HD3	14	0.67
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	17	0.66
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	23	0.66
(1,1033)	1:402:A:ILE:HG22	1:400:A:GLU:HA	15	0.66
(1,961)	1:406:A:GLU:HG3	1:402:A:ILE:HB	36	0.66
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG21	9	0.66
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	2	0.66
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD21	28	0.66
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	40	0.66
(1,787)	1:405:A:GLN:HE22	1:436:A:LEU:HD22	28	0.66
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	30	0.66
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	43	0.66
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB1	32	0.66
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	32	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	46	0.66
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	11	0.66
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	13	0.66
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	30	0.66
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	19	0.66
(2,4)	1:408:A:LEU:HD11	1:406:A:GLU:HA	43	0.65
(2,4)	1:408:A:LEU:HD12	1:406:A:GLU:HA	43	0.65
(2,4)	1:408:A:LEU:HD13	1:406:A:GLU:HA	43	0.65
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	8	0.65
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	13	0.65
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	14	0.65
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	30	0.65
(1,1162)	1:394:A:THR:HG23	1:395:A:GLN:HB2	19	0.65
(1,1130)	1:408:A:LEU:HD23	1:405:A:GLN:HG3	6	0.65
(1,1130)	1:408:A:LEU:HD23	1:405:A:GLN:HG3	39	0.65
(1,1127)	1:420:A:ILE:HG22	1:422:A:ASP:HB3	15	0.65
(1,1124)	1:429:A:LEU:HD23	1:425:A:LYS:HB2	46	0.65
(1,961)	1:406:A:GLU:HG3	1:402:A:ILE:HB	37	0.65
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG23	11	0.65
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG23	49	0.65
(1,875)	1:417:A:GLN:HA	1:420:A:ILE:HD11	15	0.65
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	27	0.65
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	31	0.65
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	20	0.65
(1,781)	1:413:A:HIS:HD2	1:412:A:LEU:HA	35	0.65
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	4	0.65
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB3	36	0.65
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB3	50	0.65
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	32	0.65
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	7	0.64
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	22	0.64
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	2	0.64
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	21	0.64
(1,1137)	1:398:A:ILE:HD11	1:401:A:GLU:HB2	18	0.64
(1,1137)	1:398:A:ILE:HD11	1:401:A:GLU:HB2	48	0.64
(1,1131)	1:416:A:LEU:HD23	1:425:A:LYS:HD3	12	0.64
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	49	0.64
(1,1033)	1:416:A:LEU:HD21	1:413:A:HIS:HA	40	0.64
(1,1002)	1:420:A:ILE:HG22	1:416:A:LEU:HA	28	0.64
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	44	0.64
(1,961)	1:406:A:GLU:HG3	1:402:A:ILE:HB	19	0.64
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	21	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,929)	1:425:A:LYS:HD2	1:416:A:LEU:HD23	41	0.64
(1,909)	1:440:A:LYS:HE3	1:398:A:ILE:HG22	9	0.64
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG22	45	0.64
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	39	0.64
(1,781)	1:413:A:HIS:HD2	1:412:A:LEU:HA	9	0.64
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	47	0.64
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD11	12	0.64
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD12	12	0.64
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD13	12	0.64
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD11	12	0.64
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD12	12	0.64
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD13	12	0.64
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD11	12	0.64
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD12	12	0.64
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD13	12	0.64
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	39	0.64
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	27	0.63
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	1	0.63
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	5	0.63
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	45	0.63
(1,1130)	1:408:A:LEU:HD23	1:405:A:GLN:HG3	11	0.63
(1,1033)	1:402:A:ILE:HG21	1:400:A:GLU:HA	25	0.63
(1,961)	1:406:A:GLU:HG3	1:402:A:ILE:HB	5	0.63
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	45	0.63
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG13	27	0.63
(1,929)	1:425:A:LYS:HD3	1:416:A:LEU:HD22	45	0.63
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD21	40	0.63
(1,909)	1:440:A:LYS:HE3	1:398:A:ILE:HG21	28	0.63
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	22	0.63
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG23	39	0.63
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB1	45	0.63
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	24	0.63
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	20	0.63
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	41	0.63
(1,753)	1:434:A:ARG:H	1:433:A:GLN:HG2	1	0.63
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	20	0.63
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	15	0.63
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	22	0.63
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	6	0.62
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	10	0.62
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	20	0.62
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	24	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	1:398:A:ILE:H	1:399:A:LYS:HD2	49	0.62
(1,1162)	1:394:A:THR:HG22	1:393:A:GLU:HB3	47	0.62
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	47	0.62
(1,1128)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	34	0.62
(1,1128)	1:408:A:LEU:HD23	1:405:A:GLN:HG3	43	0.62
(1,1119)	1:432:A:VAL:HG12	1:431:A:GLU:HB3	45	0.62
(1,1033)	1:402:A:ILE:HG21	1:400:A:GLU:HA	18	0.62
(1,1033)	1:402:A:ILE:HG21	1:400:A:GLU:HA	29	0.62
(1,1033)	1:416:A:LEU:HD21	1:413:A:HIS:HA	33	0.62
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	50	0.62
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG21	25	0.62
(1,907)	1:405:A:GLN:HG3	1:408:A:LEU:HD21	40	0.62
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG22	2	0.62
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD21	6	0.62
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	38	0.62
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	37	0.62
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	19	0.62
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	2	0.62
(1,781)	1:413:A:HIS:HD2	1:412:A:LEU:HA	32	0.62
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD21	45	0.62
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD22	45	0.62
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD23	45	0.62
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	1	0.62
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	8	0.62
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	44	0.62
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	18	0.62
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	10	0.62
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	10	0.62
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	10	0.62
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	15	0.62
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	21	0.62
(1,1234)	1:433:A:GLN:HE22	1:409:A:LEU:HD12	43	0.61
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	3	0.61
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	31	0.61
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	35	0.61
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	41	0.61
(1,1162)	1:394:A:THR:HG23	1:395:A:GLN:HB2	35	0.61
(1,1141)	1:416:A:LEU:HD22	1:415:A:ASP:HB3	40	0.61
(1,1122)	1:436:A:LEU:HD11	1:433:A:GLN:HG2	29	0.61
(1,1119)	1:432:A:VAL:HG13	1:431:A:GLU:HB3	24	0.61
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG23	48	0.61
(1,911)	1:405:A:GLN:HG3	1:408:A:LEU:HD12	1	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,906)	1:404:A:ARG:HG3	1:436:A:LEU:HD22	18	0.61
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	6	0.61
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	23	0.61
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	39	0.61
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	46	0.61
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB2	13	0.61
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB2	41	0.61
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	11	0.61
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	3	0.61
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	18	0.61
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	27	0.61
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	34	0.61
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD2	45	0.61
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD2	45	0.61
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD2	45	0.61
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	16	0.61
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB2	41	0.61
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	23	0.6
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	31	0.6
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	46	0.6
(1,1206)	1:398:A:ILE:H	1:399:A:LYS:HD3	47	0.6
(1,1131)	1:416:A:LEU:HD21	1:425:A:LYS:HD2	17	0.6
(1,1131)	1:416:A:LEU:HD22	1:429:A:LEU:HG	24	0.6
(1,1130)	1:408:A:LEU:HD23	1:405:A:GLN:HG3	15	0.6
(1,1128)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	18	0.6
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	5	0.6
(1,1107)	1:398:A:ILE:HG12	1:440:A:LYS:HD3	23	0.6
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	32	0.6
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	42	0.6
(1,1066)	1:398:A:ILE:HD11	1:440:A:LYS:HA	17	0.6
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	10	0.6
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	30	0.6
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	4	0.6
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG23	20	0.6
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	2	0.6
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	10	0.6
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	18	0.6
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	24	0.6
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	25	0.6
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	27	0.6
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	35	0.6
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	41	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	47	0.6
(1,811)	1:435:A:ILE:HA	1:439:A:LEU:HB2	15	0.6
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	29	0.6
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	36	0.6
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	13	0.6
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	45	0.6
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	15	0.6
(1,247)	1:401:A:GLU:H	1:401:A:GLU:HG3	32	0.6
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	4	0.6
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	33	0.6
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	40	0.6
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	41	0.6
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	36	0.59
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	43	0.59
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	35	0.59
(1,1124)	1:429:A:LEU:HD22	1:425:A:LYS:HB2	25	0.59
(1,1066)	1:398:A:ILE:HD11	1:440:A:LYS:HA	39	0.59
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	47	0.59
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	49	0.59
(1,967)	1:405:A:GLN:HG2	1:408:A:LEU:HG	28	0.59
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG23	4	0.59
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG13	25	0.59
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG21	27	0.59
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD21	27	0.59
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD22	39	0.59
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG21	38	0.59
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HD12	48	0.59
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	8	0.59
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	13	0.59
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	33	0.59
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	34	0.59
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	42	0.59
(1,825)	1:436:A:LEU:HA	1:436:A:LEU:HG	49	0.59
(1,797)	1:395:A:GLN:HE21	1:398:A:ILE:HG23	14	0.59
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD13	19	0.59
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	17	0.59
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	40	0.59
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB2	15	0.59
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB1	43	0.59
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	38	0.59
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	49	0.59
(1,517)	1:416:A:LEU:HG	1:415:A:ASP:HB2	16	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,517)	1:416:A:LEU:HG	1:415:A:ASP:HB2	17	0.59
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	13	0.59
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	42	0.59
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	42	0.59
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	42	0.59
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	24	0.59
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	29	0.59
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	30	0.59
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	43	0.59
(1,15)	1:420:A:ILE:H	1:420:A:ILE:HG21	14	0.59
(1,1130)	1:408:A:LEU:HD23	1:405:A:GLN:HG3	38	0.58
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	50	0.58
(1,1127)	1:420:A:ILE:HG23	1:422:A:ASP:HB3	3	0.58
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	34	0.58
(1,1033)	1:402:A:ILE:HG22	1:400:A:GLU:HA	19	0.58
(1,929)	1:425:A:LYS:HD3	1:416:A:LEU:HD23	42	0.58
(1,781)	1:413:A:HIS:HD2	1:412:A:LEU:HA	15	0.58
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	23	0.58
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	35	0.58
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD11	40	0.58
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD12	40	0.58
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD13	40	0.58
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD11	40	0.58
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD12	40	0.58
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD13	40	0.58
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD11	40	0.58
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD12	40	0.58
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD13	40	0.58
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	5	0.57
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	17	0.57
(1,1113)	1:443:A:LEU:HD12	1:393:A:GLU:HB3	32	0.57
(1,1112)	1:443:A:LEU:HD12	1:393:A:GLU:HB3	32	0.57
(1,1095)	1:436:A:LEU:HD12	1:440:A:LYS:HE3	8	0.57
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	26	0.57
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	36	0.57
(1,961)	1:422:A:ASP:HB2	1:425:A:LYS:HB2	34	0.57
(1,939)	1:413:A:HIS:HB2	1:412:A:LEU:HD12	45	0.57
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG13	35	0.57
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	9	0.57
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	36	0.57
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	17	0.57
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB3	3	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD11	46	0.57
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD12	46	0.57
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD13	46	0.57
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	44	0.57
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	46	0.57
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD3	29	0.57
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD3	29	0.57
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD3	29	0.57
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	27	0.57
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	27	0.57
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	27	0.57
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD11	28	0.57
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD12	28	0.57
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD13	28	0.57
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD11	28	0.57
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD12	28	0.57
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD13	28	0.57
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD11	28	0.57
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD12	28	0.57
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD13	28	0.57
(1,119)	1:408:A:LEU:HD11	1:409:A:LEU:HG	18	0.57
(1,119)	1:408:A:LEU:HD12	1:409:A:LEU:HG	18	0.57
(1,119)	1:408:A:LEU:HD13	1:409:A:LEU:HG	18	0.57
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	20	0.57
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	49	0.57
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	14	0.56
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	21	0.56
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	24	0.56
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	26	0.56
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	28	0.56
(1,1157)	1:396:A:ALA:HB1	1:395:A:GLN:HB3	46	0.56
(1,1143)	1:398:A:ILE:HG23	1:399:A:LYS:HE2	21	0.56
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	30	0.56
(1,1130)	1:408:A:LEU:HD23	1:405:A:GLN:HG3	41	0.56
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	35	0.56
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	40	0.56
(1,1033)	1:402:A:ILE:HG22	1:400:A:GLU:HA	12	0.56
(1,1033)	1:402:A:ILE:HG22	1:400:A:GLU:HA	20	0.56
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	38	0.56
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD11	43	0.56
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG23	13	0.56
(1,907)	1:405:A:GLN:HG3	1:408:A:LEU:HD22	42	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,906)	1:414:A:ARG:HG3	1:416:A:LEU:HD13	37	0.56
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD11	38	0.56
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG21	14	0.56
(1,825)	1:434:A:ARG:HA	1:434:A:ARG:HG3	9	0.56
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB3	27	0.56
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	5	0.56
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	36	0.56
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	1	0.56
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	1	0.56
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	1	0.56
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	38	0.56
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG12	27	0.56
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	47	0.55
(1,1141)	1:409:A:LEU:HD22	1:410:A:ASN:HB2	14	0.55
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	37	0.55
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	2	0.55
(1,1033)	1:402:A:ILE:HG22	1:400:A:GLU:HA	45	0.55
(1,924)	1:412:A:LEU:HB2	1:429:A:LEU:HD22	6	0.55
(1,909)	1:440:A:LYS:HE2	1:436:A:LEU:HD12	30	0.55
(1,907)	1:405:A:GLN:HG3	1:408:A:LEU:HD23	4	0.55
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	5	0.55
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD21	50	0.55
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	6	0.55
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	36	0.55
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	37	0.55
(1,544)	1:444:A:ARG:H	1:395:A:GLN:HE21	25	0.55
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD11	1	0.55
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD12	1	0.55
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD13	1	0.55
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD11	1	0.55
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD12	1	0.55
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD13	1	0.55
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD11	1	0.55
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD12	1	0.55
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD13	1	0.55
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	10	0.55
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	43	0.55
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	13	0.55
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	41	0.55
(1,1130)	1:408:A:LEU:HD23	1:405:A:GLN:HG3	7	0.54
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	22	0.54
(1,1130)	1:408:A:LEU:HD22	1:405:A:GLN:HG3	24	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1130)	1:408:A:LEU:HD22	1:405:A:GLN:HG3	35	0.54
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	50	0.54
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD13	22	0.54
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG13	27	0.54
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	32	0.54
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB3	11	0.54
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	21	0.54
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	14	0.54
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	25	0.54
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	25	0.54
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	25	0.54
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	11	0.54
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	17	0.54
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	20	0.54
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	37	0.54
(1,425)	1:413:A:HIS:HD2	1:416:A:LEU:HD21	15	0.54
(1,425)	1:413:A:HIS:HD2	1:416:A:LEU:HD22	15	0.54
(1,425)	1:413:A:HIS:HD2	1:416:A:LEU:HD23	15	0.54
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	7	0.54
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	7	0.54
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	7	0.54
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	24	0.54
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	24	0.54
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	24	0.54
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	45	0.54
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	45	0.54
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	45	0.54
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	7	0.54
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	45	0.54
(1,1227)	1:413:A:HIS:H	1:413:A:HIS:HE1	18	0.53
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	46	0.53
(1,1227)	1:413:A:HIS:H	1:413:A:HIS:HE1	47	0.53
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	18	0.53
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	38	0.53
(1,1157)	1:396:A:ALA:HB1	1:400:A:GLU:HB2	41	0.53
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	41	0.53
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	10	0.53
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	32	0.53
(1,1033)	1:402:A:ILE:HG21	1:400:A:GLU:HA	35	0.53
(1,1033)	1:402:A:ILE:HG22	1:400:A:GLU:HA	37	0.53
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	38	0.53
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	44	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	45	0.53
(1,939)	1:413:A:HIS:HB2	1:409:A:LEU:HD22	29	0.53
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG22	33	0.53
(1,924)	1:428:A:ARG:HB2	1:429:A:LEU:HD21	28	0.53
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG22	24	0.53
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB3	38	0.53
(1,825)	1:439:A:LEU:HA	1:443:A:LEU:HG	3	0.53
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	2	0.53
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD11	1	0.53
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	49	0.53
(1,754)	1:411:A:SER:H	1:412:A:LEU:HD12	35	0.53
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	41	0.53
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	16	0.53
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	30	0.53
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD2	50	0.53
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD2	50	0.53
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD2	50	0.53
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	9	0.53
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	16	0.53
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	41	0.53
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	41	0.53
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	41	0.53
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	25	0.53
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	32	0.53
(1,115)	1:398:A:ILE:HG12	1:406:A:GLU:HG3	50	0.53
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB2	27	0.53
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	20	0.53
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	44	0.52
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	49	0.52
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	33	0.52
(1,1130)	1:408:A:LEU:HD23	1:405:A:GLN:HG3	20	0.52
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	31	0.52
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	49	0.52
(1,1095)	1:436:A:LEU:HD12	1:440:A:LYS:HE3	37	0.52
(1,1033)	1:402:A:ILE:HG22	1:400:A:GLU:HA	46	0.52
(1,961)	1:406:A:GLU:HG3	1:402:A:ILE:HB	18	0.52
(1,907)	1:405:A:GLN:HG3	1:408:A:LEU:HD22	37	0.52
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG21	29	0.52
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG22	34	0.52
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	26	0.52
(1,875)	1:417:A:GLN:HA	1:420:A:ILE:HD12	48	0.52
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG23	46	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB2	33	0.52
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	33	0.52
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	1	0.52
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	2	0.52
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	41	0.52
(1,517)	1:416:A:LEU:HG	1:415:A:ASP:HB2	47	0.52
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD11	42	0.52
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD12	42	0.52
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD13	42	0.52
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD11	42	0.52
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD12	42	0.52
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD13	42	0.52
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD11	42	0.52
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD12	42	0.52
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD13	42	0.52
(1,377)	1:417:A:GLN:H	1:417:A:GLN:HG2	10	0.52
(1,320)	1:405:A:GLN:H	1:405:A:GLN:HG3	17	0.52
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	50	0.51
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	45	0.51
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	29	0.51
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	3	0.51
(1,921)	1:425:A:LYS:HD3	1:416:A:LEU:HD23	16	0.51
(1,919)	1:415:A:ASP:HB2	1:412:A:LEU:HD13	32	0.51
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG23	40	0.51
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	1	0.51
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG23	22	0.51
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	22	0.51
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	29	0.51
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	37	0.51
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	8	0.51
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	21	0.51
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD3	21	0.51
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD3	21	0.51
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD3	21	0.51
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD2	25	0.51
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD2	25	0.51
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD2	25	0.51
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	8	0.51
(1,362)	1:414:A:ARG:H	1:414:A:ARG:HG2	33	0.51
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	10	0.51
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	10	0.51
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	10	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	25	0.51
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	25	0.51
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	25	0.51
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB2	45	0.51
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	49	0.51
(1,15)	1:420:A:ILE:H	1:420:A:ILE:HG23	34	0.51
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	17	0.5
(1,1122)	1:436:A:LEU:HD12	1:433:A:GLN:HG2	47	0.5
(1,1066)	1:416:A:LEU:HD23	1:426:A:GLU:HA	47	0.5
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD11	30	0.5
(1,937)	1:425:A:LYS:HE3	1:412:A:LEU:HD21	45	0.5
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG21	43	0.5
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	46	0.5
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB2	29	0.5
(1,781)	1:413:A:HIS:HD2	1:412:A:LEU:HA	29	0.5
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	39	0.5
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	2	0.5
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	42	0.5
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	9	0.5
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	42	0.5
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD2	48	0.5
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD2	48	0.5
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD2	48	0.5
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	3	0.5
(1,425)	1:413:A:HIS:HD2	1:416:A:LEU:HD21	40	0.5
(1,425)	1:413:A:HIS:HD2	1:416:A:LEU:HD22	40	0.5
(1,425)	1:413:A:HIS:HD2	1:416:A:LEU:HD23	40	0.5
(1,425)	1:413:A:HIS:HD2	1:416:A:LEU:HD21	47	0.5
(1,425)	1:413:A:HIS:HD2	1:416:A:LEU:HD22	47	0.5
(1,425)	1:413:A:HIS:HD2	1:416:A:LEU:HD23	47	0.5
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	35	0.5
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	23	0.5
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	34	0.49
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	39	0.49
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	42	0.49
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HB2	14	0.49
(1,1162)	1:394:A:THR:HG21	1:395:A:GLN:HB3	21	0.49
(1,1157)	1:396:A:ALA:HB3	1:400:A:GLU:HB2	49	0.49
(1,1124)	1:429:A:LEU:HD22	1:425:A:LYS:HB2	29	0.49
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	49	0.49
(1,1033)	1:402:A:ILE:HG21	1:400:A:GLU:HA	6	0.49
(1,1033)	1:416:A:LEU:HD21	1:413:A:HIS:HA	17	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1033)	1:402:A:ILE:HG22	1:400:A:GLU:HA	48	0.49
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	47	0.49
(1,923)	1:441:A:ARG:HD3	1:437:A:THR:HG23	32	0.49
(1,909)	1:440:A:LYS:HE3	1:398:A:ILE:HG23	44	0.49
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG22	32	0.49
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB3	19	0.49
(1,776)	1:444:A:ARG:H	1:443:A:LEU:HB2	26	0.49
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	1	0.49
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	37	0.49
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	50	0.49
(1,754)	1:411:A:SER:H	1:412:A:LEU:HD12	41	0.49
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	31	0.49
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	1	0.49
(1,152)	1:441:A:ARG:HA	1:441:A:ARG:HD2	14	0.49
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	25	0.49
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	31	0.49
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	36	0.49
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	37	0.49
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	15	0.48
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	34	0.48
(1,1161)	1:441:A:ARG:HG2	1:445:A:GLU:HG2	5	0.48
(1,1157)	1:396:A:ALA:HB2	1:395:A:GLN:HB3	42	0.48
(1,1135)	1:409:A:LEU:HD22	1:433:A:GLN:HG3	40	0.48
(1,1133)	1:412:A:LEU:HD23	1:409:A:LEU:HG	9	0.48
(1,1133)	1:412:A:LEU:HD23	1:409:A:LEU:HG	12	0.48
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	33	0.48
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	31	0.48
(1,967)	1:405:A:GLN:HG2	1:408:A:LEU:HG	17	0.48
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG23	41	0.48
(1,919)	1:415:A:ASP:HB2	1:412:A:LEU:HD11	3	0.48
(1,907)	1:405:A:GLN:HG3	1:436:A:LEU:HD21	23	0.48
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG23	44	0.48
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	7	0.48
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG22	16	0.48
(1,866)	1:423:A:LEU:HA	1:423:A:LEU:HD12	40	0.48
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	5	0.48
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	34	0.48
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	46	0.48
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD11	27	0.48
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD12	27	0.48
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD13	27	0.48
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	47	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	26	0.48
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	48	0.48
(1,517)	1:416:A:LEU:HG	1:415:A:ASP:HB2	18	0.48
(1,517)	1:416:A:LEU:HG	1:415:A:ASP:HB2	28	0.48
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD2	27	0.48
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD2	27	0.48
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD2	27	0.48
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD2	46	0.48
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD2	46	0.48
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD2	46	0.48
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD11	44	0.48
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD12	44	0.48
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD13	44	0.48
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD11	44	0.48
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD12	44	0.48
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD13	44	0.48
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD11	44	0.48
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD12	44	0.48
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD13	44	0.48
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	12	0.48
(1,413)	1:420:A:ILE:H	1:420:A:ILE:HG12	14	0.48
(1,55)	1:417:A:GLN:HE21	1:414:A:ARG:HB3	50	0.48
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	19	0.48
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	48	0.48
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	3	0.48
(1,1201)	1:405:A:GLN:HE22	1:401:A:GLU:HG2	39	0.47
(1,1133)	1:412:A:LEU:HD21	1:409:A:LEU:HG	48	0.47
(1,1131)	1:416:A:LEU:HD22	1:425:A:LYS:HD3	39	0.47
(1,1119)	1:432:A:VAL:HG13	1:431:A:GLU:HB3	2	0.47
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	21	0.47
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	35	0.47
(1,1107)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	27	0.47
(1,1096)	1:402:A:ILE:HG13	1:440:A:LYS:HE2	7	0.47
(1,1095)	1:412:A:LEU:HD11	1:425:A:LYS:HE2	17	0.47
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	16	0.47
(1,1033)	1:402:A:ILE:HG22	1:400:A:GLU:HA	23	0.47
(1,921)	1:429:A:LEU:HG	1:416:A:LEU:HD23	42	0.47
(1,909)	1:425:A:LYS:HE3	1:412:A:LEU:HD11	26	0.47
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG23	22	0.47
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG23	34	0.47
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	49	0.47
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD11	40	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	40	0.47
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	27	0.47
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	40	0.47
(1,517)	1:416:A:LEU:HG	1:415:A:ASP:HB2	2	0.47
(1,517)	1:416:A:LEU:HG	1:415:A:ASP:HB2	39	0.47
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD3	3	0.47
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD3	3	0.47
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD3	3	0.47
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD3	19	0.47
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD3	19	0.47
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD3	19	0.47
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD2	40	0.47
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD2	40	0.47
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD2	40	0.47
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	23	0.47
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	47	0.47
(1,435)	1:405:A:GLN:HE22	1:401:A:GLU:HG2	39	0.47
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	31	0.47
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	43	0.47
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	6	0.47
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	6	0.47
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	6	0.47
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	48	0.47
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	48	0.47
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	48	0.47
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD21	33	0.47
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD22	33	0.47
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD23	33	0.47
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD21	33	0.47
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD22	33	0.47
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD23	33	0.47
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD21	33	0.47
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD22	33	0.47
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD23	33	0.47
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG12	28	0.47
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	22	0.47
(1,15)	1:420:A:ILE:H	1:420:A:ILE:HD12	48	0.47
(1,1196)	1:398:A:ILE:HD12	1:440:A:LYS:HG2	9	0.46
(1,1196)	1:398:A:ILE:HD13	1:440:A:LYS:HG2	16	0.46
(1,1133)	1:412:A:LEU:HD22	1:409:A:LEU:HG	11	0.46
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	16	0.46
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	31	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	19	0.46
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	38	0.46
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG22	11	0.46
(1,920)	1:417:A:GLN:HB2	1:420:A:ILE:HD12	34	0.46
(1,909)	1:440:A:LYS:HE2	1:436:A:LEU:HD13	34	0.46
(1,907)	1:405:A:GLN:HG3	1:408:A:LEU:HD22	8	0.46
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG21	2	0.46
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG23	6	0.46
(1,825)	1:439:A:LEU:HA	1:443:A:LEU:HG	16	0.46
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	31	0.46
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	33	0.46
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	38	0.46
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	29	0.46
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	43	0.46
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	24	0.46
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	32	0.46
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	1	0.46
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	33	0.46
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD3	43	0.46
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD3	43	0.46
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD3	43	0.46
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD11	3	0.46
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD12	3	0.46
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD13	3	0.46
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD11	3	0.46
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD12	3	0.46
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD13	3	0.46
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD11	3	0.46
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD12	3	0.46
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD13	3	0.46
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD11	26	0.46
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD12	26	0.46
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD13	26	0.46
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD11	26	0.46
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD12	26	0.46
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD13	26	0.46
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD11	26	0.46
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD12	26	0.46
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD13	26	0.46
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	4	0.46
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	4	0.46
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	4	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	21	0.46
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	21	0.46
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	21	0.46
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	28	0.46
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	28	0.46
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	28	0.46
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	32	0.46
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	32	0.46
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	32	0.46
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	37	0.46
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	37	0.46
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	37	0.46
(1,115)	1:398:A:ILE:HG13	1:406:A:GLU:HG3	28	0.46
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	19	0.46
(1,15)	1:420:A:ILE:H	1:420:A:ILE:HD11	15	0.46
(1,1227)	1:413:A:HIS:H	1:413:A:HIS:HE1	38	0.45
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	10	0.45
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	13	0.45
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	50	0.45
(1,1206)	1:398:A:ILE:H	1:399:A:LYS:HD2	36	0.45
(1,1196)	1:402:A:ILE:HD13	1:440:A:LYS:HG2	42	0.45
(1,1143)	1:398:A:ILE:HG21	1:399:A:LYS:HE3	11	0.45
(1,1124)	1:429:A:LEU:HD22	1:425:A:LYS:HB2	19	0.45
(1,1033)	1:402:A:ILE:HG21	1:400:A:GLU:HA	41	0.45
(1,907)	1:405:A:GLN:HG3	1:408:A:LEU:HD21	3	0.45
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG23	9	0.45
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB1	47	0.45
(1,811)	1:426:A:GLU:HA	1:425:A:LYS:HB2	45	0.45
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	49	0.45
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	15	0.45
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	36	0.45
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	44	0.45
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	6	0.45
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	38	0.45
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	4	0.45
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	35	0.45
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD11	37	0.45
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD12	37	0.45
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD13	37	0.45
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD11	37	0.45
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD12	37	0.45
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD13	37	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD11	37	0.45
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD12	37	0.45
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD13	37	0.45
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	18	0.45
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	31	0.45
(1,390)	1:445:A:GLU:H	1:445:A:GLU:HB2	25	0.45
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	3	0.45
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	22	0.45
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	22	0.45
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	22	0.45
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	21	0.45
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG12	23	0.45
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	43	0.45
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	13	0.45
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	19	0.45
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	19	0.44
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	43	0.44
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	49	0.44
(1,1207)	1:412:A:LEU:H	1:429:A:LEU:HB3	27	0.44
(1,1157)	1:396:A:ALA:HB2	1:395:A:GLN:HB3	28	0.44
(1,1141)	1:416:A:LEU:HD21	1:415:A:ASP:HB3	9	0.44
(1,1133)	1:412:A:LEU:HD23	1:429:A:LEU:HG	4	0.44
(1,1133)	1:412:A:LEU:HD21	1:409:A:LEU:HG	15	0.44
(1,1124)	1:429:A:LEU:HD23	1:425:A:LYS:HB2	24	0.44
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	23	0.44
(1,1033)	1:416:A:LEU:HD23	1:413:A:HIS:HA	42	0.44
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	35	0.44
(1,1006)	1:412:A:LEU:HD12	1:413:A:HIS:HA	25	0.44
(1,974)	1:403:A:ARG:HD2	1:400:A:GLU:HG2	28	0.44
(1,961)	1:406:A:GLU:HG3	1:402:A:ILE:HB	17	0.44
(1,961)	1:422:A:ASP:HB2	1:425:A:LYS:HB2	46	0.44
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	20	0.44
(1,937)	1:425:A:LYS:HE3	1:412:A:LEU:HD23	26	0.44
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HD12	20	0.44
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	33	0.44
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	40	0.44
(1,517)	1:416:A:LEU:HG	1:415:A:ASP:HB2	45	0.44
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD3	13	0.44
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD3	13	0.44
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD3	13	0.44
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD3	35	0.44
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD3	35	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD3	35	0.44
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD2	49	0.44
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD2	49	0.44
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD2	49	0.44
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	35	0.44
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	32	0.44
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	7	0.44
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	13	0.44
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	18	0.44
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	39	0.44
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG12	42	0.44
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	35	0.44
(1,22)	1:395:A:GLN:HE21	1:398:A:ILE:HG21	7	0.44
(1,22)	1:395:A:GLN:HE21	1:398:A:ILE:HG22	7	0.44
(1,22)	1:395:A:GLN:HE21	1:398:A:ILE:HG23	7	0.44
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	14	0.44
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB3	35	0.44
(1,1227)	1:413:A:HIS:H	1:413:A:HIS:HE1	40	0.43
(1,1196)	1:398:A:ILE:HD12	1:399:A:LYS:HG2	47	0.43
(1,1137)	1:412:A:LEU:HD23	1:432:A:VAL:HB	25	0.43
(1,1137)	1:398:A:ILE:HD13	1:401:A:GLU:HB2	39	0.43
(1,1130)	1:408:A:LEU:HD22	1:405:A:GLN:HG3	19	0.43
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	18	0.43
(1,1033)	1:402:A:ILE:HG21	1:400:A:GLU:HA	21	0.43
(1,1002)	1:420:A:ILE:HG21	1:421:A:LYS:HA	3	0.43
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	21	0.43
(1,974)	1:403:A:ARG:HD2	1:400:A:GLU:HG2	50	0.43
(1,961)	1:422:A:ASP:HB2	1:425:A:LYS:HB2	10	0.43
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD13	3	0.43
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD12	15	0.43
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG23	49	0.43
(1,920)	1:417:A:GLN:HB2	1:420:A:ILE:HD12	48	0.43
(1,907)	1:406:A:GLU:HB2	1:436:A:LEU:HD22	21	0.43
(1,868)	1:421:A:LYS:HA	1:423:A:LEU:HD22	12	0.43
(1,786)	1:407:A:PHE:HE2	1:403:A:ARG:HB3	17	0.43
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	42	0.43
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	3	0.43
(1,754)	1:411:A:SER:H	1:409:A:LEU:HD22	27	0.43
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	39	0.43
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD2	17	0.43
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD2	17	0.43
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD2	17	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD3	34	0.43
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD3	34	0.43
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD3	34	0.43
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	4	0.43
(1,360)	1:414:A:ARG:H	1:414:A:ARG:HD3	9	0.43
(1,360)	1:414:A:ARG:H	1:414:A:ARG:HD2	25	0.43
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	2	0.43
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	50	0.43
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	13	0.43
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	13	0.43
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	13	0.43
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	13	0.43
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	13	0.43
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	13	0.43
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	13	0.43
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	13	0.43
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	13	0.43
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	46	0.43
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	36	0.43
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	43	0.43
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	50	0.43
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	11	0.43
(1,1227)	1:413:A:HIS:H	1:413:A:HIS:HE1	15	0.42
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	6	0.42
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	22	0.42
(1,1206)	1:398:A:ILE:H	1:399:A:LYS:HD3	17	0.42
(1,1162)	1:394:A:THR:HG23	1:395:A:GLN:HB2	4	0.42
(1,1128)	1:408:A:LEU:HD11	1:432:A:VAL:HB	12	0.42
(1,1095)	1:436:A:LEU:HD11	1:440:A:LYS:HE3	39	0.42
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	17	0.42
(1,1017)	1:398:A:ILE:HG13	1:436:A:LEU:HA	26	0.42
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG21	41	0.42
(1,911)	1:405:A:GLN:HG3	1:408:A:LEU:HD22	37	0.42
(1,899)	1:433:A:GLN:HB3	1:409:A:LEU:HD11	19	0.42
(1,899)	1:433:A:GLN:HB3	1:409:A:LEU:HD13	31	0.42
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	8	0.42
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG23	49	0.42
(1,825)	1:439:A:LEU:HA	1:443:A:LEU:HG	32	0.42
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	8	0.42
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	23	0.42
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	36	0.42
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	26	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	36	0.42
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	49	0.42
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	8	0.42
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	5	0.42
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	45	0.42
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	45	0.42
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	45	0.42
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD11	36	0.42
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD12	36	0.42
(1,506)	1:432:A:VAL:HG21	1:429:A:LEU:HD13	36	0.42
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD11	36	0.42
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD12	36	0.42
(1,506)	1:432:A:VAL:HG22	1:429:A:LEU:HD13	36	0.42
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD11	36	0.42
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD12	36	0.42
(1,506)	1:432:A:VAL:HG23	1:429:A:LEU:HD13	36	0.42
(1,390)	1:445:A:GLU:H	1:445:A:GLU:HB2	48	0.42
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	7	0.42
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	16	0.42
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	16	0.42
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	16	0.42
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	46	0.42
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	46	0.42
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	46	0.42
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	4	0.42
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	32	0.42
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	37	0.42
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	17	0.42
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG13	26	0.42
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	7	0.42
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	26	0.42
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	30	0.41
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	41	0.41
(1,1201)	1:405:A:GLN:HE22	1:401:A:GLU:HG2	19	0.41
(1,1131)	1:416:A:LEU:HD23	1:425:A:LYS:HD3	36	0.41
(1,1124)	1:429:A:LEU:HD21	1:425:A:LYS:HB2	39	0.41
(1,1122)	1:436:A:LEU:HD11	1:433:A:GLN:HG2	22	0.41
(1,1122)	1:436:A:LEU:HD11	1:433:A:GLN:HG2	38	0.41
(1,1113)	1:436:A:LEU:HD23	1:432:A:VAL:HB	30	0.41
(1,1112)	1:436:A:LEU:HD23	1:432:A:VAL:HB	30	0.41
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	10	0.41
(1,961)	1:422:A:ASP:HB2	1:425:A:LYS:HB2	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD13	23	0.41
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG12	9	0.41
(1,929)	1:425:A:LYS:HD2	1:416:A:LEU:HD23	29	0.41
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG22	48	0.41
(1,825)	1:439:A:LEU:HA	1:443:A:LEU:HG	11	0.41
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	26	0.41
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	4	0.41
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	2	0.41
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	10	0.41
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	14	0.41
(1,731)	1:441:A:ARG:H	1:438:A:ALA:HB3	22	0.41
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	24	0.41
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	25	0.41
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD3	4	0.41
(1,517)	1:416:A:LEU:HG	1:415:A:ASP:HB2	11	0.41
(1,517)	1:416:A:LEU:HG	1:415:A:ASP:HB2	31	0.41
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD3	7	0.41
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD3	7	0.41
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD3	7	0.41
(1,435)	1:405:A:GLN:HE22	1:401:A:GLU:HG2	19	0.41
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	11	0.41
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB3	1	0.41
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	17	0.41
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	17	0.41
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	17	0.41
(1,117)	1:398:A:ILE:HG13	1:399:A:LYS:HE3	18	0.41
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB3	34	0.41
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	41	0.41
(1,115)	1:398:A:ILE:HG13	1:406:A:GLU:HG3	27	0.41
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	10	0.41
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HB3	30	0.4
(1,1196)	1:398:A:ILE:HD12	1:440:A:LYS:HG2	38	0.4
(1,1162)	1:394:A:THR:HG22	1:393:A:GLU:HB3	1	0.4
(1,1113)	1:443:A:LEU:HD12	1:393:A:GLU:HB3	24	0.4
(1,1113)	1:436:A:LEU:HD21	1:432:A:VAL:HB	34	0.4
(1,1112)	1:443:A:LEU:HD12	1:393:A:GLU:HB3	24	0.4
(1,1112)	1:436:A:LEU:HD21	1:432:A:VAL:HB	34	0.4
(1,1111)	1:398:A:ILE:HG12	1:440:A:LYS:HD3	23	0.4
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	4	0.4
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	35	0.4
(1,1071)	1:409:A:LEU:HD22	1:410:A:ASN:HA	29	0.4
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	37	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	48	0.4
(1,967)	1:405:A:GLN:HG2	1:408:A:LEU:HG	40	0.4
(1,939)	1:413:A:HIS:HB2	1:409:A:LEU:HD23	41	0.4
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG21	16	0.4
(1,921)	1:409:A:LEU:HG	1:412:A:LEU:HD21	4	0.4
(1,907)	1:405:A:GLN:HG3	1:436:A:LEU:HD23	31	0.4
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	36	0.4
(1,825)	1:439:A:LEU:HA	1:443:A:LEU:HG	1	0.4
(1,786)	1:405:A:GLN:HE22	1:402:A:ILE:HB	34	0.4
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	15	0.4
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	9	0.4
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	16	0.4
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	42	0.4
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	45	0.4
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	9	0.4
(1,642)	1:416:A:LEU:H	1:412:A:LEU:HB2	42	0.4
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	26	0.4
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	41	0.4
(1,413)	1:420:A:ILE:H	1:420:A:ILE:HG12	48	0.4
(1,390)	1:445:A:GLU:H	1:445:A:GLU:HB2	5	0.4
(1,362)	1:414:A:ARG:H	1:414:A:ARG:HG2	21	0.4
(1,360)	1:414:A:ARG:H	1:414:A:ARG:HD3	27	0.4
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	8	0.4
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	37	0.4
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	41	0.4
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	27	0.4
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	27	0.4
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	27	0.4
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	36	0.4
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	36	0.4
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	36	0.4
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	40	0.4
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	40	0.4
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	40	0.4
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	6	0.4
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	15	0.4
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	37	0.4
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	48	0.4
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	6	0.4
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	23	0.4
(1,1227)	1:413:A:HIS:H	1:429:A:LEU:H	33	0.39
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	11	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	29	0.39
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HB2	40	0.39
(1,1196)	1:398:A:ILE:HD11	1:440:A:LYS:HG2	15	0.39
(1,1162)	1:394:A:THR:HG23	1:395:A:GLN:HB3	37	0.39
(1,1162)	1:394:A:THR:HG21	1:395:A:GLN:HB3	50	0.39
(1,1137)	1:398:A:ILE:HD11	1:401:A:GLU:HB2	13	0.39
(1,1131)	1:416:A:LEU:HD21	1:425:A:LYS:HD3	31	0.39
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	2	0.39
(1,1107)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	25	0.39
(1,1033)	1:416:A:LEU:HD21	1:413:A:HIS:HA	3	0.39
(1,1017)	1:398:A:ILE:HG13	1:436:A:LEU:HA	2	0.39
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	31	0.39
(1,1017)	1:398:A:ILE:HG13	1:436:A:LEU:HA	33	0.39
(1,1002)	1:420:A:ILE:HG22	1:416:A:LEU:HA	24	0.39
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	23	0.39
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD12	12	0.39
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	25	0.39
(1,906)	1:404:A:ARG:HG3	1:402:A:ILE:HG23	43	0.39
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD22	13	0.39
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	44	0.39
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG22	1	0.39
(1,808)	1:416:A:LEU:HA	1:417:A:GLN:HG2	38	0.39
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD11	17	0.39
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB2	18	0.39
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	33	0.39
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	5	0.39
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD11	12	0.39
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD12	12	0.39
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD13	12	0.39
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	15	0.39
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	23	0.39
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD3	19	0.39
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	25	0.39
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	48	0.39
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	9	0.39
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	25	0.39
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD3	9	0.39
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD3	14	0.39
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG21	9	0.39
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG22	9	0.39
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG23	9	0.39
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG21	9	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG22	9	0.39
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG23	9	0.39
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG21	9	0.39
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG22	9	0.39
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG23	9	0.39
(1,465)	1:395:A:GLN:HE21	1:443:A:LEU:HB3	4	0.39
(1,360)	1:414:A:ARG:H	1:414:A:ARG:HD2	33	0.39
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	5	0.39
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	18	0.39
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	40	0.39
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	2	0.39
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	2	0.39
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	2	0.39
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	3	0.39
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	3	0.39
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	3	0.39
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	11	0.39
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	11	0.39
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	11	0.39
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	38	0.39
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	42	0.39
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	49	0.39
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	49	0.39
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	49	0.39
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	49	0.39
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	49	0.39
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	49	0.39
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	49	0.39
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	49	0.39
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	49	0.39
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	24	0.39
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG13	2	0.39
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	31	0.39
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG13	33	0.39
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	2	0.39
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	8	0.39
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	33	0.39
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB3	30	0.39
(1,1161)	1:404:A:ARG:HG3	1:405:A:GLN:HG3	19	0.38
(1,1141)	1:416:A:LEU:HD21	1:415:A:ASP:HB3	1	0.38
(1,1137)	1:412:A:LEU:HD22	1:432:A:VAL:HB	3	0.38
(1,1113)	1:436:A:LEU:HD21	1:432:A:VAL:HB	20	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1113)	1:436:A:LEU:HD22	1:432:A:VAL:HB	33	0.38
(1,1112)	1:436:A:LEU:HD21	1:432:A:VAL:HB	20	0.38
(1,1112)	1:436:A:LEU:HD22	1:432:A:VAL:HB	33	0.38
(1,1033)	1:402:A:ILE:HG22	1:400:A:GLU:HA	34	0.38
(1,1017)	1:398:A:ILE:HG13	1:436:A:LEU:HA	1	0.38
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	9	0.38
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	45	0.38
(1,1017)	1:398:A:ILE:HG13	1:436:A:LEU:HA	46	0.38
(1,961)	1:422:A:ASP:HB2	1:425:A:LYS:HB2	26	0.38
(1,924)	1:412:A:LEU:HB2	1:429:A:LEU:HD22	10	0.38
(1,921)	1:409:A:LEU:HG	1:412:A:LEU:HD23	12	0.38
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD22	3	0.38
(1,911)	1:405:A:GLN:HG3	1:436:A:LEU:HD21	23	0.38
(1,825)	1:439:A:LEU:HA	1:442:A:LYS:HD2	5	0.38
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	32	0.38
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	34	0.38
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	31	0.38
(1,733)	1:440:A:LYS:H	1:440:A:LYS:HB3	47	0.38
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	12	0.38
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	45	0.38
(1,645)	1:404:A:ARG:H	1:403:A:ARG:HB2	31	0.38
(1,642)	1:416:A:LEU:H	1:412:A:LEU:HB2	26	0.38
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	31	0.38
(1,472)	1:410:A:ASN:HD22	1:414:A:ARG:HB2	38	0.38
(1,390)	1:445:A:GLU:H	1:445:A:GLU:HB2	10	0.38
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	14	0.38
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	20	0.38
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	21	0.38
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	22	0.38
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	26	0.38
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	27	0.38
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	46	0.38
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	23	0.38
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB3	32	0.38
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	12	0.38
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	12	0.38
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	12	0.38
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	35	0.38
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	35	0.38
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	35	0.38
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	38	0.38
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	38	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	38	0.38
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	3	0.38
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	12	0.38
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	30	0.38
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	34	0.38
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	41	0.38
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	47	0.38
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG13	1	0.38
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	9	0.38
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	45	0.38
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG13	46	0.38
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	5	0.38
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB3	24	0.38
(1,1227)	1:413:A:HIS:H	1:413:A:HIS:HE1	32	0.37
(1,1141)	1:416:A:LEU:HD22	1:415:A:ASP:HB3	50	0.37
(1,1137)	1:412:A:LEU:HD22	1:432:A:VAL:HB	36	0.37
(1,1119)	1:432:A:VAL:HG11	1:431:A:GLU:HB3	25	0.37
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	24	0.37
(1,1033)	1:416:A:LEU:HD23	1:413:A:HIS:HA	14	0.37
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	8	0.37
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	21	0.37
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	36	0.37
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	40	0.37
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	4	0.37
(1,948)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	35	0.37
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD13	21	0.37
(1,924)	1:412:A:LEU:HB2	1:429:A:LEU:HD22	22	0.37
(1,923)	1:413:A:HIS:HB2	1:412:A:LEU:HG	40	0.37
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD22	36	0.37
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	13	0.37
(1,776)	1:444:A:ARG:H	1:443:A:LEU:HB2	2	0.37
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	1	0.37
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	2	0.37
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	27	0.37
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	31	0.37
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	50	0.37
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	8	0.37
(1,331)	1:413:A:HIS:H	1:412:A:LEU:HG	29	0.37
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	39	0.37
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	45	0.37
(1,229)	1:396:A:ALA:H	1:394:A:THR:HB	41	0.37
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	46	0.37
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	8	0.37
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	8	0.37
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	8	0.37
(1,55)	1:417:A:GLN:HE21	1:414:A:ARG:HB3	5	0.37
(1,55)	1:417:A:GLN:HE21	1:414:A:ARG:HB3	27	0.37
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	17	0.37
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	29	0.37
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	33	0.37
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	38	0.37
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	40	0.37
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	8	0.37
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	21	0.37
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	36	0.37
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	40	0.37
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	20	0.37
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	22	0.37
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	24	0.37
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	14	0.37
(2,2)	1:415:A:ASP:HB3	1:420:A:ILE:HG13	48	0.36
(1,1161)	1:441:A:ARG:HG2	1:445:A:GLU:HG2	41	0.36
(1,1141)	1:402:A:ILE:HG21	1:399:A:LYS:HE2	43	0.36
(1,1137)	1:398:A:ILE:HD13	1:401:A:GLU:HB2	45	0.36
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	16	0.36
(1,974)	1:403:A:ARG:HD2	1:400:A:GLU:HG3	7	0.36
(1,924)	1:412:A:LEU:HB2	1:429:A:LEU:HD23	13	0.36
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD23	1	0.36
(1,911)	1:405:A:GLN:HG3	1:408:A:LEU:HD22	8	0.36
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG22	31	0.36
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB3	30	0.36
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB3	42	0.36
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	27	0.36
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	44	0.36
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	23	0.36
(1,733)	1:440:A:LYS:H	1:440:A:LYS:HB3	41	0.36
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	34	0.36
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG2	11	0.36
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD3	24	0.36
(1,390)	1:445:A:GLU:H	1:445:A:GLU:HB2	45	0.36
(1,360)	1:414:A:ARG:H	1:414:A:ARG:HD2	28	0.36
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	39	0.36
(1,331)	1:413:A:HIS:H	1:412:A:LEU:HG	35	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:405:A:GLN:H	1:405:A:GLN:HG3	26	0.36
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	12	0.36
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	13	0.36
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	14	0.36
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	35	0.36
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	42	0.36
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	49	0.36
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	40	0.36
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	50	0.36
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	20	0.36
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	20	0.36
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	20	0.36
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	34	0.36
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	34	0.36
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	34	0.36
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	34	0.36
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	34	0.36
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	34	0.36
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	34	0.36
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	34	0.36
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	34	0.36
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	1	0.36
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	5	0.36
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	36	0.36
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	16	0.36
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	28	0.36
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	29	0.36
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB3	36	0.36
(1,1201)	1:405:A:GLN:HE22	1:401:A:GLU:HG3	11	0.35
(1,1137)	1:398:A:ILE:HD13	1:401:A:GLU:HB2	41	0.35
(1,1122)	1:416:A:LEU:HD11	1:426:A:GLU:HG3	15	0.35
(1,1107)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	45	0.35
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	8	0.35
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	11	0.35
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	12	0.35
(1,1017)	1:398:A:ILE:HG13	1:436:A:LEU:HA	24	0.35
(1,967)	1:415:A:ASP:HB2	1:425:A:LYS:HB3	36	0.35
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD13	16	0.35
(1,911)	1:405:A:GLN:HG3	1:408:A:LEU:HD21	3	0.35
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	12	0.35
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD22	34	0.35
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG23	19	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG21	37	0.35
(1,842)	1:437:A:THR:HB	1:434:A:ARG:HB2	4	0.35
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	37	0.35
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	25	0.35
(1,733)	1:440:A:LYS:H	1:440:A:LYS:HB3	39	0.35
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD21	42	0.35
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD22	42	0.35
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD23	42	0.35
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	21	0.35
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	24	0.35
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD3	7	0.35
(1,642)	1:416:A:LEU:H	1:412:A:LEU:HB3	35	0.35
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	32	0.35
(1,435)	1:405:A:GLN:HE22	1:401:A:GLU:HG3	11	0.35
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	20	0.35
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	46	0.35
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	34	0.35
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	36	0.35
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	17	0.35
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	31	0.35
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	29	0.35
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	29	0.35
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	29	0.35
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	30	0.35
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	30	0.35
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	30	0.35
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	11	0.35
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	16	0.35
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	22	0.35
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	45	0.35
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	11	0.35
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	12	0.35
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG13	24	0.35
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	4	0.35
(1,1236)	1:430:A:TRP:HE1	1:434:A:ARG:HA	3	0.34
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	36	0.34
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	48	0.34
(1,967)	1:405:A:GLN:HG2	1:408:A:LEU:HG	16	0.34
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	20	0.34
(1,937)	1:440:A:LYS:HE3	1:402:A:ILE:HD11	8	0.34
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	46	0.34
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG21	13	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB2	14	0.34
(1,825)	1:439:A:LEU:HA	1:443:A:LEU:HG	14	0.34
(1,825)	1:439:A:LEU:HA	1:443:A:LEU:HG	50	0.34
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	2	0.34
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	22	0.34
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	7	0.34
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	45	0.34
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	6	0.34
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	27	0.34
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	33	0.34
(1,734)	1:399:A:LYS:H	1:399:A:LYS:HD3	17	0.34
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	6	0.34
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD3	27	0.34
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	23	0.34
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	27	0.34
(1,642)	1:416:A:LEU:H	1:412:A:LEU:HB2	43	0.34
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG21	12	0.34
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG22	12	0.34
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG23	12	0.34
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG21	12	0.34
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG22	12	0.34
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG23	12	0.34
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG21	12	0.34
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG22	12	0.34
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG23	12	0.34
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	6	0.34
(1,413)	1:420:A:ILE:H	1:420:A:ILE:HG12	34	0.34
(1,390)	1:445:A:GLU:H	1:445:A:GLU:HB2	26	0.34
(1,390)	1:445:A:GLU:H	1:445:A:GLU:HB2	46	0.34
(1,362)	1:414:A:ARG:H	1:414:A:ARG:HG2	50	0.34
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	13	0.34
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	21	0.34
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	23	0.34
(1,294)	1:409:A:LEU:H	1:408:A:LEU:HD11	18	0.34
(1,294)	1:409:A:LEU:H	1:408:A:LEU:HD12	18	0.34
(1,294)	1:409:A:LEU:H	1:408:A:LEU:HD13	18	0.34
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	19	0.34
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	37	0.34
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	43	0.34
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	14	0.34
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	14	0.34
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	14	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	47	0.34
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	47	0.34
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	47	0.34
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	47	0.34
(1,114)	1:398:A:ILE:HG12	1:401:A:GLU:HB2	21	0.34
(1,55)	1:417:A:GLN:HE21	1:414:A:ARG:HB2	11	0.34
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	26	0.34
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB3	11	0.34
(1,1201)	1:405:A:GLN:HE22	1:401:A:GLU:HG3	6	0.33
(1,1201)	1:405:A:GLN:HE22	1:401:A:GLU:HG3	30	0.33
(1,1196)	1:398:A:ILE:HD13	1:399:A:LYS:HG2	17	0.33
(1,1127)	1:420:A:ILE:HG22	1:422:A:ASP:HB3	24	0.33
(1,1113)	1:436:A:LEU:HD23	1:432:A:VAL:HB	7	0.33
(1,1113)	1:443:A:LEU:HD12	1:393:A:GLU:HB3	27	0.33
(1,1112)	1:436:A:LEU:HD23	1:432:A:VAL:HB	7	0.33
(1,1112)	1:443:A:LEU:HD12	1:393:A:GLU:HB3	27	0.33
(1,1089)	1:432:A:VAL:HB	1:405:A:GLN:HG2	19	0.33
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	3	0.33
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	5	0.33
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	10	0.33
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	22	0.33
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	29	0.33
(1,967)	1:405:A:GLN:HG2	1:408:A:LEU:HG	31	0.33
(1,967)	1:405:A:GLN:HG2	1:408:A:LEU:HG	42	0.33
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD12	1	0.33
(1,924)	1:412:A:LEU:HB2	1:429:A:LEU:HD22	20	0.33
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD23	5	0.33
(1,910)	1:399:A:LYS:HG2	1:398:A:ILE:HD13	17	0.33
(1,907)	1:406:A:GLU:HB2	1:436:A:LEU:HD22	45	0.33
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD21	6	0.33
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD22	13	0.33
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG21	11	0.33
(1,842)	1:437:A:THR:HB	1:434:A:ARG:HB2	28	0.33
(1,842)	1:413:A:HIS:HA	1:412:A:LEU:HB2	40	0.33
(1,825)	1:439:A:LEU:HA	1:442:A:LYS:HD2	20	0.33
(1,786)	1:405:A:GLN:HE22	1:402:A:ILE:HB	47	0.33
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	8	0.33
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	40	0.33
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	26	0.33
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	50	0.33
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	8	0.33
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	24	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	31	0.33
(1,754)	1:411:A:SER:H	1:408:A:LEU:HD12	45	0.33
(1,751)	1:398:A:ILE:HA	1:439:A:LEU:HD22	35	0.33
(1,739)	1:439:A:LEU:H	1:439:A:LEU:HD12	4	0.33
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	40	0.33
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	25	0.33
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	42	0.33
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	47	0.33
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	50	0.33
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	5	0.33
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	30	0.33
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD3	28	0.33
(1,435)	1:405:A:GLN:HE22	1:401:A:GLU:HG3	6	0.33
(1,435)	1:405:A:GLN:HE22	1:401:A:GLU:HG3	30	0.33
(1,360)	1:414:A:ARG:H	1:414:A:ARG:HD2	48	0.33
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	31	0.33
(1,331)	1:413:A:HIS:H	1:412:A:LEU:HG	27	0.33
(1,253)	1:442:A:LYS:H	1:442:A:LYS:HD3	7	0.33
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	5	0.33
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	10	0.33
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	27	0.33
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	38	0.33
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	39	0.33
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	42	0.33
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	2	0.33
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	23	0.33
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	6	0.33
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	6	0.33
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	6	0.33
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	24	0.33
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	24	0.33
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	24	0.33
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD21	30	0.33
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD22	30	0.33
(1,81)	1:432:A:VAL:HG11	1:412:A:LEU:HD23	30	0.33
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD21	30	0.33
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD22	30	0.33
(1,81)	1:432:A:VAL:HG12	1:412:A:LEU:HD23	30	0.33
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD21	30	0.33
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD22	30	0.33
(1,81)	1:432:A:VAL:HG13	1:412:A:LEU:HD23	30	0.33
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	49	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	50	0.33
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	3	0.33
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	5	0.33
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	10	0.33
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	22	0.33
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	29	0.33
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	50	0.33
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	3	0.32
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	5	0.32
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	29	0.32
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	30	0.32
(1,1192)	1:420:A:ILE:HG22	1:420:A:ILE:HG13	3	0.32
(1,1192)	1:420:A:ILE:HG22	1:420:A:ILE:HG13	23	0.32
(1,1162)	1:394:A:THR:HG23	1:393:A:GLU:HB3	3	0.32
(1,1162)	1:394:A:THR:HG21	1:393:A:GLU:HB3	44	0.32
(1,1141)	1:409:A:LEU:HD22	1:410:A:ASN:HB2	7	0.32
(1,1125)	1:409:A:LEU:HD12	1:433:A:GLN:HB2	15	0.32
(1,1117)	1:412:A:LEU:HD22	1:408:A:LEU:HB2	35	0.32
(1,1107)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	35	0.32
(1,1091)	1:425:A:LYS:HB2	1:422:A:ASP:HB3	23	0.32
(1,1033)	1:402:A:ILE:HG23	1:400:A:GLU:HA	43	0.32
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	6	0.32
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	20	0.32
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	43	0.32
(1,963)	1:410:A:ASN:HB2	1:409:A:LEU:HB3	31	0.32
(1,937)	1:440:A:LYS:HE3	1:402:A:ILE:HD13	28	0.32
(1,907)	1:405:A:GLN:HG3	1:436:A:LEU:HD23	14	0.32
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD21	30	0.32
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD21	33	0.32
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	2	0.32
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	18	0.32
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD22	32	0.32
(1,825)	1:439:A:LEU:HA	1:443:A:LEU:HG	40	0.32
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	29	0.32
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	46	0.32
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	33	0.32
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	23	0.32
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	24	0.32
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	20	0.32
(1,765)	1:405:A:GLN:H	1:405:A:GLN:HG3	17	0.32
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	1	0.32
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	9	0.32
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	20	0.32
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	36	0.32
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	39	0.32
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	40	0.32
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	49	0.32
(1,724)	1:405:A:GLN:H	1:405:A:GLN:HE22	26	0.32
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD21	30	0.32
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD22	30	0.32
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD23	30	0.32
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	49	0.32
(1,668)	1:441:A:ARG:H	1:442:A:LYS:HG3	9	0.32
(1,616)	1:439:A:LEU:H	1:442:A:LYS:HD3	16	0.32
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD3	36	0.32
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	4	0.32
(1,390)	1:445:A:GLU:H	1:445:A:GLU:HB2	37	0.32
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	26	0.32
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	4	0.32
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	8	0.32
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	37	0.32
(1,331)	1:413:A:HIS:H	1:412:A:LEU:HG	45	0.32
(1,320)	1:405:A:GLN:H	1:405:A:GLN:HG3	28	0.32
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	24	0.32
(1,253)	1:442:A:LYS:H	1:442:A:LYS:HD2	45	0.32
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	8	0.32
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB3	20	0.32
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB3	28	0.32
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	44	0.32
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	15	0.32
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	15	0.32
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	15	0.32
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	6	0.32
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	27	0.32
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	21	0.32
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	21	0.32
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	21	0.32
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	41	0.32
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	41	0.32
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	41	0.32
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	8	0.32
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	9	0.32
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	20	0.32
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	43	0.32
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB3	50	0.32
(1,1225)	1:427:A:GLU:H	1:416:A:LEU:HD12	40	0.31
(1,1225)	1:427:A:GLU:H	1:416:A:LEU:HD13	47	0.31
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	23	0.31
(1,1192)	1:420:A:ILE:HG22	1:420:A:ILE:HG13	20	0.31
(1,1122)	1:416:A:LEU:HD13	1:426:A:GLU:HG3	39	0.31
(1,1033)	1:402:A:ILE:HG21	1:400:A:GLU:HA	4	0.31
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	15	0.31
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	28	0.31
(1,1017)	1:398:A:ILE:HG13	1:436:A:LEU:HA	39	0.31
(1,1017)	1:398:A:ILE:HG13	1:436:A:LEU:HA	44	0.31
(1,961)	1:422:A:ASP:HB2	1:425:A:LYS:HB2	1	0.31
(1,924)	1:412:A:LEU:HB2	1:429:A:LEU:HD22	19	0.31
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	11	0.31
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	17	0.31
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD21	31	0.31
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG22	4	0.31
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG23	18	0.31
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB2	12	0.31
(1,842)	1:413:A:HIS:HA	1:412:A:LEU:HB2	5	0.31
(1,842)	1:413:A:HIS:HA	1:412:A:LEU:HB2	13	0.31
(1,842)	1:413:A:HIS:HA	1:412:A:LEU:HB2	30	0.31
(1,808)	1:424:A:SER:HA	1:427:A:GLU:HG2	4	0.31
(1,808)	1:416:A:LEU:HA	1:417:A:GLN:HG2	9	0.31
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	31	0.31
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	34	0.31
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	2	0.31
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	7	0.31
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	24	0.31
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	6	0.31
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	8	0.31
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	10	0.31
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	11	0.31
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	12	0.31
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	14	0.31
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	17	0.31
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	19	0.31
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	21	0.31
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	22	0.31
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	24	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	28	0.31
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	29	0.31
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	30	0.31
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	41	0.31
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	46	0.31
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	48	0.31
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG23	47	0.31
(1,739)	1:439:A:LEU:H	1:439:A:LEU:HD12	49	0.31
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	32	0.31
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	9	0.31
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	34	0.31
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB3	7	0.31
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	24	0.31
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	29	0.31
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD2	4	0.31
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	6	0.31
(1,294)	1:409:A:LEU:H	1:408:A:LEU:HD11	34	0.31
(1,294)	1:409:A:LEU:H	1:408:A:LEU:HD12	34	0.31
(1,294)	1:409:A:LEU:H	1:408:A:LEU:HD13	34	0.31
(1,229)	1:396:A:ALA:H	1:394:A:THR:HA	27	0.31
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	6	0.31
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB3	9	0.31
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	24	0.31
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	26	0.31
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	41	0.31
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	26	0.31
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	26	0.31
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	26	0.31
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	44	0.31
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	44	0.31
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	44	0.31
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	1	0.31
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	1	0.31
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	1	0.31
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	32	0.31
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	32	0.31
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	32	0.31
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	14	0.31
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	14	0.31
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	14	0.31
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	14	0.31
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	14	0.31
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	14	0.31
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	14	0.31
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	14	0.31
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	20	0.31
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	20	0.31
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	20	0.31
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	20	0.31
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	20	0.31
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	20	0.31
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	20	0.31
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	20	0.31
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	20	0.31
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	20	0.31
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	31	0.31
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	15	0.31
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	28	0.31
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG13	39	0.31
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG13	44	0.31
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	2	0.31
(1,1236)	1:430:A:TRP:HE1	1:434:A:ARG:HA	50	0.3
(1,1227)	1:413:A:HIS:H	1:413:A:HIS:HE1	12	0.3
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	19	0.3
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	42	0.3
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	44	0.3
(1,1161)	1:404:A:ARG:HG3	1:405:A:GLN:HG3	12	0.3
(1,1141)	1:402:A:ILE:HG23	1:399:A:LYS:HE2	37	0.3
(1,1130)	1:408:A:LEU:HD21	1:405:A:GLN:HG3	46	0.3
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	46	0.3
(1,1109)	1:402:A:ILE:HG13	1:406:A:GLU:HB2	48	0.3
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	32	0.3
(1,1017)	1:398:A:ILE:HG13	1:436:A:LEU:HA	41	0.3
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	49	0.3
(1,967)	1:405:A:GLN:HG2	1:408:A:LEU:HG	2	0.3
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD13	5	0.3
(1,923)	1:413:A:HIS:HB2	1:412:A:LEU:HG	48	0.3
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	13	0.3
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	8	0.3
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	9	0.3
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	22	0.3
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD22	43	0.3
(1,860)	1:429:A:LEU:HA	1:429:A:LEU:HG	9	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,860)	1:429:A:LEU:HA	1:429:A:LEU:HG	11	0.3
(1,860)	1:429:A:LEU:HA	1:429:A:LEU:HG	42	0.3
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB3	25	0.3
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	19	0.3
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	37	0.3
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB3	9	0.3
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	21	0.3
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	28	0.3
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	14	0.3
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	33	0.3
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	42	0.3
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	45	0.3
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	1	0.3
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	49	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	2	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	3	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	5	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	13	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	18	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	23	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	26	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	27	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	34	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	35	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	37	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	38	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	42	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	43	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	44	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	45	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	47	0.3
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	49	0.3
(1,754)	1:411:A:SER:H	1:408:A:LEU:HD13	29	0.3
(1,739)	1:439:A:LEU:H	1:439:A:LEU:HD11	10	0.3
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG23	34	0.3
(1,722)	1:403:A:ARG:H	1:404:A:ARG:HG3	38	0.3
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD21	1	0.3
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD22	1	0.3
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD23	1	0.3
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	3	0.3
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	7	0.3
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	39	0.3
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	24	0.3
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	23	0.3
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	29	0.3
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	14	0.3
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	46	0.3
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	48	0.3
(1,390)	1:445:A:GLU:H	1:445:A:GLU:HB2	27	0.3
(1,362)	1:414:A:ARG:H	1:414:A:ARG:HG2	6	0.3
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	7	0.3
(1,341)	1:422:A:ASP:H	1:421:A:LYS:HA	23	0.3
(1,253)	1:442:A:LYS:H	1:442:A:LYS:HD3	28	0.3
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB3	12	0.3
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	21	0.3
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	29	0.3
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	30	0.3
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	34	0.3
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	45	0.3
(1,117)	1:398:A:ILE:HG12	1:399:A:LYS:HE3	49	0.3
(1,114)	1:398:A:ILE:HG12	1:401:A:GLU:HB2	4	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	2	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	2	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	2	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	7	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	7	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	7	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	8	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	8	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	8	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	11	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	11	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	11	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	15	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	15	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	15	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	20	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	20	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	20	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	22	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	22	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	22	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	25	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	25	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	25	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	28	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	28	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	28	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	30	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	30	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	30	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	31	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	31	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	31	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	35	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	35	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	35	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	37	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	37	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	37	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	38	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	38	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	38	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	39	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	39	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	39	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	40	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	40	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	40	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	44	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	44	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	44	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	46	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	46	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	46	0.3
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	49	0.3
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	49	0.3
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	49	0.3
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	2	0.3
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	32	0.3
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG13	41	0.3
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	49	0.3
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	7	0.3
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	8	0.3
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	43	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:427:A:GLU:H	1:416:A:LEU:HD12	25	0.29
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	26	0.29
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	49	0.29
(1,1192)	1:420:A:ILE:HG23	1:420:A:ILE:HG13	15	0.29
(1,1192)	1:420:A:ILE:HG21	1:420:A:ILE:HG13	34	0.29
(1,1162)	1:394:A:THR:HG23	1:395:A:GLN:HB2	45	0.29
(1,1141)	1:409:A:LEU:HD21	1:410:A:ASN:HB2	47	0.29
(1,1134)	1:416:A:LEU:HD23	1:422:A:ASP:HB3	37	0.29
(1,1131)	1:416:A:LEU:HD21	1:425:A:LYS:HD3	28	0.29
(1,1127)	1:420:A:ILE:HG22	1:422:A:ASP:HB3	25	0.29
(1,1122)	1:436:A:LEU:HD11	1:433:A:GLN:HG2	9	0.29
(1,1117)	1:398:A:ILE:HD12	1:436:A:LEU:HB2	45	0.29
(1,1109)	1:439:A:LEU:HD21	1:401:A:GLU:HB2	20	0.29
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	33	0.29
(1,1107)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	13	0.29
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	14	0.29
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	9	0.29
(1,967)	1:405:A:GLN:HG2	1:408:A:LEU:HG	35	0.29
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD13	38	0.29
(1,924)	1:412:A:LEU:HB2	1:429:A:LEU:HD22	8	0.29
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	8	0.29
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG13	23	0.29
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG13	28	0.29
(1,909)	1:440:A:LYS:HE2	1:436:A:LEU:HD12	48	0.29
(1,907)	1:405:A:GLN:HG3	1:436:A:LEU:HD23	12	0.29
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD21	3	0.29
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	25	0.29
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD21	33	0.29
(1,860)	1:429:A:LEU:HA	1:429:A:LEU:HG	32	0.29
(1,860)	1:429:A:LEU:HA	1:429:A:LEU:HG	41	0.29
(1,860)	1:429:A:LEU:HA	1:429:A:LEU:HG	45	0.29
(1,860)	1:429:A:LEU:HA	1:429:A:LEU:HG	48	0.29
(1,856)	1:409:A:LEU:HA	1:409:A:LEU:HG	45	0.29
(1,848)	1:424:A:SER:HA	1:427:A:GLU:HB3	35	0.29
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB2	13	0.29
(1,842)	1:405:A:GLN:HA	1:408:A:LEU:HB3	46	0.29
(1,794)	1:430:A:TRP:HD1	1:427:A:GLU:HA	26	0.29
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	41	0.29
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	2	0.29
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	18	0.29
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	35	0.29
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	48	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	45	0.29
(1,776)	1:444:A:ARG:H	1:443:A:LEU:HB2	41	0.29
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	32	0.29
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG12	26	0.29
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	4	0.29
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	15	0.29
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	16	0.29
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	25	0.29
(1,756)	1:403:A:ARG:H	1:403:A:ARG:HA	50	0.29
(1,739)	1:439:A:LEU:H	1:439:A:LEU:HD11	6	0.29
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	18	0.29
(1,731)	1:441:A:ARG:H	1:442:A:LYS:HG3	20	0.29
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD21	11	0.29
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD22	11	0.29
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD23	11	0.29
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD3	37	0.29
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	1	0.29
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	21	0.29
(1,472)	1:410:A:ASN:HD22	1:414:A:ARG:HB2	48	0.29
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD11	11	0.29
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD12	11	0.29
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD13	11	0.29
(1,415)	1:420:A:ILE:H	1:420:A:ILE:HB	20	0.29
(1,414)	1:420:A:ILE:H	1:420:A:ILE:HG13	40	0.29
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	37	0.29
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	16	0.29
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	18	0.29
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	22	0.29
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	30	0.29
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	33	0.29
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	46	0.29
(1,294)	1:409:A:LEU:H	1:408:A:LEU:HD11	43	0.29
(1,294)	1:409:A:LEU:H	1:408:A:LEU:HD12	43	0.29
(1,294)	1:409:A:LEU:H	1:408:A:LEU:HD13	43	0.29
(1,253)	1:442:A:LYS:H	1:442:A:LYS:HD2	35	0.29
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	33	0.29
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	38	0.29
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	18	0.29
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	36	0.29
(1,117)	1:398:A:ILE:HG13	1:399:A:LYS:HE3	13	0.29
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	49	0.29
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	3	0.29
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	3	0.29
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	10	0.29
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	10	0.29
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	10	0.29
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	12	0.29
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	12	0.29
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	12	0.29
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	14	0.29
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	14	0.29
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	14	0.29
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	17	0.29
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	17	0.29
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	17	0.29
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	27	0.29
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	27	0.29
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	27	0.29
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	33	0.29
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	33	0.29
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	33	0.29
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	36	0.29
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	36	0.29
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	36	0.29
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	42	0.29
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	42	0.29
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	42	0.29
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	45	0.29
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	45	0.29
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	45	0.29
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	48	0.29
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	48	0.29
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	48	0.29
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	22	0.29
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	22	0.29
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	22	0.29
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	22	0.29
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	22	0.29
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	22	0.29
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	22	0.29
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	22	0.29
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	22	0.29
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	14	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	31	0.29
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	34	0.29
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	46	0.29
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	2	0.28
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	8	0.28
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	18	0.28
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	46	0.28
(1,1201)	1:405:A:GLN:HE22	1:401:A:GLU:HG2	16	0.28
(1,1200)	1:442:A:LYS:H	1:442:A:LYS:HB3	50	0.28
(1,1141)	1:416:A:LEU:HD22	1:415:A:ASP:HB3	31	0.28
(1,1131)	1:416:A:LEU:HD23	1:425:A:LYS:HD3	43	0.28
(1,1124)	1:429:A:LEU:HD22	1:425:A:LYS:HB2	27	0.28
(1,1124)	1:429:A:LEU:HD22	1:425:A:LYS:HB2	36	0.28
(1,1119)	1:432:A:VAL:HG13	1:431:A:GLU:HB3	27	0.28
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	18	0.28
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	16	0.28
(1,924)	1:428:A:ARG:HB3	1:429:A:LEU:HD23	1	0.28
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD23	42	0.28
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD23	19	0.28
(1,919)	1:415:A:ASP:HB2	1:412:A:LEU:HD11	24	0.28
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD21	42	0.28
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD21	45	0.28
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	3	0.28
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	15	0.28
(1,906)	1:414:A:ARG:HG3	1:412:A:LEU:HD12	20	0.28
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD22	19	0.28
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD22	23	0.28
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	26	0.28
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD21	28	0.28
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD21	50	0.28
(1,873)	1:425:A:LYS:HA	1:412:A:LEU:HD23	23	0.28
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG22	41	0.28
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG22	50	0.28
(1,866)	1:423:A:LEU:HA	1:423:A:LEU:HD13	8	0.28
(1,866)	1:423:A:LEU:HA	1:423:A:LEU:HD13	10	0.28
(1,860)	1:429:A:LEU:HA	1:429:A:LEU:HG	4	0.28
(1,860)	1:429:A:LEU:HA	1:429:A:LEU:HG	12	0.28
(1,860)	1:429:A:LEU:HA	1:429:A:LEU:HG	16	0.28
(1,860)	1:429:A:LEU:HA	1:429:A:LEU:HG	40	0.28
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB1	27	0.28
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB3	33	0.28
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB1	42	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,842)	1:437:A:THR:HB	1:434:A:ARG:HB2	15	0.28
(1,842)	1:413:A:HIS:HA	1:412:A:LEU:HB2	43	0.28
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	32	0.28
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	38	0.28
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	47	0.28
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	49	0.28
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	5	0.28
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	41	0.28
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	21	0.28
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	11	0.28
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	19	0.28
(1,756)	1:442:A:LYS:H	1:442:A:LYS:HA	32	0.28
(1,739)	1:439:A:LEU:H	1:439:A:LEU:HD11	2	0.28
(1,739)	1:439:A:LEU:H	1:439:A:LEU:HD13	13	0.28
(1,739)	1:439:A:LEU:H	1:439:A:LEU:HD13	42	0.28
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	1	0.28
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	17	0.28
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD21	17	0.28
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD22	17	0.28
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD23	17	0.28
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD21	36	0.28
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD22	36	0.28
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD23	36	0.28
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD21	43	0.28
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD22	43	0.28
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD23	43	0.28
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	8	0.28
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	18	0.28
(1,642)	1:416:A:LEU:H	1:412:A:LEU:HB2	8	0.28
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	20	0.28
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG21	40	0.28
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG22	40	0.28
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG23	40	0.28
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG21	40	0.28
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG22	40	0.28
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG23	40	0.28
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG21	40	0.28
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG22	40	0.28
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG23	40	0.28
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD11	19	0.28
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD12	19	0.28
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD13	19	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:405:A:GLN:HE22	1:401:A:GLU:HG2	16	0.28
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	22	0.28
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	49	0.28
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	2	0.28
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	11	0.28
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	13	0.28
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	15	0.28
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	27	0.28
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	38	0.28
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	41	0.28
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	46	0.28
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	47	0.28
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	25	0.28
(1,253)	1:442:A:LYS:H	1:442:A:LYS:HD2	21	0.28
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	13	0.28
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	21	0.28
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	2	0.28
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	11	0.28
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	15	0.28
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	35	0.28
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	47	0.28
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	39	0.28
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	10	0.28
(1,114)	1:398:A:ILE:HG13	1:401:A:GLU:HB2	42	0.28
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	5	0.28
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	5	0.28
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	5	0.28
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	13	0.28
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	13	0.28
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	13	0.28
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	16	0.28
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	16	0.28
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	16	0.28
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	23	0.28
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	23	0.28
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	23	0.28
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	26	0.28
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	26	0.28
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	26	0.28
(1,92)	1:408:A:LEU:HD21	1:408:A:LEU:HA	34	0.28
(1,92)	1:408:A:LEU:HD22	1:408:A:LEU:HA	34	0.28
(1,92)	1:408:A:LEU:HD23	1:408:A:LEU:HA	34	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	50	0.28
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	50	0.28
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	50	0.28
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	7	0.28
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	7	0.28
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	7	0.28
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	7	0.28
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	7	0.28
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	7	0.28
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	7	0.28
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	7	0.28
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	7	0.28
(1,53)	1:441:A:ARG:HG2	1:398:A:ILE:HG13	44	0.28
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	18	0.28
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	39	0.28
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	45	0.28
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB3	41	0.28
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	10	0.27
(1,1227)	1:413:A:HIS:H	1:413:A:HIS:HE1	25	0.27
(1,1213)	1:431:A:GLU:H	1:428:A:ARG:HB3	20	0.27
(1,1209)	1:429:A:LEU:H	1:427:A:GLU:HB3	41	0.27
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	24	0.27
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	31	0.27
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	33	0.27
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	38	0.27
(1,1200)	1:442:A:LYS:H	1:442:A:LYS:HB3	24	0.27
(1,1200)	1:442:A:LYS:H	1:442:A:LYS:HB3	30	0.27
(1,1141)	1:416:A:LEU:HD23	1:415:A:ASP:HB3	13	0.27
(1,1111)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	27	0.27
(1,1068)	1:441:A:ARG:HG2	1:437:A:THR:HB	11	0.27
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	7	0.27
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	30	0.27
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	50	0.27
(1,975)	1:403:A:ARG:HD3	1:400:A:GLU:HG3	5	0.27
(1,947)	1:399:A:LYS:HE2	1:398:A:ILE:HG12	35	0.27
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD11	33	0.27
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	14	0.27
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	26	0.27
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	47	0.27
(1,911)	1:406:A:GLU:HB3	1:409:A:LEU:HD11	31	0.27
(1,910)	1:399:A:LYS:HG3	1:402:A:ILE:HG22	15	0.27
(1,909)	1:440:A:LYS:HE3	1:436:A:LEU:HD13	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,907)	1:406:A:GLU:HB2	1:436:A:LEU:HD22	27	0.27
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	36	0.27
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG23	27	0.27
(1,860)	1:429:A:LEU:HA	1:429:A:LEU:HG	15	0.27
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB1	37	0.27
(1,842)	1:437:A:THR:HB	1:434:A:ARG:HB2	14	0.27
(1,842)	1:437:A:THR:HB	1:434:A:ARG:HB2	37	0.27
(1,808)	1:424:A:SER:HA	1:427:A:GLU:HG2	10	0.27
(1,794)	1:430:A:TRP:HD1	1:433:A:GLN:HA	22	0.27
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB2	8	0.27
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	1	0.27
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	10	0.27
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	11	0.27
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	20	0.27
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	41	0.27
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	46	0.27
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	50	0.27
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	3	0.27
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	14	0.27
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	19	0.27
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	35	0.27
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	47	0.27
(1,739)	1:439:A:LEU:H	1:439:A:LEU:HD12	23	0.27
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG21	31	0.27
(1,739)	1:439:A:LEU:H	1:439:A:LEU:HD13	32	0.27
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	13	0.27
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	19	0.27
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	32	0.27
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	37	0.27
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD2	27	0.27
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	37	0.27
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG21	28	0.27
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG22	28	0.27
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG23	28	0.27
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG21	28	0.27
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG22	28	0.27
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG23	28	0.27
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG21	28	0.27
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG22	28	0.27
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG23	28	0.27
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD21	48	0.27
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD22	48	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD23	48	0.27
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	25	0.27
(1,362)	1:414:A:ARG:H	1:414:A:ARG:HG2	1	0.27
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	1	0.27
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	2	0.27
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	5	0.27
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	24	0.27
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	43	0.27
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	6	0.27
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	7	0.27
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	19	0.27
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	24	0.27
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	25	0.27
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	45	0.27
(1,331)	1:413:A:HIS:H	1:412:A:LEU:HG	41	0.27
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	24	0.27
(1,253)	1:442:A:LYS:H	1:442:A:LYS:HD2	19	0.27
(1,253)	1:442:A:LYS:H	1:442:A:LYS:HD3	30	0.27
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	46	0.27
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	13	0.27
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	14	0.27
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	22	0.27
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	37	0.27
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	50	0.27
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	50	0.27
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	50	0.27
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	25	0.27
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	4	0.27
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	4	0.27
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	4	0.27
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	9	0.27
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	9	0.27
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	9	0.27
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	19	0.27
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	19	0.27
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	19	0.27
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	29	0.27
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	29	0.27
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	29	0.27
(1,92)	1:408:A:LEU:HD11	1:408:A:LEU:HA	47	0.27
(1,92)	1:408:A:LEU:HD12	1:408:A:LEU:HA	47	0.27
(1,92)	1:408:A:LEU:HD13	1:408:A:LEU:HA	47	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:408:A:LEU:HD11	1:412:A:LEU:HD21	45	0.27
(1,83)	1:408:A:LEU:HD11	1:412:A:LEU:HD22	45	0.27
(1,83)	1:408:A:LEU:HD11	1:412:A:LEU:HD23	45	0.27
(1,83)	1:408:A:LEU:HD12	1:412:A:LEU:HD21	45	0.27
(1,83)	1:408:A:LEU:HD12	1:412:A:LEU:HD22	45	0.27
(1,83)	1:408:A:LEU:HD12	1:412:A:LEU:HD23	45	0.27
(1,83)	1:408:A:LEU:HD13	1:412:A:LEU:HD21	45	0.27
(1,83)	1:408:A:LEU:HD13	1:412:A:LEU:HD22	45	0.27
(1,83)	1:408:A:LEU:HD13	1:412:A:LEU:HD23	45	0.27
(1,72)	1:440:A:LYS:HE2	1:441:A:ARG:HG2	44	0.27
(1,55)	1:417:A:GLN:HE21	1:414:A:ARG:HB3	21	0.27
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	7	0.27
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	30	0.27
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	50	0.27
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	6	0.26
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	12	0.26
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	21	0.26
(1,1122)	1:416:A:LEU:HD11	1:426:A:GLU:HG3	5	0.26
(1,1122)	1:436:A:LEU:HD12	1:433:A:GLN:HG2	49	0.26
(1,1119)	1:432:A:VAL:HG11	1:431:A:GLU:HB3	35	0.26
(1,1114)	1:432:A:VAL:HG13	1:409:A:LEU:HB2	25	0.26
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	25	0.26
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD21	8	0.26
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	19	0.26
(1,909)	1:440:A:LYS:HE2	1:436:A:LEU:HD12	33	0.26
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	10	0.26
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG23	7	0.26
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG22	44	0.26
(1,842)	1:437:A:THR:HB	1:434:A:ARG:HB2	23	0.26
(1,842)	1:413:A:HIS:HA	1:412:A:LEU:HB2	25	0.26
(1,842)	1:437:A:THR:HB	1:434:A:ARG:HB2	32	0.26
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	33	0.26
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	32	0.26
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	42	0.26
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	37	0.26
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	3	0.26
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	21	0.26
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	27	0.26
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	28	0.26
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG21	9	0.26
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	8	0.26
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	14	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	30	0.26
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	33	0.26
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD11	25	0.26
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD12	25	0.26
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD13	25	0.26
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	44	0.26
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	44	0.26
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	44	0.26
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	13	0.26
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	3	0.26
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	5	0.26
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	28	0.26
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	39	0.26
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	42	0.26
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD2	34	0.26
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	40	0.26
(1,344)	1:412:A:LEU:H	1:411:A:SER:HB2	35	0.26
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	10	0.26
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD21	12	0.26
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD22	12	0.26
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD23	12	0.26
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	15	0.26
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	33	0.26
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	37	0.26
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	44	0.26
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	25	0.26
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	1	0.26
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	15	0.26
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	22	0.26
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	36	0.26
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	37	0.26
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	25	0.26
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	33	0.26
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	48	0.26
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG3	13	0.26
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	14	0.26
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	18	0.26
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	20	0.26
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	26	0.26
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG3	41	0.26
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	33	0.26
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	33	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	33	0.26
(1,117)	1:398:A:ILE:HG13	1:399:A:LYS:HE3	44	0.26
(1,114)	1:398:A:ILE:HG13	1:401:A:GLU:HB2	23	0.26
(1,72)	1:440:A:LYS:HE3	1:441:A:ARG:HG2	22	0.26
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	25	0.26
(2,13)	1:395:A:GLN:HE21	1:443:A:LEU:HA	5	0.25
(1,1234)	1:433:A:GLN:HE22	1:409:A:LEU:HD11	15	0.25
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	7	0.25
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	22	0.25
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	34	0.25
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	39	0.25
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	47	0.25
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	50	0.25
(1,1206)	1:398:A:ILE:H	1:399:A:LYS:HD2	24	0.25
(1,1206)	1:398:A:ILE:H	1:443:A:LEU:HG	46	0.25
(1,1200)	1:442:A:LYS:H	1:442:A:LYS:HB3	41	0.25
(1,1196)	1:398:A:ILE:HD11	1:440:A:LYS:HG2	6	0.25
(1,1186)	1:429:A:LEU:HD21	1:416:A:LEU:HD12	17	0.25
(1,1161)	1:404:A:ARG:HG3	1:405:A:GLN:HG3	35	0.25
(1,1157)	1:396:A:ALA:HB1	1:395:A:GLN:HB3	33	0.25
(1,1133)	1:412:A:LEU:HD21	1:409:A:LEU:HG	30	0.25
(1,1128)	1:408:A:LEU:HD12	1:432:A:VAL:HB	2	0.25
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	30	0.25
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	34	0.25
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	47	0.25
(1,1063)	1:408:A:LEU:HD12	1:411:A:SER:HB2	34	0.25
(1,1045)	1:435:A:ILE:HG13	1:431:A:GLU:HA	23	0.25
(1,1045)	1:435:A:ILE:HG13	1:431:A:GLU:HA	24	0.25
(1,1045)	1:435:A:ILE:HG13	1:431:A:GLU:HA	45	0.25
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	11	0.25
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	30	0.25
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG21	15	0.25
(1,924)	1:428:A:ARG:HB3	1:429:A:LEU:HD22	7	0.25
(1,924)	1:428:A:ARG:HB3	1:429:A:LEU:HD21	37	0.25
(1,923)	1:413:A:HIS:HB2	1:412:A:LEU:HG	3	0.25
(1,921)	1:409:A:LEU:HG	1:412:A:LEU:HD21	40	0.25
(1,899)	1:433:A:GLN:HB3	1:409:A:LEU:HD11	2	0.25
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	21	0.25
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG22	30	0.25
(1,860)	1:429:A:LEU:HA	1:429:A:LEU:HG	25	0.25
(1,860)	1:429:A:LEU:HA	1:429:A:LEU:HG	29	0.25
(1,860)	1:429:A:LEU:HA	1:429:A:LEU:HG	35	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,842)	1:413:A:HIS:HA	1:425:A:LYS:HB2	50	0.25
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	19	0.25
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	20	0.25
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	45	0.25
(1,788)	1:405:A:GLN:HE22	1:435:A:ILE:HD11	17	0.25
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	35	0.25
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	3	0.25
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	12	0.25
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	26	0.25
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	29	0.25
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	36	0.25
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	36	0.25
(1,776)	1:444:A:ARG:H	1:443:A:LEU:HB3	34	0.25
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	2	0.25
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG23	18	0.25
(1,739)	1:439:A:LEU:H	1:439:A:LEU:HD11	25	0.25
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	50	0.25
(1,722)	1:403:A:ARG:H	1:404:A:ARG:HG3	32	0.25
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD21	3	0.25
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD22	3	0.25
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD23	3	0.25
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	37	0.25
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD11	49	0.25
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD12	49	0.25
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD13	49	0.25
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD2	10	0.25
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	3	0.25
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	10	0.25
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	17	0.25
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	43	0.25
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	10	0.25
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG21	1	0.25
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG22	1	0.25
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG23	1	0.25
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG21	1	0.25
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG22	1	0.25
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG23	1	0.25
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG21	1	0.25
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG22	1	0.25
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG23	1	0.25
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD21	9	0.25
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD22	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD23	9	0.25
(1,415)	1:420:A:ILE:H	1:420:A:ILE:HB	40	0.25
(1,360)	1:414:A:ARG:H	1:414:A:ARG:HD2	11	0.25
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	5	0.25
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	9	0.25
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	23	0.25
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	34	0.25
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD21	9	0.25
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD22	9	0.25
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD23	9	0.25
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD21	32	0.25
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD22	32	0.25
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD23	32	0.25
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	3	0.25
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	4	0.25
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	19	0.25
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	22	0.25
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	26	0.25
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	32	0.25
(1,249)	1:401:A:GLU:HA	1:401:A:GLU:HB3	50	0.25
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	3	0.25
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	49	0.25
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG3	4	0.25
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	16	0.25
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	21	0.25
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	27	0.25
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	31	0.25
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG3	35	0.25
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	36	0.25
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	43	0.25
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	49	0.25
(1,117)	1:398:A:ILE:HG13	1:399:A:LYS:HE3	39	0.25
(1,114)	1:398:A:ILE:HG12	1:401:A:GLU:HB2	12	0.25
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	50	0.25
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	50	0.25
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	50	0.25
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	50	0.25
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	50	0.25
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	50	0.25
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	50	0.25
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	50	0.25
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	50	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:440:A:LYS:HE2	1:441:A:ARG:HG2	19	0.25
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	46	0.25
(1,1227)	1:413:A:HIS:H	1:413:A:HIS:HE1	4	0.24
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	1	0.24
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	32	0.24
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	37	0.24
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	40	0.24
(1,1196)	1:398:A:ILE:HD12	1:440:A:LYS:HG2	10	0.24
(1,1196)	1:398:A:ILE:HD13	1:440:A:LYS:HG2	11	0.24
(1,1165)	1:446:A:ALA:HB1	1:445:A:GLU:HB2	4	0.24
(1,1165)	1:446:A:ALA:HB1	1:445:A:GLU:HB2	13	0.24
(1,1157)	1:396:A:ALA:HB1	1:395:A:GLN:HB3	24	0.24
(1,1119)	1:432:A:VAL:HG11	1:431:A:GLU:HB3	31	0.24
(1,1109)	1:439:A:LEU:HD22	1:401:A:GLU:HB2	8	0.24
(1,1107)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	14	0.24
(1,1099)	1:408:A:LEU:HD13	1:408:A:LEU:HG	47	0.24
(1,1089)	1:432:A:VAL:HB	1:405:A:GLN:HG2	46	0.24
(1,1066)	1:398:A:ILE:HD12	1:440:A:LYS:HA	38	0.24
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG11	32	0.24
(1,923)	1:441:A:ARG:HD2	1:437:A:THR:HG23	12	0.24
(1,923)	1:413:A:HIS:HB2	1:412:A:LEU:HG	46	0.24
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	45	0.24
(1,907)	1:406:A:GLU:HB2	1:436:A:LEU:HD23	25	0.24
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	1	0.24
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG22	36	0.24
(1,866)	1:423:A:LEU:HA	1:423:A:LEU:HD12	31	0.24
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB3	44	0.24
(1,825)	1:439:A:LEU:HA	1:443:A:LEU:HG	36	0.24
(1,825)	1:439:A:LEU:HA	1:443:A:LEU:HG	37	0.24
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	30	0.24
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	4	0.24
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	9	0.24
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	19	0.24
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	22	0.24
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	25	0.24
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	30	0.24
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	20	0.24
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	46	0.24
(1,758)	1:428:A:ARG:H	1:428:A:ARG:HB2	45	0.24
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG21	19	0.24
(1,738)	1:440:A:LYS:HA	1:443:A:LEU:HB2	26	0.24
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	43	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD3	46	0.24
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	16	0.24
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	18	0.24
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	44	0.24
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	22	0.24
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD2	23	0.24
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD3	45	0.24
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	35	0.24
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	35	0.24
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	35	0.24
(1,500)	1:413:A:HIS:HB2	1:410:A:ASN:HA	8	0.24
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD21	4	0.24
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD22	4	0.24
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD23	4	0.24
(1,472)	1:410:A:ASN:HD22	1:414:A:ARG:HB2	14	0.24
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD11	4	0.24
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD12	4	0.24
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD13	4	0.24
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	3	0.24
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	3	0.24
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	21	0.24
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	32	0.24
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	49	0.24
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	10	0.24
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	23	0.24
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	28	0.24
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	30	0.24
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	42	0.24
(1,253)	1:442:A:LYS:H	1:442:A:LYS:HD2	4	0.24
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	6	0.24
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	45	0.24
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	7	0.24
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	2	0.24
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	6	0.24
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	10	0.24
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	25	0.24
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG3	42	0.24
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	13	0.24
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	13	0.24
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	13	0.24
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	49	0.24
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	49	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	49	0.24
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	9	0.24
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	49	0.24
(1,2)	1:445:A:GLU:H	1:444:A:ARG:HG2	16	0.24
(1,1236)	1:430:A:TRP:HE1	1:434:A:ARG:HA	45	0.23
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	10	0.23
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	11	0.23
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	14	0.23
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	20	0.23
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	25	0.23
(1,1159)	1:421:A:LYS:HG3	1:421:A:LYS:HD2	14	0.23
(1,1159)	1:440:A:LYS:HG2	1:440:A:LYS:HD3	41	0.23
(1,1143)	1:398:A:ILE:HG23	1:399:A:LYS:HE2	38	0.23
(1,1141)	1:416:A:LEU:HD21	1:415:A:ASP:HB3	48	0.23
(1,1132)	1:408:A:LEU:HD12	1:405:A:GLN:HB3	1	0.23
(1,1109)	1:409:A:LEU:HD23	1:406:A:GLU:HB3	16	0.23
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	19	0.23
(1,1107)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	5	0.23
(1,1107)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	21	0.23
(1,1102)	1:402:A:ILE:HG23	1:402:A:ILE:HB	30	0.23
(1,1100)	1:443:A:LEU:HD23	1:443:A:LEU:HG	15	0.23
(1,1100)	1:435:A:ILE:HD11	1:435:A:ILE:HG12	32	0.23
(1,1100)	1:435:A:ILE:HD13	1:435:A:ILE:HG12	45	0.23
(1,1099)	1:408:A:LEU:HD23	1:408:A:LEU:HG	8	0.23
(1,1099)	1:408:A:LEU:HD12	1:408:A:LEU:HG	15	0.23
(1,1099)	1:408:A:LEU:HD22	1:408:A:LEU:HG	21	0.23
(1,1099)	1:408:A:LEU:HD12	1:408:A:LEU:HG	37	0.23
(1,1099)	1:408:A:LEU:HD13	1:408:A:LEU:HG	45	0.23
(1,1066)	1:398:A:ILE:HD12	1:440:A:LYS:HA	48	0.23
(1,1045)	1:435:A:ILE:HG13	1:431:A:GLU:HA	27	0.23
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	23	0.23
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG11	40	0.23
(1,924)	1:428:A:ARG:HB3	1:429:A:LEU:HD23	21	0.23
(1,923)	1:413:A:HIS:HB2	1:412:A:LEU:HG	42	0.23
(1,919)	1:415:A:ASP:HB2	1:412:A:LEU:HD13	4	0.23
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD21	20	0.23
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	49	0.23
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB1	26	0.23
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB3	30	0.23
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB1	34	0.23
(1,842)	1:413:A:HIS:HA	1:412:A:LEU:HB2	20	0.23
(1,825)	1:439:A:LEU:HA	1:443:A:LEU:HG	31	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,808)	1:424:A:SER:HA	1:427:A:GLU:HG2	13	0.23
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	31	0.23
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	35	0.23
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB2	40	0.23
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	13	0.23
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	23	0.23
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	43	0.23
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	31	0.23
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	1	0.23
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	48	0.23
(1,758)	1:442:A:LYS:H	1:442:A:LYS:HB2	7	0.23
(1,758)	1:428:A:ARG:H	1:428:A:ARG:HB2	14	0.23
(1,722)	1:403:A:ARG:H	1:404:A:ARG:HG3	8	0.23
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD21	20	0.23
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD22	20	0.23
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD23	20	0.23
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD11	24	0.23
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD12	24	0.23
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD13	24	0.23
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD2	2	0.23
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD3	23	0.23
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD2	42	0.23
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	13	0.23
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	18	0.23
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	50	0.23
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD2	25	0.23
(1,500)	1:413:A:HIS:HB2	1:410:A:ASN:HA	13	0.23
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	29	0.23
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD11	17	0.23
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD12	17	0.23
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD13	17	0.23
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	6	0.23
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	33	0.23
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	34	0.23
(1,341)	1:422:A:ASP:H	1:421:A:LYS:HA	25	0.23
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	14	0.23
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	42	0.23
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	43	0.23
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	9	0.23
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	34	0.23
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	36	0.23
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	40	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	49	0.23
(1,253)	1:442:A:LYS:H	1:442:A:LYS:HD2	48	0.23
(1,249)	1:401:A:GLU:HA	1:401:A:GLU:HB3	1	0.23
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	19	0.23
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	20	0.23
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	41	0.23
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	4	0.23
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	9	0.23
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	12	0.23
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	29	0.23
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	30	0.23
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG3	34	0.23
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	38	0.23
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	40	0.23
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	48	0.23
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	23	0.23
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	23	0.23
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	23	0.23
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	13	0.23
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	23	0.23
(1,22)	1:395:A:GLN:HE21	1:398:A:ILE:HG21	14	0.23
(1,22)	1:395:A:GLN:HE21	1:398:A:ILE:HG22	14	0.23
(1,22)	1:395:A:GLN:HE21	1:398:A:ILE:HG23	14	0.23
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	36	0.23
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB2	39	0.23
(1,1209)	1:429:A:LEU:H	1:427:A:GLU:HB3	50	0.22
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	9	0.22
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	16	0.22
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	43	0.22
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	48	0.22
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	33	0.22
(1,1196)	1:398:A:ILE:HD13	1:399:A:LYS:HG3	44	0.22
(1,1161)	1:441:A:ARG:HG2	1:445:A:GLU:HG2	44	0.22
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	33	0.22
(1,1159)	1:440:A:LYS:HG2	1:440:A:LYS:HD3	13	0.22
(1,1159)	1:421:A:LYS:HG3	1:421:A:LYS:HD2	18	0.22
(1,1159)	1:440:A:LYS:HG3	1:440:A:LYS:HD2	32	0.22
(1,1132)	1:408:A:LEU:HD13	1:405:A:GLN:HB3	21	0.22
(1,1109)	1:402:A:ILE:HG21	1:406:A:GLU:HB2	27	0.22
(1,1109)	1:439:A:LEU:HD23	1:401:A:GLU:HB2	50	0.22
(1,1107)	1:398:A:ILE:HG12	1:440:A:LYS:HD3	42	0.22
(1,1100)	1:435:A:ILE:HD11	1:435:A:ILE:HG12	25	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1100)	1:435:A:ILE:HD12	1:435:A:ILE:HG12	29	0.22
(1,1100)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	35	0.22
(1,1100)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	42	0.22
(1,1099)	1:408:A:LEU:HD12	1:408:A:LEU:HG	5	0.22
(1,1099)	1:408:A:LEU:HD13	1:408:A:LEU:HG	6	0.22
(1,1099)	1:408:A:LEU:HD13	1:408:A:LEU:HG	11	0.22
(1,1099)	1:408:A:LEU:HD11	1:408:A:LEU:HG	17	0.22
(1,1099)	1:408:A:LEU:HD22	1:408:A:LEU:HG	22	0.22
(1,1099)	1:408:A:LEU:HD23	1:408:A:LEU:HG	23	0.22
(1,1099)	1:408:A:LEU:HD12	1:408:A:LEU:HG	25	0.22
(1,1099)	1:408:A:LEU:HD13	1:408:A:LEU:HG	30	0.22
(1,1099)	1:408:A:LEU:HD11	1:408:A:LEU:HG	39	0.22
(1,1099)	1:408:A:LEU:HD21	1:408:A:LEU:HG	40	0.22
(1,1099)	1:408:A:LEU:HD12	1:408:A:LEU:HG	42	0.22
(1,1099)	1:408:A:LEU:HD12	1:408:A:LEU:HG	46	0.22
(1,1097)	1:416:A:LEU:HD12	1:416:A:LEU:HB3	16	0.22
(1,1097)	1:443:A:LEU:HD11	1:443:A:LEU:HG	42	0.22
(1,1066)	1:398:A:ILE:HD12	1:440:A:LYS:HA	11	0.22
(1,1045)	1:435:A:ILE:HG13	1:431:A:GLU:HA	25	0.22
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	27	0.22
(1,948)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	42	0.22
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD23	11	0.22
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	7	0.22
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	38	0.22
(1,911)	1:405:A:GLN:HG3	1:436:A:LEU:HD23	14	0.22
(1,907)	1:405:A:GLN:HG3	1:408:A:LEU:HD22	9	0.22
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	5	0.22
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	44	0.22
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	46	0.22
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD22	49	0.22
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG22	8	0.22
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG23	21	0.22
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG21	35	0.22
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG23	42	0.22
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	9	0.22
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	12	0.22
(1,794)	1:430:A:TRP:HD1	1:433:A:GLN:HA	15	0.22
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	21	0.22
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	38	0.22
(1,794)	1:430:A:TRP:HD1	1:433:A:GLN:HA	40	0.22
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	46	0.22
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	44	0.22
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	6	0.22
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	10	0.22
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	30	0.22
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	39	0.22
(1,758)	1:442:A:LYS:H	1:442:A:LYS:HB2	30	0.22
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG23	7	0.22
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG21	27	0.22
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG21	28	0.22
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG23	39	0.22
(1,730)	1:438:A:ALA:H	1:435:A:ILE:HG22	17	0.22
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	50	0.22
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	15	0.22
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	15	0.22
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	15	0.22
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	28	0.22
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	28	0.22
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	28	0.22
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD2	11	0.22
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD2	38	0.22
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	44	0.22
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	33	0.22
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	34	0.22
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	47	0.22
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	49	0.22
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD2	7	0.22
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD2	16	0.22
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD2	31	0.22
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD2	40	0.22
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD2	44	0.22
(1,544)	1:444:A:ARG:H	1:395:A:GLN:HE21	18	0.22
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG21	42	0.22
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG22	42	0.22
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG23	42	0.22
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG21	42	0.22
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG22	42	0.22
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG23	42	0.22
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG21	42	0.22
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG22	42	0.22
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG23	42	0.22
(1,517)	1:416:A:LEU:HG	1:415:A:ASP:HB2	35	0.22
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD2	28	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD2	28	0.22
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD2	28	0.22
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD21	11	0.22
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD22	11	0.22
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD23	11	0.22
(1,472)	1:410:A:ASN:HD22	1:414:A:ARG:HB2	6	0.22
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB2	21	0.22
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD11	37	0.22
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD12	37	0.22
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD13	37	0.22
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	44	0.22
(1,344)	1:412:A:LEU:H	1:411:A:SER:HB2	17	0.22
(1,344)	1:412:A:LEU:H	1:411:A:SER:HB2	19	0.22
(1,341)	1:422:A:ASP:H	1:421:A:LYS:HA	3	0.22
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	20	0.22
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	35	0.22
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	40	0.22
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	50	0.22
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD21	11	0.22
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD22	11	0.22
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD23	11	0.22
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	5	0.22
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD2	9	0.22
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	10	0.22
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD2	28	0.22
(1,253)	1:442:A:LYS:H	1:442:A:LYS:HD2	5	0.22
(1,253)	1:442:A:LYS:H	1:442:A:LYS:HD2	12	0.22
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	43	0.22
(1,205)	1:430:A:TRP:H	1:429:A:LEU:HB2	16	0.22
(1,192)	1:400:A:GLU:H	1:400:A:GLU:HB3	37	0.22
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	1	0.22
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	3	0.22
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	15	0.22
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG3	23	0.22
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	24	0.22
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	28	0.22
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	33	0.22
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	46	0.22
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	50	0.22
(1,146)	1:441:A:ARG:H	1:441:A:ARG:HG2	14	0.22
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	9	0.22
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	9	0.22
(1,117)	1:398:A:ILE:HG12	1:399:A:LYS:HE2	19	0.22
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	8	0.22
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	18	0.22
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	46	0.22
(1,114)	1:398:A:ILE:HG12	1:401:A:GLU:HB2	36	0.22
(1,92)	1:408:A:LEU:HD21	1:408:A:LEU:HA	43	0.22
(1,92)	1:408:A:LEU:HD22	1:408:A:LEU:HA	43	0.22
(1,92)	1:408:A:LEU:HD23	1:408:A:LEU:HA	43	0.22
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	18	0.22
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	18	0.22
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	18	0.22
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	18	0.22
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	18	0.22
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	18	0.22
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	18	0.22
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	18	0.22
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	18	0.22
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	48	0.22
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	48	0.22
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	48	0.22
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	48	0.22
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	48	0.22
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	48	0.22
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	48	0.22
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	48	0.22
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	48	0.22
(1,79)	1:430:A:TRP:HB3	1:427:A:GLU:HA	12	0.22
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	27	0.22
(1,35)	1:398:A:ILE:HA	1:401:A:GLU:HG2	32	0.22
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	21	0.22
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	30	0.22
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	33	0.22
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	37	0.22
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB2	7	0.22
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB2	13	0.22
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB2	45	0.22
(2,2)	1:415:A:ASP:HB3	1:420:A:ILE:HG13	34	0.21
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	15	0.21
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	28	0.21
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	45	0.21
(1,1199)	1:414:A:ARG:HB3	1:414:A:ARG:HG2	50	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	7	0.21
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	45	0.21
(1,1160)	1:414:A:ARG:HG2	1:414:A:ARG:HB3	50	0.21
(1,1159)	1:440:A:LYS:HG3	1:440:A:LYS:HD2	22	0.21
(1,1159)	1:421:A:LYS:HG3	1:421:A:LYS:HD2	33	0.21
(1,1159)	1:399:A:LYS:HG3	1:399:A:LYS:HD2	40	0.21
(1,1159)	1:399:A:LYS:HG2	1:399:A:LYS:HD3	43	0.21
(1,1159)	1:421:A:LYS:HG2	1:421:A:LYS:HD3	49	0.21
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	39	0.21
(1,1100)	1:435:A:ILE:HD12	1:435:A:ILE:HG12	11	0.21
(1,1100)	1:435:A:ILE:HD12	1:435:A:ILE:HG12	16	0.21
(1,1100)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	19	0.21
(1,1100)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	48	0.21
(1,1099)	1:408:A:LEU:HD12	1:408:A:LEU:HG	2	0.21
(1,1099)	1:408:A:LEU:HD12	1:408:A:LEU:HG	3	0.21
(1,1099)	1:408:A:LEU:HD13	1:408:A:LEU:HG	4	0.21
(1,1099)	1:408:A:LEU:HD13	1:408:A:LEU:HG	7	0.21
(1,1099)	1:408:A:LEU:HD11	1:408:A:LEU:HG	10	0.21
(1,1099)	1:408:A:LEU:HD11	1:408:A:LEU:HG	12	0.21
(1,1099)	1:408:A:LEU:HD12	1:408:A:LEU:HG	14	0.21
(1,1099)	1:408:A:LEU:HD22	1:408:A:LEU:HG	16	0.21
(1,1099)	1:408:A:LEU:HD12	1:408:A:LEU:HG	19	0.21
(1,1099)	1:408:A:LEU:HD11	1:408:A:LEU:HG	20	0.21
(1,1099)	1:408:A:LEU:HD22	1:408:A:LEU:HG	24	0.21
(1,1099)	1:408:A:LEU:HD12	1:408:A:LEU:HG	26	0.21
(1,1099)	1:408:A:LEU:HD12	1:408:A:LEU:HG	27	0.21
(1,1099)	1:408:A:LEU:HD13	1:408:A:LEU:HG	28	0.21
(1,1099)	1:408:A:LEU:HD11	1:408:A:LEU:HG	29	0.21
(1,1099)	1:408:A:LEU:HD13	1:408:A:LEU:HG	32	0.21
(1,1099)	1:408:A:LEU:HD23	1:408:A:LEU:HG	35	0.21
(1,1099)	1:408:A:LEU:HD11	1:408:A:LEU:HG	36	0.21
(1,1099)	1:408:A:LEU:HD12	1:408:A:LEU:HG	38	0.21
(1,1099)	1:408:A:LEU:HD13	1:408:A:LEU:HG	44	0.21
(1,1099)	1:408:A:LEU:HD11	1:408:A:LEU:HG	48	0.21
(1,1099)	1:408:A:LEU:HD13	1:408:A:LEU:HG	49	0.21
(1,1097)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	9	0.21
(1,1097)	1:436:A:LEU:HD22	1:436:A:LEU:HG	25	0.21
(1,1097)	1:416:A:LEU:HD12	1:416:A:LEU:HG	32	0.21
(1,1097)	1:436:A:LEU:HD13	1:436:A:LEU:HG	45	0.21
(1,1097)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	48	0.21
(1,1045)	1:435:A:ILE:HG13	1:431:A:GLU:HA	50	0.21
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1006)	1:412:A:LEU:HD11	1:413:A:HIS:HA	33	0.21
(1,988)	1:406:A:GLU:HB2	1:403:A:ARG:HA	28	0.21
(1,929)	1:425:A:LYS:HD3	1:416:A:LEU:HD23	16	0.21
(1,924)	1:412:A:LEU:HB2	1:429:A:LEU:HD23	2	0.21
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	36	0.21
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG13	42	0.21
(1,909)	1:440:A:LYS:HE3	1:436:A:LEU:HD11	15	0.21
(1,907)	1:405:A:GLN:HG3	1:436:A:LEU:HD21	2	0.21
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD22	29	0.21
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD21	30	0.21
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD22	45	0.21
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB2	9	0.21
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB2	10	0.21
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	32	0.21
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB2	50	0.21
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	16	0.21
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB2	31	0.21
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	37	0.21
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	8	0.21
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	21	0.21
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	34	0.21
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	43	0.21
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	6	0.21
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	35	0.21
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	39	0.21
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG23	1	0.21
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG23	21	0.21
(1,739)	1:439:A:LEU:H	1:439:A:LEU:HD12	37	0.21
(1,738)	1:440:A:LYS:HA	1:443:A:LEU:HB3	24	0.21
(1,735)	1:440:A:LYS:H	1:440:A:LYS:HG2	38	0.21
(1,730)	1:438:A:ALA:H	1:435:A:ILE:HG23	26	0.21
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD21	29	0.21
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD22	29	0.21
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD23	29	0.21
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	14	0.21
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	35	0.21
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	14	0.21
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	14	0.21
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	14	0.21
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD2	34	0.21
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	36	0.21
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	45	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	11	0.21
(1,616)	1:439:A:LEU:H	1:442:A:LYS:HD3	35	0.21
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	18	0.21
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD3	2	0.21
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD2	10	0.21
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD3	6	0.21
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD3	6	0.21
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD3	6	0.21
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD3	32	0.21
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD3	32	0.21
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD3	32	0.21
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD21	16	0.21
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD22	16	0.21
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD23	16	0.21
(1,362)	1:414:A:ARG:H	1:414:A:ARG:HG2	25	0.21
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	42	0.21
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	6	0.21
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	14	0.21
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	18	0.21
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	43	0.21
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	48	0.21
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	5	0.21
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	7	0.21
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	8	0.21
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	11	0.21
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	19	0.21
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	32	0.21
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	45	0.21
(1,121)	1:429:A:LEU:HD11	1:433:A:GLN:HG3	37	0.21
(1,121)	1:429:A:LEU:HD12	1:433:A:GLN:HG3	37	0.21
(1,121)	1:429:A:LEU:HD13	1:433:A:GLN:HG3	37	0.21
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	31	0.21
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	31	0.21
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	31	0.21
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	12	0.21
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	13	0.21
(1,38)	1:425:A:LYS:HA	1:425:A:LYS:HG2	31	0.21
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	44	0.21
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	25	0.21
(1,5)	1:394:A:THR:H	1:393:A:GLU:HB3	24	0.21
(2,3)	1:406:A:GLU:HB3	1:410:A:ASN:HA	42	0.2
(1,1282)	1:446:A:ALA:H	1:444:A:ARG:HG3	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	13	0.2
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	17	0.2
(1,1200)	1:442:A:LYS:H	1:442:A:LYS:HB3	36	0.2
(1,1199)	1:428:A:ARG:HB3	1:428:A:ARG:HG2	7	0.2
(1,1199)	1:403:A:ARG:HB2	1:403:A:ARG:HG3	24	0.2
(1,1199)	1:428:A:ARG:HB2	1:428:A:ARG:HG2	29	0.2
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	40	0.2
(1,1199)	1:403:A:ARG:HB3	1:403:A:ARG:HG2	49	0.2
(1,1196)	1:398:A:ILE:HD13	1:440:A:LYS:HG2	4	0.2
(1,1165)	1:446:A:ALA:HB1	1:445:A:GLU:HB2	14	0.2
(1,1161)	1:441:A:ARG:HG2	1:445:A:GLU:HG2	36	0.2
(1,1160)	1:403:A:ARG:HG2	1:403:A:ARG:HB3	21	0.2
(1,1160)	1:403:A:ARG:HG3	1:403:A:ARG:HB2	24	0.2
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	26	0.2
(1,1160)	1:428:A:ARG:HG3	1:428:A:ARG:HB3	29	0.2
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	40	0.2
(1,1160)	1:403:A:ARG:HG2	1:403:A:ARG:HB3	49	0.2
(1,1159)	1:440:A:LYS:HG2	1:440:A:LYS:HD3	1	0.2
(1,1159)	1:440:A:LYS:HG3	1:440:A:LYS:HD2	7	0.2
(1,1159)	1:421:A:LYS:HG3	1:421:A:LYS:HD2	8	0.2
(1,1159)	1:399:A:LYS:HG2	1:399:A:LYS:HD3	17	0.2
(1,1159)	1:421:A:LYS:HG3	1:421:A:LYS:HD2	31	0.2
(1,1159)	1:440:A:LYS:HG2	1:440:A:LYS:HD3	37	0.2
(1,1159)	1:440:A:LYS:HG2	1:440:A:LYS:HD3	39	0.2
(1,1157)	1:396:A:ALA:HB3	1:395:A:GLN:HB3	50	0.2
(1,1134)	1:416:A:LEU:HD21	1:415:A:ASP:HB2	25	0.2
(1,1132)	1:408:A:LEU:HD11	1:405:A:GLN:HB3	36	0.2
(1,1122)	1:436:A:LEU:HD11	1:433:A:GLN:HG2	40	0.2
(1,1107)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	2	0.2
(1,1107)	1:398:A:ILE:HG13	1:440:A:LYS:HD2	19	0.2
(1,1100)	1:435:A:ILE:HD11	1:435:A:ILE:HG12	9	0.2
(1,1100)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	40	0.2
(1,1099)	1:408:A:LEU:HD12	1:408:A:LEU:HG	1	0.2
(1,1099)	1:408:A:LEU:HD11	1:408:A:LEU:HG	13	0.2
(1,1099)	1:408:A:LEU:HD23	1:408:A:LEU:HG	18	0.2
(1,1099)	1:408:A:LEU:HD12	1:408:A:LEU:HG	31	0.2
(1,1099)	1:408:A:LEU:HD11	1:408:A:LEU:HG	33	0.2
(1,1099)	1:408:A:LEU:HD13	1:408:A:LEU:HG	41	0.2
(1,1099)	1:408:A:LEU:HD13	1:408:A:LEU:HG	50	0.2
(1,1089)	1:401:A:GLU:HB3	1:405:A:GLN:HG2	24	0.2
(1,1013)	1:409:A:LEU:HD13	1:406:A:GLU:HA	29	0.2
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	39	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,967)	1:405:A:GLN:HG2	1:408:A:LEU:HG	11	0.2
(1,967)	1:405:A:GLN:HG2	1:408:A:LEU:HG	12	0.2
(1,961)	1:422:A:ASP:HB2	1:425:A:LYS:HB2	8	0.2
(1,924)	1:428:A:ARG:HB2	1:429:A:LEU:HD21	17	0.2
(1,924)	1:412:A:LEU:HB2	1:429:A:LEU:HD21	31	0.2
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	10	0.2
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	16	0.2
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	29	0.2
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	35	0.2
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	50	0.2
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG23	26	0.2
(1,842)	1:413:A:HIS:HA	1:412:A:LEU:HB2	16	0.2
(1,825)	1:439:A:LEU:HA	1:443:A:LEU:HG	43	0.2
(1,808)	1:416:A:LEU:HA	1:417:A:GLN:HG3	39	0.2
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	6	0.2
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	10	0.2
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	48	0.2
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	50	0.2
(1,796)	1:395:A:GLN:HE21	1:398:A:ILE:HD11	9	0.2
(1,793)	1:413:A:HIS:HD2	1:425:A:LYS:HB2	50	0.2
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	7	0.2
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	15	0.2
(1,776)	1:444:A:ARG:H	1:443:A:LEU:HB2	42	0.2
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG23	12	0.2
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG23	38	0.2
(1,739)	1:439:A:LEU:H	1:439:A:LEU:HD12	43	0.2
(1,724)	1:405:A:GLN:H	1:405:A:GLN:HE22	17	0.2
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	3	0.2
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	3	0.2
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	3	0.2
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	5	0.2
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	5	0.2
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	5	0.2
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	20	0.2
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	20	0.2
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	20	0.2
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	14	0.2
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	12	0.2
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	19	0.2
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	31	0.2
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	4	0.2
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	11	0.2
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	13	0.2
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	14	0.2
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	16	0.2
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	20	0.2
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	30	0.2
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	48	0.2
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	50	0.2
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	7	0.2
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	7	0.2
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	7	0.2
(1,391)	1:417:A:GLN:H	1:417:A:GLN:HB3	5	0.2
(1,362)	1:414:A:ARG:H	1:414:A:ARG:HG2	40	0.2
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	8	0.2
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	21	0.2
(1,253)	1:442:A:LYS:H	1:442:A:LYS:HD3	17	0.2
(1,249)	1:401:A:GLU:HA	1:401:A:GLU:HB3	37	0.2
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	17	0.2
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	40	0.2
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	42	0.2
(1,229)	1:396:A:ALA:H	1:394:A:THR:HA	45	0.2
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	22	0.2
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	47	0.2
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	39	0.2
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	39	0.2
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	39	0.2
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	24	0.2
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	33	0.2
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	35	0.2
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	39	0.2
(1,92)	1:408:A:LEU:HD21	1:408:A:LEU:HA	18	0.2
(1,92)	1:408:A:LEU:HD22	1:408:A:LEU:HA	18	0.2
(1,92)	1:408:A:LEU:HD23	1:408:A:LEU:HA	18	0.2
(1,83)	1:408:A:LEU:HD11	1:412:A:LEU:HD21	35	0.2
(1,83)	1:408:A:LEU:HD11	1:412:A:LEU:HD22	35	0.2
(1,83)	1:408:A:LEU:HD11	1:412:A:LEU:HD23	35	0.2
(1,83)	1:408:A:LEU:HD12	1:412:A:LEU:HD21	35	0.2
(1,83)	1:408:A:LEU:HD12	1:412:A:LEU:HD22	35	0.2
(1,83)	1:408:A:LEU:HD12	1:412:A:LEU:HD23	35	0.2
(1,83)	1:408:A:LEU:HD13	1:412:A:LEU:HD21	35	0.2
(1,83)	1:408:A:LEU:HD13	1:412:A:LEU:HD22	35	0.2
(1,83)	1:408:A:LEU:HD13	1:412:A:LEU:HD23	35	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	15	0.2
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	15	0.2
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	15	0.2
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	15	0.2
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	15	0.2
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	15	0.2
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	15	0.2
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	15	0.2
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	15	0.2
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	38	0.2
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	38	0.2
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	38	0.2
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	38	0.2
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	38	0.2
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	38	0.2
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	38	0.2
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	38	0.2
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	38	0.2
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	3	0.2
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	15	0.2
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	18	0.2
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	26	0.2
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	27	0.2
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	48	0.2
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB2	19	0.2
(1,1227)	1:413:A:HIS:H	1:413:A:HIS:HE1	11	0.19
(1,1225)	1:427:A:GLU:H	1:416:A:LEU:HD11	30	0.19
(1,1209)	1:429:A:LEU:H	1:427:A:GLU:HB3	35	0.19
(1,1199)	1:428:A:ARG:HB2	1:428:A:ARG:HG3	3	0.19
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	17	0.19
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	25	0.19
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	32	0.19
(1,1199)	1:403:A:ARG:HB2	1:403:A:ARG:HG3	41	0.19
(1,1196)	1:398:A:ILE:HD12	1:440:A:LYS:HG2	45	0.19
(1,1160)	1:428:A:ARG:HG3	1:428:A:ARG:HB2	3	0.19
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	6	0.19
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	17	0.19
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	25	0.19
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	27	0.19
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	32	0.19
(1,1160)	1:403:A:ARG:HG3	1:403:A:ARG:HB2	41	0.19
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	46	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1159)	1:399:A:LYS:HG2	1:399:A:LYS:HD3	6	0.19
(1,1159)	1:421:A:LYS:HG3	1:421:A:LYS:HD2	9	0.19
(1,1159)	1:399:A:LYS:HG3	1:399:A:LYS:HD2	12	0.19
(1,1159)	1:421:A:LYS:HG2	1:421:A:LYS:HD3	15	0.19
(1,1159)	1:421:A:LYS:HG3	1:421:A:LYS:HD2	19	0.19
(1,1159)	1:399:A:LYS:HG3	1:399:A:LYS:HD2	23	0.19
(1,1159)	1:399:A:LYS:HG3	1:399:A:LYS:HD2	27	0.19
(1,1159)	1:421:A:LYS:HG2	1:421:A:LYS:HD3	46	0.19
(1,1159)	1:440:A:LYS:HG3	1:440:A:LYS:HD2	50	0.19
(1,1124)	1:429:A:LEU:HD23	1:425:A:LYS:HB2	2	0.19
(1,1111)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	25	0.19
(1,1109)	1:409:A:LEU:HD11	1:432:A:VAL:HB	6	0.19
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	17	0.19
(1,1100)	1:443:A:LEU:HD22	1:443:A:LEU:HB3	12	0.19
(1,1100)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	18	0.19
(1,1100)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	27	0.19
(1,1100)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	34	0.19
(1,1100)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	41	0.19
(1,1099)	1:408:A:LEU:HD12	1:408:A:LEU:HG	9	0.19
(1,1099)	1:408:A:LEU:HD21	1:408:A:LEU:HG	43	0.19
(1,1097)	1:416:A:LEU:HD11	1:416:A:LEU:HB3	15	0.19
(1,1097)	1:416:A:LEU:HD12	1:416:A:LEU:HB2	18	0.19
(1,1097)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	27	0.19
(1,1097)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	34	0.19
(1,1097)	1:423:A:LEU:HD21	1:423:A:LEU:HB3	35	0.19
(1,1097)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	41	0.19
(1,1068)	1:441:A:ARG:HG2	1:437:A:THR:HB	12	0.19
(1,1045)	1:435:A:ILE:HG13	1:431:A:GLU:HA	7	0.19
(1,1006)	1:412:A:LEU:HD13	1:413:A:HIS:HA	9	0.19
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	17	0.19
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	19	0.19
(1,924)	1:428:A:ARG:HB3	1:429:A:LEU:HD23	46	0.19
(1,924)	1:428:A:ARG:HB2	1:429:A:LEU:HD21	49	0.19
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD21	47	0.19
(1,916)	1:405:A:GLN:HG2	1:408:A:LEU:HD22	5	0.19
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	1	0.19
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	40	0.19
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD21	17	0.19
(1,866)	1:423:A:LEU:HA	1:423:A:LEU:HD12	7	0.19
(1,866)	1:423:A:LEU:HA	1:423:A:LEU:HD12	46	0.19
(1,856)	1:409:A:LEU:HA	1:409:A:LEU:HG	32	0.19
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB2	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB1	29	0.19
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB1	49	0.19
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	7	0.19
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	22	0.19
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	17	0.19
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	5	0.19
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	42	0.19
(1,776)	1:444:A:ARG:H	1:443:A:LEU:HB2	45	0.19
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	12	0.19
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG21	20	0.19
(1,722)	1:403:A:ARG:H	1:404:A:ARG:HG3	33	0.19
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD11	10	0.19
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD12	10	0.19
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD13	10	0.19
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	41	0.19
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	48	0.19
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	36	0.19
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	36	0.19
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	36	0.19
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD3	22	0.19
(1,642)	1:416:A:LEU:H	1:412:A:LEU:HB2	17	0.19
(1,642)	1:416:A:LEU:H	1:412:A:LEU:HB2	37	0.19
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	7	0.19
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	24	0.19
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	30	0.19
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	15	0.19
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	29	0.19
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	33	0.19
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	34	0.19
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	38	0.19
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	41	0.19
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	47	0.19
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	49	0.19
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	50	0.19
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD21	15	0.19
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD22	15	0.19
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD23	15	0.19
(1,472)	1:410:A:ASN:HD22	1:414:A:ARG:HB2	15	0.19
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD11	43	0.19
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD12	43	0.19
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD13	43	0.19
(1,391)	1:417:A:GLN:H	1:417:A:GLN:HB2	30	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,391)	1:417:A:GLN:H	1:417:A:GLN:HB2	47	0.19
(1,362)	1:414:A:ARG:H	1:414:A:ARG:HG2	34	0.19
(1,362)	1:414:A:ARG:H	1:414:A:ARG:HG2	48	0.19
(1,360)	1:414:A:ARG:H	1:414:A:ARG:HD2	12	0.19
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	31	0.19
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	36	0.19
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD21	15	0.19
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD22	15	0.19
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD23	15	0.19
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD21	16	0.19
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD22	16	0.19
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD23	16	0.19
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD21	18	0.19
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD22	18	0.19
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD23	18	0.19
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	2	0.19
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	7	0.19
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB3	17	0.19
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	38	0.19
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	47	0.19
(1,253)	1:442:A:LYS:H	1:442:A:LYS:HD2	20	0.19
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	29	0.19
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	35	0.19
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	48	0.19
(1,229)	1:396:A:ALA:H	1:394:A:THR:HA	21	0.19
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	44	0.19
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	48	0.19
(1,114)	1:398:A:ILE:HG13	1:401:A:GLU:HB2	27	0.19
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	4	0.19
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	4	0.19
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	4	0.19
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	4	0.19
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	4	0.19
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	4	0.19
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	4	0.19
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	4	0.19
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	4	0.19
(1,72)	1:440:A:LYS:HE2	1:441:A:ARG:HG2	28	0.19
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	23	0.19
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	1	0.19
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	42	0.19
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	38	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:394:A:THR:H	1:393:A:GLU:HB3	32	0.19
(1,2)	1:445:A:GLU:H	1:444:A:ARG:HG2	40	0.19
(1,1201)	1:405:A:GLN:HE22	1:431:A:GLU:HG3	44	0.18
(1,1199)	1:428:A:ARG:HB3	1:428:A:ARG:HG2	6	0.18
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	9	0.18
(1,1199)	1:428:A:ARG:HB2	1:428:A:ARG:HG3	13	0.18
(1,1199)	1:428:A:ARG:HB3	1:428:A:ARG:HG2	27	0.18
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	31	0.18
(1,1199)	1:403:A:ARG:HB2	1:403:A:ARG:HG3	35	0.18
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	42	0.18
(1,1161)	1:441:A:ARG:HG2	1:445:A:GLU:HG2	20	0.18
(1,1160)	1:403:A:ARG:HG2	1:403:A:ARG:HB3	8	0.18
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	9	0.18
(1,1160)	1:428:A:ARG:HG3	1:428:A:ARG:HB2	13	0.18
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	31	0.18
(1,1160)	1:403:A:ARG:HG3	1:403:A:ARG:HB2	35	0.18
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	42	0.18
(1,1159)	1:421:A:LYS:HG2	1:421:A:LYS:HD3	3	0.18
(1,1159)	1:421:A:LYS:HG2	1:421:A:LYS:HD3	30	0.18
(1,1159)	1:421:A:LYS:HG2	1:421:A:LYS:HD3	44	0.18
(1,1137)	1:412:A:LEU:HD23	1:432:A:VAL:HB	1	0.18
(1,1133)	1:412:A:LEU:HD22	1:409:A:LEU:HG	3	0.18
(1,1122)	1:416:A:LEU:HD11	1:426:A:GLU:HG3	16	0.18
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	49	0.18
(1,1107)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	40	0.18
(1,1101)	1:398:A:ILE:HG22	1:398:A:ILE:HB	44	0.18
(1,1100)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	4	0.18
(1,1100)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	23	0.18
(1,1097)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	4	0.18
(1,1097)	1:416:A:LEU:HD13	1:416:A:LEU:HB3	11	0.18
(1,1097)	1:416:A:LEU:HD12	1:416:A:LEU:HB2	12	0.18
(1,1097)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	23	0.18
(1,1008)	1:412:A:LEU:HD12	1:413:A:HIS:HA	30	0.18
(1,1000)	1:420:A:ILE:HG21	1:420:A:ILE:HA	7	0.18
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	12	0.18
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	37	0.18
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	49	0.18
(1,986)	1:422:A:ASP:HB3	1:416:A:LEU:HA	37	0.18
(1,937)	1:425:A:LYS:HE3	1:412:A:LEU:HD23	41	0.18
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG21	32	0.18
(1,924)	1:412:A:LEU:HB2	1:429:A:LEU:HD22	30	0.18
(1,920)	1:432:A:VAL:HB	1:412:A:LEU:HD23	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	21	0.18
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	41	0.18
(1,907)	1:405:A:GLN:HG3	1:436:A:LEU:HD21	36	0.18
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD22	37	0.18
(1,866)	1:423:A:LEU:HA	1:423:A:LEU:HD11	2	0.18
(1,856)	1:409:A:LEU:HA	1:409:A:LEU:HG	25	0.18
(1,848)	1:424:A:SER:HA	1:427:A:GLU:HB3	24	0.18
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB3	46	0.18
(1,842)	1:437:A:THR:HB	1:434:A:ARG:HB2	9	0.18
(1,842)	1:413:A:HIS:HA	1:412:A:LEU:HB2	12	0.18
(1,842)	1:437:A:THR:HB	1:434:A:ARG:HB2	21	0.18
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	3	0.18
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	12	0.18
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	14	0.18
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	16	0.18
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	17	0.18
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	18	0.18
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	41	0.18
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB3	35	0.18
(1,769)	1:429:A:LEU:H	1:428:A:ARG:HA	37	0.18
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	9	0.18
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	25	0.18
(1,752)	1:398:A:ILE:HA	1:398:A:ILE:HG13	27	0.18
(1,735)	1:440:A:LYS:H	1:440:A:LYS:HG2	42	0.18
(1,726)	1:446:A:ALA:H	1:445:A:GLU:HA	27	0.18
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD21	37	0.18
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD22	37	0.18
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD23	37	0.18
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	33	0.18
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	46	0.18
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	22	0.18
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	22	0.18
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	22	0.18
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD11	35	0.18
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD12	35	0.18
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD13	35	0.18
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD2	6	0.18
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	33	0.18
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	2	0.18
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	38	0.18
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	22	0.18
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	39	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD2	32	0.18
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD3	46	0.18
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG21	44	0.18
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG22	44	0.18
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG23	44	0.18
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG21	44	0.18
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG22	44	0.18
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG23	44	0.18
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG21	44	0.18
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG22	44	0.18
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG23	44	0.18
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD21	38	0.18
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD22	38	0.18
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD23	38	0.18
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	2	0.18
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	22	0.18
(1,464)	1:410:A:ASN:HD21	1:414:A:ARG:HB3	28	0.18
(1,391)	1:417:A:GLN:H	1:417:A:GLN:HB3	14	0.18
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	27	0.18
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	30	0.18
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD21	48	0.18
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD22	48	0.18
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD23	48	0.18
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	1	0.18
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	11	0.18
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	12	0.18
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	13	0.18
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	31	0.18
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	47	0.18
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	29	0.18
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	49	0.18
(1,221)	1:410:A:ASN:H	1:410:A:ASN:HB3	7	0.18
(1,121)	1:429:A:LEU:HD11	1:433:A:GLN:HG3	4	0.18
(1,121)	1:429:A:LEU:HD12	1:433:A:GLN:HG3	4	0.18
(1,121)	1:429:A:LEU:HD13	1:433:A:GLN:HG3	4	0.18
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	26	0.18
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	37	0.18
(1,83)	1:408:A:LEU:HD11	1:412:A:LEU:HD21	41	0.18
(1,83)	1:408:A:LEU:HD11	1:412:A:LEU:HD22	41	0.18
(1,83)	1:408:A:LEU:HD11	1:412:A:LEU:HD23	41	0.18
(1,83)	1:408:A:LEU:HD12	1:412:A:LEU:HD21	41	0.18
(1,83)	1:408:A:LEU:HD12	1:412:A:LEU:HD22	41	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:408:A:LEU:HD12	1:412:A:LEU:HD23	41	0.18
(1,83)	1:408:A:LEU:HD13	1:412:A:LEU:HD21	41	0.18
(1,83)	1:408:A:LEU:HD13	1:412:A:LEU:HD22	41	0.18
(1,83)	1:408:A:LEU:HD13	1:412:A:LEU:HD23	41	0.18
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	47	0.18
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	47	0.18
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	47	0.18
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	47	0.18
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	47	0.18
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	47	0.18
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	47	0.18
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	47	0.18
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	47	0.18
(1,38)	1:425:A:LYS:HA	1:425:A:LYS:HG2	45	0.18
(1,26)	1:400:A:GLU:HA	1:403:A:ARG:HD3	24	0.18
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	1	0.18
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	22	0.18
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	28	0.18
(1,15)	1:420:A:ILE:H	1:420:A:ILE:HD13	44	0.18
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB2	2	0.18
(1,1200)	1:442:A:LYS:H	1:442:A:LYS:HB3	11	0.17
(1,1199)	1:414:A:ARG:HB3	1:414:A:ARG:HG2	2	0.17
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	18	0.17
(1,1199)	1:428:A:ARG:HB3	1:428:A:ARG:HG2	26	0.17
(1,1199)	1:414:A:ARG:HB3	1:414:A:ARG:HG2	28	0.17
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	48	0.17
(1,1196)	1:398:A:ILE:HD13	1:440:A:LYS:HG2	36	0.17
(1,1168)	1:402:A:ILE:HG13	1:436:A:LEU:HD22	42	0.17
(1,1161)	1:441:A:ARG:HG2	1:445:A:GLU:HG2	8	0.17
(1,1160)	1:414:A:ARG:HG2	1:414:A:ARG:HB3	2	0.17
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	18	0.17
(1,1160)	1:414:A:ARG:HG2	1:414:A:ARG:HB3	28	0.17
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	47	0.17
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	48	0.17
(1,1159)	1:399:A:LYS:HG2	1:399:A:LYS:HD3	25	0.17
(1,1159)	1:421:A:LYS:HG2	1:421:A:LYS:HD3	26	0.17
(1,1159)	1:399:A:LYS:HG2	1:399:A:LYS:HD3	29	0.17
(1,1159)	1:421:A:LYS:HG3	1:421:A:LYS:HD2	47	0.17
(1,1157)	1:396:A:ALA:HB2	1:400:A:GLU:HB2	26	0.17
(1,1141)	1:409:A:LEU:HD21	1:410:A:ASN:HB2	28	0.17
(1,1132)	1:408:A:LEU:HD22	1:404:A:ARG:HB3	46	0.17
(1,1131)	1:416:A:LEU:HD23	1:425:A:LYS:HD3	47	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1117)	1:412:A:LEU:HD22	1:408:A:LEU:HB2	43	0.17
(1,1113)	1:436:A:LEU:HD23	1:432:A:VAL:HB	6	0.17
(1,1112)	1:436:A:LEU:HD23	1:432:A:VAL:HB	6	0.17
(1,1101)	1:436:A:LEU:HD21	1:436:A:LEU:HB3	50	0.17
(1,1100)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	7	0.17
(1,1100)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	10	0.17
(1,1100)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	17	0.17
(1,1100)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	21	0.17
(1,1100)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	24	0.17
(1,1097)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	10	0.17
(1,1097)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	17	0.17
(1,1097)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	21	0.17
(1,1097)	1:423:A:LEU:HD22	1:423:A:LEU:HB3	29	0.17
(1,1071)	1:443:A:LEU:HD23	1:393:A:GLU:HA	32	0.17
(1,1045)	1:435:A:ILE:HG13	1:431:A:GLU:HA	14	0.17
(1,1000)	1:420:A:ILE:HG23	1:420:A:ILE:HA	31	0.17
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	20	0.17
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	28	0.17
(1,938)	1:409:A:LEU:HG	1:408:A:LEU:HD13	12	0.17
(1,931)	1:406:A:GLU:HG3	1:432:A:VAL:HG21	21	0.17
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD22	15	0.17
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD23	30	0.17
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	30	0.17
(1,866)	1:423:A:LEU:HA	1:423:A:LEU:HD12	41	0.17
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB1	5	0.17
(1,825)	1:439:A:LEU:HA	1:443:A:LEU:HG	15	0.17
(1,825)	1:439:A:LEU:HA	1:443:A:LEU:HG	29	0.17
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	1	0.17
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	4	0.17
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	21	0.17
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	37	0.17
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	38	0.17
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	23	0.17
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	36	0.17
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB2	1	0.17
(1,781)	1:413:A:HIS:HD2	1:414:A:ARG:HA	23	0.17
(1,774)	1:419:A:GLY:H	1:420:A:ILE:HD11	32	0.17
(1,769)	1:429:A:LEU:H	1:428:A:ARG:HA	1	0.17
(1,769)	1:429:A:LEU:H	1:428:A:ARG:HA	21	0.17
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	17	0.17
(1,753)	1:434:A:ARG:H	1:433:A:GLN:HG2	35	0.17
(1,735)	1:440:A:LYS:H	1:440:A:LYS:HG2	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,735)	1:440:A:LYS:H	1:440:A:LYS:HG2	23	0.17
(1,726)	1:446:A:ALA:H	1:445:A:GLU:HA	29	0.17
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD11	9	0.17
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD12	9	0.17
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD13	9	0.17
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	7	0.17
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	7	0.17
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	7	0.17
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	40	0.17
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	40	0.17
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	40	0.17
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	4	0.17
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	9	0.17
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	40	0.17
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	41	0.17
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	10	0.17
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	5	0.17
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	6	0.17
(1,612)	1:432:A:VAL:H	1:432:A:VAL:HB	43	0.17
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD2	42	0.17
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD2	42	0.17
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD2	42	0.17
(1,510)	1:432:A:VAL:HG11	1:405:A:GLN:HA	33	0.17
(1,510)	1:432:A:VAL:HG12	1:405:A:GLN:HA	33	0.17
(1,510)	1:432:A:VAL:HG13	1:405:A:GLN:HA	33	0.17
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD11	30	0.17
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD12	30	0.17
(1,463)	1:433:A:GLN:HE21	1:409:A:LEU:HD13	30	0.17
(1,396)	1:416:A:LEU:H	1:416:A:LEU:HB3	24	0.17
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	10	0.17
(1,342)	1:422:A:ASP:H	1:421:A:LYS:HB3	33	0.17
(1,342)	1:422:A:ASP:H	1:421:A:LYS:HB3	49	0.17
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	48	0.17
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD21	40	0.17
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD22	40	0.17
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD23	40	0.17
(1,320)	1:405:A:GLN:H	1:405:A:GLN:HG3	32	0.17
(1,249)	1:401:A:GLU:HA	1:401:A:GLU:HB3	22	0.17
(1,249)	1:401:A:GLU:HA	1:401:A:GLU:HB3	45	0.17
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	2	0.17
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	9	0.17
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	24	0.17
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	30	0.17
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	34	0.17
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	39	0.17
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	50	0.17
(1,155)	1:440:A:LYS:HA	1:440:A:LYS:HG2	17	0.17
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	22	0.17
(1,114)	1:398:A:ILE:HG12	1:401:A:GLU:HB2	49	0.17
(1,72)	1:440:A:LYS:HE2	1:441:A:ARG:HG2	4	0.17
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	10	0.17
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	13	0.17
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	31	0.17
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	35	0.17
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	42	0.17
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	43	0.17
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	45	0.17
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	23	0.16
(2,3)	1:406:A:GLU:HB3	1:410:A:ASN:HA	10	0.16
(1,1207)	1:412:A:LEU:H	1:408:A:LEU:HB2	4	0.16
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	15	0.16
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	16	0.16
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	19	0.16
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	38	0.16
(1,1199)	1:428:A:ARG:HB3	1:428:A:ARG:HG2	47	0.16
(1,1196)	1:398:A:ILE:HD13	1:440:A:LYS:HG2	35	0.16
(1,1165)	1:446:A:ALA:HB1	1:445:A:GLU:HB2	23	0.16
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	15	0.16
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	16	0.16
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	19	0.16
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	38	0.16
(1,1159)	1:440:A:LYS:HG2	1:440:A:LYS:HD3	28	0.16
(1,1159)	1:399:A:LYS:HG3	1:399:A:LYS:HD2	48	0.16
(1,1157)	1:396:A:ALA:HB2	1:400:A:GLU:HB2	29	0.16
(1,1131)	1:416:A:LEU:HD21	1:425:A:LYS:HD3	44	0.16
(1,1128)	1:408:A:LEU:HD11	1:432:A:VAL:HB	8	0.16
(1,1119)	1:432:A:VAL:HG11	1:431:A:GLU:HB3	23	0.16
(1,1117)	1:412:A:LEU:HD23	1:408:A:LEU:HB2	3	0.16
(1,1101)	1:436:A:LEU:HD22	1:436:A:LEU:HB3	33	0.16
(1,1100)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	1	0.16
(1,1100)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	5	0.16
(1,1100)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	6	0.16
(1,1100)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1100)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	14	0.16
(1,1100)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	20	0.16
(1,1100)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	30	0.16
(1,1100)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	31	0.16
(1,1100)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	39	0.16
(1,1097)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	1	0.16
(1,1097)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	5	0.16
(1,1097)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	6	0.16
(1,1097)	1:423:A:LEU:HD23	1:423:A:LEU:HB3	7	0.16
(1,1097)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	13	0.16
(1,1097)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	14	0.16
(1,1097)	1:423:A:LEU:HD23	1:423:A:LEU:HB3	19	0.16
(1,1097)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	20	0.16
(1,1097)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	30	0.16
(1,1097)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	39	0.16
(1,1091)	1:425:A:LYS:HB2	1:422:A:ASP:HB3	40	0.16
(1,1048)	1:398:A:ILE:HD11	1:399:A:LYS:HA	35	0.16
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	42	0.16
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	1	0.16
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	18	0.16
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	22	0.16
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	27	0.16
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	33	0.16
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	38	0.16
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	45	0.16
(1,924)	1:412:A:LEU:HB2	1:429:A:LEU:HD21	34	0.16
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD22	41	0.16
(1,910)	1:440:A:LYS:HG2	1:398:A:ILE:HD13	35	0.16
(1,909)	1:440:A:LYS:HE3	1:436:A:LEU:HD12	16	0.16
(1,866)	1:423:A:LEU:HA	1:423:A:LEU:HD13	30	0.16
(1,866)	1:423:A:LEU:HA	1:423:A:LEU:HD12	35	0.16
(1,813)	1:406:A:GLU:HA	1:405:A:GLN:HB3	18	0.16
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	24	0.16
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	28	0.16
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	39	0.16
(1,794)	1:430:A:TRP:HD1	1:433:A:GLN:HA	43	0.16
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	49	0.16
(1,776)	1:444:A:ARG:H	1:443:A:LEU:HB2	22	0.16
(1,769)	1:429:A:LEU:H	1:428:A:ARG:HA	9	0.16
(1,769)	1:426:A:GLU:H	1:423:A:LEU:HA	10	0.16
(1,769)	1:429:A:LEU:H	1:428:A:ARG:HA	40	0.16
(1,769)	1:407:A:PHE:H	1:404:A:ARG:HA	42	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,769)	1:429:A:LEU:H	1:428:A:ARG:HA	43	0.16
(1,769)	1:426:A:GLU:H	1:423:A:LEU:HA	46	0.16
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	22	0.16
(1,765)	1:405:A:GLN:H	1:405:A:GLN:HG3	26	0.16
(1,764)	1:405:A:GLN:H	1:406:A:GLU:HG2	31	0.16
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG23	22	0.16
(1,737)	1:440:A:LYS:H	1:398:A:ILE:HD12	23	0.16
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	19	0.16
(1,726)	1:446:A:ALA:H	1:445:A:GLU:HA	14	0.16
(1,726)	1:446:A:ALA:H	1:445:A:GLU:HA	32	0.16
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	5	0.16
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	22	0.16
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	16	0.16
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	16	0.16
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	16	0.16
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	21	0.16
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	21	0.16
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	21	0.16
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	31	0.16
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	31	0.16
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	31	0.16
(1,646)	1:404:A:ARG:H	1:404:A:ARG:HG2	33	0.16
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	19	0.16
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG21	3	0.16
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG22	3	0.16
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG23	3	0.16
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG21	3	0.16
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG22	3	0.16
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG23	3	0.16
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG21	3	0.16
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG22	3	0.16
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG23	3	0.16
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG21	26	0.16
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG22	26	0.16
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG23	26	0.16
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG21	26	0.16
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG22	26	0.16
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG23	26	0.16
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG21	26	0.16
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG22	26	0.16
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG23	26	0.16
(1,515)	1:437:A:THR:HG21	1:441:A:ARG:HD3	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,515)	1:437:A:THR:HG22	1:441:A:ARG:HD3	10	0.16
(1,515)	1:437:A:THR:HG23	1:441:A:ARG:HD3	10	0.16
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD21	32	0.16
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD22	32	0.16
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD23	32	0.16
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD21	47	0.16
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD22	47	0.16
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD23	47	0.16
(1,472)	1:410:A:ASN:HD22	1:414:A:ARG:HB2	7	0.16
(1,471)	1:433:A:GLN:HE22	1:429:A:LEU:HD11	1	0.16
(1,471)	1:433:A:GLN:HE22	1:429:A:LEU:HD12	1	0.16
(1,471)	1:433:A:GLN:HE22	1:429:A:LEU:HD13	1	0.16
(1,471)	1:433:A:GLN:HE22	1:429:A:LEU:HD11	23	0.16
(1,471)	1:433:A:GLN:HE22	1:429:A:LEU:HD12	23	0.16
(1,471)	1:433:A:GLN:HE22	1:429:A:LEU:HD13	23	0.16
(1,471)	1:433:A:GLN:HE22	1:429:A:LEU:HD11	50	0.16
(1,471)	1:433:A:GLN:HE22	1:429:A:LEU:HD12	50	0.16
(1,471)	1:433:A:GLN:HE22	1:429:A:LEU:HD13	50	0.16
(1,429)	1:407:A:PHE:HD1	1:408:A:LEU:HA	17	0.16
(1,429)	1:407:A:PHE:HD2	1:408:A:LEU:HA	17	0.16
(1,362)	1:414:A:ARG:H	1:414:A:ARG:HG2	4	0.16
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	28	0.16
(1,342)	1:422:A:ASP:H	1:421:A:LYS:HB3	46	0.16
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD21	25	0.16
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD22	25	0.16
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD23	25	0.16
(1,253)	1:442:A:LYS:H	1:442:A:LYS:HD2	14	0.16
(1,238)	1:411:A:SER:H	1:411:A:SER:HB3	19	0.16
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	19	0.16
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	43	0.16
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	50	0.16
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	11	0.16
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	11	0.16
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	11	0.16
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	11	0.16
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	11	0.16
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	11	0.16
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	11	0.16
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	11	0.16
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	11	0.16
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	42	0.16
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	14	0.16
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	16	0.16
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	20	0.16
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	32	0.16
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	34	0.16
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	16	0.16
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB2	12	0.16
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB2	38	0.16
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	39	0.15
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	46	0.15
(2,3)	1:406:A:GLU:HB3	1:410:A:ASN:HA	34	0.15
(2,3)	1:406:A:GLU:HB3	1:410:A:ASN:HA	48	0.15
(1,1227)	1:413:A:HIS:H	1:413:A:HIS:HE1	16	0.15
(1,1209)	1:429:A:LEU:H	1:427:A:GLU:HB3	30	0.15
(1,1199)	1:414:A:ARG:HB3	1:414:A:ARG:HG2	10	0.15
(1,1199)	1:428:A:ARG:HB2	1:428:A:ARG:HG2	23	0.15
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	30	0.15
(1,1199)	1:428:A:ARG:HB2	1:428:A:ARG:HG3	34	0.15
(1,1161)	1:404:A:ARG:HG3	1:405:A:GLN:HG3	24	0.15
(1,1160)	1:414:A:ARG:HG2	1:414:A:ARG:HB3	10	0.15
(1,1160)	1:428:A:ARG:HG3	1:428:A:ARG:HB3	23	0.15
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	30	0.15
(1,1160)	1:428:A:ARG:HG3	1:428:A:ARG:HB2	34	0.15
(1,1159)	1:399:A:LYS:HG2	1:399:A:LYS:HD3	36	0.15
(1,1157)	1:396:A:ALA:HB1	1:395:A:GLN:HB3	1	0.15
(1,1141)	1:416:A:LEU:HD21	1:415:A:ASP:HB3	18	0.15
(1,1132)	1:408:A:LEU:HD23	1:404:A:ARG:HB3	8	0.15
(1,1119)	1:432:A:VAL:HG13	1:431:A:GLU:HB3	10	0.15
(1,1111)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	45	0.15
(1,1109)	1:439:A:LEU:HD22	1:401:A:GLU:HB2	29	0.15
(1,1107)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	34	0.15
(1,1101)	1:436:A:LEU:HD12	1:436:A:LEU:HB2	13	0.15
(1,1101)	1:436:A:LEU:HD23	1:436:A:LEU:HB3	19	0.15
(1,1101)	1:436:A:LEU:HD21	1:436:A:LEU:HB3	23	0.15
(1,1101)	1:436:A:LEU:HD23	1:436:A:LEU:HB3	30	0.15
(1,1100)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	22	0.15
(1,1100)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	28	0.15
(1,1100)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	37	0.15
(1,1099)	1:408:A:LEU:HD22	1:408:A:LEU:HG	34	0.15
(1,1097)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	22	0.15
(1,1097)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	28	0.15
(1,1097)	1:423:A:LEU:HD22	1:423:A:LEU:HB3	31	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1049)	1:435:A:ILE:HG13	1:431:A:GLU:HA	24	0.15
(1,1049)	1:435:A:ILE:HG13	1:431:A:GLU:HA	45	0.15
(1,1045)	1:435:A:ILE:HG13	1:431:A:GLU:HA	8	0.15
(1,1000)	1:420:A:ILE:HG22	1:420:A:ILE:HA	2	0.15
(1,1000)	1:420:A:ILE:HG23	1:420:A:ILE:HA	30	0.15
(1,1000)	1:420:A:ILE:HG22	1:420:A:ILE:HA	46	0.15
(1,988)	1:406:A:GLU:HB2	1:403:A:ARG:HA	32	0.15
(1,986)	1:410:A:ASN:HB2	1:407:A:PHE:HA	44	0.15
(1,974)	1:403:A:ARG:HD3	1:400:A:GLU:HG2	21	0.15
(1,963)	1:410:A:ASN:HB2	1:409:A:LEU:HB3	23	0.15
(1,924)	1:412:A:LEU:HB2	1:429:A:LEU:HD22	23	0.15
(1,924)	1:428:A:ARG:HB3	1:429:A:LEU:HD23	24	0.15
(1,924)	1:412:A:LEU:HB2	1:429:A:LEU:HD23	43	0.15
(1,921)	1:409:A:LEU:HG	1:412:A:LEU:HD21	30	0.15
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD21	10	0.15
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	9	0.15
(1,910)	1:440:A:LYS:HG2	1:436:A:LEU:HD11	47	0.15
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	35	0.15
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG22	29	0.15
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG22	45	0.15
(1,868)	1:416:A:LEU:HA	1:420:A:ILE:HG21	47	0.15
(1,866)	1:423:A:LEU:HA	1:423:A:LEU:HD11	26	0.15
(1,813)	1:406:A:GLU:HA	1:405:A:GLN:HB3	37	0.15
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	26	0.15
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	43	0.15
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	44	0.15
(1,794)	1:430:A:TRP:HD1	1:433:A:GLN:HA	3	0.15
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	35	0.15
(1,786)	1:405:A:GLN:HE22	1:439:A:LEU:HB2	37	0.15
(1,778)	1:428:A:ARG:H	1:428:A:ARG:HG2	34	0.15
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	12	0.15
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	1	0.15
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	2	0.15
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	7	0.15
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	8	0.15
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	11	0.15
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	13	0.15
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	16	0.15
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	23	0.15
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	24	0.15
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	34	0.15
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG23	33	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,734)	1:399:A:LYS:H	1:399:A:LYS:HD3	28	0.15
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	48	0.15
(1,726)	1:446:A:ALA:H	1:445:A:GLU:HA	13	0.15
(1,726)	1:446:A:ALA:H	1:445:A:GLU:HA	33	0.15
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD11	34	0.15
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD12	34	0.15
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD13	34	0.15
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	13	0.15
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	1	0.15
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	1	0.15
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	1	0.15
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	37	0.15
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	37	0.15
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	37	0.15
(1,642)	1:416:A:LEU:H	1:412:A:LEU:HB2	23	0.15
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	21	0.15
(1,633)	1:426:A:GLU:H	1:428:A:ARG:HB2	15	0.15
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD3	26	0.15
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	36	0.15
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG21	37	0.15
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG22	37	0.15
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG23	37	0.15
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG21	37	0.15
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG22	37	0.15
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG23	37	0.15
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG21	37	0.15
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG22	37	0.15
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG23	37	0.15
(1,500)	1:413:A:HIS:HB2	1:410:A:ASN:HA	49	0.15
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD21	12	0.15
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD22	12	0.15
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD23	12	0.15
(1,395)	1:416:A:LEU:H	1:415:A:ASP:HB2	42	0.15
(1,370)	1:419:A:GLY:H	1:419:A:GLY:HA2	23	0.15
(1,370)	1:419:A:GLY:H	1:419:A:GLY:HA2	47	0.15
(1,361)	1:414:A:ARG:H	1:414:A:ARG:HB3	18	0.15
(1,361)	1:414:A:ARG:H	1:414:A:ARG:HB3	37	0.15
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	17	0.15
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	23	0.15
(1,344)	1:412:A:LEU:H	1:411:A:SER:HB2	23	0.15
(1,342)	1:422:A:ASP:H	1:421:A:LYS:HB3	4	0.15
(1,342)	1:422:A:ASP:H	1:421:A:LYS:HB3	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,342)	1:422:A:ASP:H	1:421:A:LYS:HB3	22	0.15
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	1	0.15
(1,337)	1:437:A:THR:H	1:436:A:LEU:HB2	12	0.15
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	16	0.15
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	50	0.15
(1,249)	1:401:A:GLU:HA	1:401:A:GLU:HB3	3	0.15
(1,249)	1:401:A:GLU:HA	1:401:A:GLU:HB2	32	0.15
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	10	0.15
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	26	0.15
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	47	0.15
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HB2	4	0.15
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	15	0.15
(1,114)	1:398:A:ILE:HG12	1:401:A:GLU:HB2	10	0.15
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	16	0.15
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	16	0.15
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	16	0.15
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	16	0.15
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	16	0.15
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	16	0.15
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	16	0.15
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	16	0.15
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	16	0.15
(1,79)	1:430:A:TRP:HB3	1:427:A:GLU:HA	39	0.15
(1,38)	1:425:A:LYS:HA	1:425:A:LYS:HG2	24	0.15
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	6	0.15
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	17	0.15
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	19	0.15
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	38	0.15
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	39	0.15
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	40	0.15
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	41	0.15
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	7	0.14
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	17	0.14
(2,3)	1:406:A:GLU:HB3	1:410:A:ASN:HA	12	0.14
(2,3)	1:406:A:GLU:HB3	1:410:A:ASN:HA	36	0.14
(2,3)	1:406:A:GLU:HB3	1:410:A:ASN:HA	47	0.14
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	5	0.14
(1,1199)	1:428:A:ARG:HB3	1:428:A:ARG:HG2	46	0.14
(1,1161)	1:441:A:ARG:HG2	1:445:A:GLU:HG2	4	0.14
(1,1161)	1:441:A:ARG:HG2	1:445:A:GLU:HG2	10	0.14
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	5	0.14
(1,1132)	1:408:A:LEU:HD22	1:404:A:ARG:HB3	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1127)	1:420:A:ILE:HG22	1:422:A:ASP:HB3	4	0.14
(1,1127)	1:420:A:ILE:HG21	1:422:A:ASP:HB3	35	0.14
(1,1117)	1:412:A:LEU:HD22	1:408:A:LEU:HB2	2	0.14
(1,1117)	1:412:A:LEU:HD23	1:408:A:LEU:HB2	29	0.14
(1,1109)	1:402:A:ILE:HG12	1:406:A:GLU:HB2	38	0.14
(1,1107)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	16	0.14
(1,1107)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	50	0.14
(1,1101)	1:436:A:LEU:HD11	1:436:A:LEU:HB2	4	0.14
(1,1101)	1:436:A:LEU:HD12	1:436:A:LEU:HB2	7	0.14
(1,1101)	1:436:A:LEU:HD23	1:436:A:LEU:HB3	12	0.14
(1,1101)	1:398:A:ILE:HG22	1:440:A:LYS:HB3	24	0.14
(1,1101)	1:436:A:LEU:HD12	1:436:A:LEU:HB2	25	0.14
(1,1101)	1:436:A:LEU:HD23	1:436:A:LEU:HB3	48	0.14
(1,1100)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	2	0.14
(1,1100)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	38	0.14
(1,1100)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	43	0.14
(1,1100)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	46	0.14
(1,1100)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	50	0.14
(1,1097)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	2	0.14
(1,1097)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	38	0.14
(1,1097)	1:423:A:LEU:HD21	1:423:A:LEU:HB3	40	0.14
(1,1097)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	43	0.14
(1,1097)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	46	0.14
(1,1097)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	50	0.14
(1,1095)	1:398:A:ILE:HG22	1:440:A:LYS:HE3	9	0.14
(1,1045)	1:435:A:ILE:HG13	1:431:A:GLU:HA	31	0.14
(1,1006)	1:412:A:LEU:HD13	1:413:A:HIS:HA	12	0.14
(1,1000)	1:420:A:ILE:HG21	1:420:A:ILE:HA	10	0.14
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	7	0.14
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	13	0.14
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	29	0.14
(1,988)	1:406:A:GLU:HB2	1:403:A:ARG:HA	25	0.14
(1,974)	1:403:A:ARG:HD2	1:400:A:GLU:HG3	18	0.14
(1,933)	1:409:A:LEU:HG	1:432:A:VAL:HG12	42	0.14
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	5	0.14
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	6	0.14
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	12	0.14
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	20	0.14
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	22	0.14
(1,910)	1:440:A:LYS:HG2	1:436:A:LEU:HD11	10	0.14
(1,875)	1:413:A:HIS:HA	1:416:A:LEU:HD23	42	0.14
(1,866)	1:423:A:LEU:HA	1:423:A:LEU:HD12	28	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB2	1	0.14
(1,842)	1:437:A:THR:HB	1:434:A:ARG:HB2	1	0.14
(1,842)	1:437:A:THR:HB	1:434:A:ARG:HB2	7	0.14
(1,825)	1:439:A:LEU:HA	1:442:A:LYS:HD3	7	0.14
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	34	0.14
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	47	0.14
(1,797)	1:395:A:GLN:HE21	1:398:A:ILE:HG23	3	0.14
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	28	0.14
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	41	0.14
(1,786)	1:405:A:GLN:HE22	1:402:A:ILE:HB	25	0.14
(1,782)	1:407:A:PHE:HD2	1:403:A:ARG:HB3	39	0.14
(1,769)	1:429:A:LEU:H	1:428:A:ARG:HA	20	0.14
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	13	0.14
(1,758)	1:428:A:ARG:H	1:428:A:ARG:HB2	21	0.14
(1,758)	1:428:A:ARG:H	1:428:A:ARG:HB2	28	0.14
(1,753)	1:434:A:ARG:H	1:433:A:GLN:HG2	6	0.14
(1,753)	1:434:A:ARG:H	1:433:A:GLN:HG2	12	0.14
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	5	0.14
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	15	0.14
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	18	0.14
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	19	0.14
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	20	0.14
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	25	0.14
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	33	0.14
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	35	0.14
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	36	0.14
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	37	0.14
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	38	0.14
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	40	0.14
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	42	0.14
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	49	0.14
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG22	17	0.14
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG22	35	0.14
(1,739)	1:439:A:LEU:H	1:439:A:LEU:HD12	50	0.14
(1,735)	1:440:A:LYS:H	1:440:A:LYS:HG2	34	0.14
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	27	0.14
(1,726)	1:446:A:ALA:H	1:445:A:GLU:HA	34	0.14
(1,726)	1:446:A:ALA:H	1:445:A:GLU:HA	50	0.14
(1,724)	1:405:A:GLN:H	1:405:A:GLN:HE22	28	0.14
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD21	7	0.14
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD22	7	0.14
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD23	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD11	26	0.14
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD12	26	0.14
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD13	26	0.14
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	40	0.14
(1,642)	1:416:A:LEU:H	1:412:A:LEU:HB2	28	0.14
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG2	25	0.14
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	27	0.14
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD2	47	0.14
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD3	48	0.14
(1,500)	1:413:A:HIS:HB2	1:410:A:ASN:HA	31	0.14
(1,370)	1:419:A:GLY:H	1:419:A:GLY:HA2	27	0.14
(1,360)	1:414:A:ARG:H	1:414:A:ARG:HD2	47	0.14
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	36	0.14
(1,342)	1:422:A:ASP:H	1:421:A:LYS:HB2	9	0.14
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD21	38	0.14
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD22	38	0.14
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD23	38	0.14
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD21	39	0.14
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD22	39	0.14
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD23	39	0.14
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD21	47	0.14
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD22	47	0.14
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD23	47	0.14
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	6	0.14
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	11	0.14
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	15	0.14
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	23	0.14
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	38	0.14
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	7	0.14
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	14	0.14
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	28	0.14
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	32	0.14
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB2	44	0.14
(1,229)	1:396:A:ALA:H	1:394:A:THR:HA	4	0.14
(1,229)	1:396:A:ALA:H	1:394:A:THR:HA	17	0.14
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	7	0.14
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	31	0.14
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	40	0.14
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	45	0.14
(1,89)	1:394:A:THR:HG23	1:394:A:THR:HB	4	0.14
(1,89)	1:394:A:THR:HG21	1:394:A:THR:HB	37	0.14
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	5	0.14
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	5	0.14
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	5	0.14
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	5	0.14
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	5	0.14
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	5	0.14
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	5	0.14
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	5	0.14
(1,72)	1:440:A:LYS:HE3	1:441:A:ARG:HG2	49	0.14
(1,38)	1:425:A:LYS:HA	1:425:A:LYS:HG2	36	0.14
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	4	0.14
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	49	0.14
(1,19)	1:413:A:HIS:HD2	1:429:A:LEU:HB3	21	0.14
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	48	0.14
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD11	15	0.14
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD12	15	0.14
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD13	15	0.14
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	1	0.13
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	10	0.13
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	19	0.13
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	31	0.13
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	33	0.13
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	49	0.13
(2,3)	1:406:A:GLU:HB3	1:410:A:ASN:HA	1	0.13
(1,1282)	1:446:A:ALA:H	1:444:A:ARG:HG2	35	0.13
(1,1225)	1:427:A:GLU:H	1:416:A:LEU:HD13	18	0.13
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	36	0.13
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	39	0.13
(1,1196)	1:402:A:ILE:HD12	1:440:A:LYS:HG2	23	0.13
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	36	0.13
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	39	0.13
(1,1159)	1:399:A:LYS:HG2	1:399:A:LYS:HD3	2	0.13
(1,1159)	1:399:A:LYS:HG2	1:399:A:LYS:HD3	10	0.13
(1,1159)	1:399:A:LYS:HG2	1:399:A:LYS:HD3	24	0.13
(1,1143)	1:398:A:ILE:HG22	1:399:A:LYS:HE2	20	0.13
(1,1116)	1:435:A:ILE:HD13	1:431:A:GLU:HG2	47	0.13
(1,1113)	1:436:A:LEU:HD23	1:432:A:VAL:HB	11	0.13
(1,1113)	1:436:A:LEU:HD23	1:432:A:VAL:HB	22	0.13
(1,1112)	1:436:A:LEU:HD23	1:432:A:VAL:HB	11	0.13
(1,1112)	1:436:A:LEU:HD23	1:432:A:VAL:HB	22	0.13
(1,1109)	1:439:A:LEU:HD21	1:401:A:GLU:HB2	11	0.13
(1,1107)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	41	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1101)	1:436:A:LEU:HD22	1:436:A:LEU:HB3	18	0.13
(1,1101)	1:436:A:LEU:HD21	1:436:A:LEU:HB3	27	0.13
(1,1101)	1:436:A:LEU:HD12	1:436:A:LEU:HB2	45	0.13
(1,1100)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	8	0.13
(1,1100)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	36	0.13
(1,1100)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	44	0.13
(1,1097)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	8	0.13
(1,1097)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	36	0.13
(1,1097)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	44	0.13
(1,1095)	1:398:A:ILE:HG21	1:440:A:LYS:HE3	28	0.13
(1,1049)	1:435:A:ILE:HG13	1:431:A:GLU:HA	27	0.13
(1,999)	1:412:A:LEU:HB2	1:412:A:LEU:HA	39	0.13
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	35	0.13
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	42	0.13
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	48	0.13
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	50	0.13
(1,974)	1:403:A:ARG:HD3	1:400:A:GLU:HG2	49	0.13
(1,967)	1:405:A:GLN:HG2	1:408:A:LEU:HG	39	0.13
(1,963)	1:410:A:ASN:HB2	1:409:A:LEU:HB3	18	0.13
(1,937)	1:440:A:LYS:HE2	1:402:A:ILE:HD12	2	0.13
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	4	0.13
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	31	0.13
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	33	0.13
(1,842)	1:437:A:THR:HB	1:434:A:ARG:HB2	11	0.13
(1,813)	1:397:A:GLY:HA2	1:400:A:GLU:HB2	4	0.13
(1,813)	1:406:A:GLU:HA	1:405:A:GLN:HB2	12	0.13
(1,808)	1:416:A:LEU:HA	1:417:A:GLN:HG3	45	0.13
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	49	0.13
(1,769)	1:407:A:PHE:H	1:404:A:ARG:HA	28	0.13
(1,764)	1:405:A:GLN:H	1:403:A:ARG:HB2	26	0.13
(1,762)	1:436:A:LEU:H	1:432:A:VAL:HG11	9	0.13
(1,758)	1:442:A:LYS:H	1:441:A:ARG:HB2	4	0.13
(1,758)	1:442:A:LYS:H	1:441:A:ARG:HB2	48	0.13
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	3	0.13
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	4	0.13
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	6	0.13
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	10	0.13
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	12	0.13
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	14	0.13
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	17	0.13
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	21	0.13
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	22	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	30	0.13
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	39	0.13
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	43	0.13
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	46	0.13
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	48	0.13
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	50	0.13
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG23	8	0.13
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG21	30	0.13
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG23	41	0.13
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG23	46	0.13
(1,737)	1:440:A:LYS:H	1:398:A:ILE:HD13	27	0.13
(1,735)	1:440:A:LYS:H	1:440:A:LYS:HG2	48	0.13
(1,726)	1:446:A:ALA:H	1:445:A:GLU:HA	37	0.13
(1,654)	1:399:A:LYS:H	1:395:A:GLN:HB3	46	0.13
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD21	14	0.13
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD22	14	0.13
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD23	14	0.13
(1,472)	1:410:A:ASN:HD22	1:414:A:ARG:HB2	46	0.13
(1,469)	1:394:A:THR:HA	1:396:A:ALA:HB1	41	0.13
(1,469)	1:394:A:THR:HA	1:396:A:ALA:HB2	41	0.13
(1,469)	1:394:A:THR:HA	1:396:A:ALA:HB3	41	0.13
(1,344)	1:412:A:LEU:H	1:411:A:SER:HB2	15	0.13
(1,342)	1:422:A:ASP:H	1:421:A:LYS:HB3	17	0.13
(1,342)	1:422:A:ASP:H	1:421:A:LYS:HB3	21	0.13
(1,341)	1:422:A:ASP:H	1:421:A:LYS:HA	44	0.13
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD21	4	0.13
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD22	4	0.13
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD23	4	0.13
(1,308)	1:439:A:LEU:H	1:440:A:LYS:HD3	16	0.13
(1,303)	1:430:A:TRP:HE1	1:433:A:GLN:HB2	12	0.13
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	1	0.13
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	2	0.13
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	25	0.13
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	32	0.13
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	42	0.13
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	49	0.13
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	8	0.13
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	12	0.13
(1,238)	1:411:A:SER:H	1:411:A:SER:HB3	15	0.13
(1,211)	1:430:A:TRP:H	1:427:A:GLU:HA	39	0.13
(1,121)	1:429:A:LEU:HD11	1:433:A:GLN:HG3	47	0.13
(1,121)	1:429:A:LEU:HD12	1:433:A:GLN:HG3	47	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:429:A:LEU:HD13	1:433:A:GLN:HG3	47	0.13
(1,117)	1:398:A:ILE:HG13	1:399:A:LYS:HE3	3	0.13
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	3	0.13
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	14	0.13
(1,89)	1:394:A:THR:HG22	1:394:A:THR:HA	35	0.13
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	7	0.13
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	12	0.13
(1,17)	1:441:A:ARG:H	1:445:A:GLU:HG3	21	0.13
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB2	18	0.13
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD11	23	0.13
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD12	23	0.13
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD13	23	0.13
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD11	42	0.13
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD12	42	0.13
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD13	42	0.13
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	2	0.12
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	14	0.12
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	34	0.12
(2,3)	1:406:A:GLU:HB3	1:410:A:ASN:HA	6	0.12
(2,3)	1:406:A:GLU:HB3	1:410:A:ASN:HA	9	0.12
(2,3)	1:406:A:GLU:HB3	1:410:A:ASN:HA	19	0.12
(1,1196)	1:398:A:ILE:HD12	1:399:A:LYS:HG2	30	0.12
(1,1161)	1:441:A:ARG:HG2	1:445:A:GLU:HG2	27	0.12
(1,1159)	1:399:A:LYS:HG2	1:399:A:LYS:HD3	34	0.12
(1,1157)	1:396:A:ALA:HB2	1:395:A:GLN:HB3	21	0.12
(1,1150)	1:442:A:LYS:HD3	1:442:A:LYS:HB3	37	0.12
(1,1150)	1:442:A:LYS:HD2	1:442:A:LYS:HB3	49	0.12
(1,1137)	1:412:A:LEU:HD21	1:432:A:VAL:HB	44	0.12
(1,1125)	1:409:A:LEU:HD12	1:433:A:GLN:HB2	16	0.12
(1,1117)	1:412:A:LEU:HD22	1:408:A:LEU:HB2	40	0.12
(1,1111)	1:398:A:ILE:HG13	1:440:A:LYS:HD3	35	0.12
(1,1104)	1:435:A:ILE:HG22	1:435:A:ILE:HB	25	0.12
(1,1101)	1:436:A:LEU:HD23	1:436:A:LEU:HB3	5	0.12
(1,1101)	1:436:A:LEU:HD21	1:436:A:LEU:HB3	8	0.12
(1,1101)	1:436:A:LEU:HD21	1:436:A:LEU:HB3	21	0.12
(1,1101)	1:436:A:LEU:HD21	1:436:A:LEU:HB3	35	0.12
(1,1101)	1:398:A:ILE:HG21	1:440:A:LYS:HB3	36	0.12
(1,1101)	1:436:A:LEU:HD21	1:436:A:LEU:HB3	38	0.12
(1,1101)	1:436:A:LEU:HD21	1:436:A:LEU:HB3	40	0.12
(1,1101)	1:436:A:LEU:HD21	1:436:A:LEU:HB3	42	0.12
(1,1100)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	26	0.12
(1,1100)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	49	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1097)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	26	0.12
(1,1097)	1:416:A:LEU:HD12	1:416:A:LEU:HB2	37	0.12
(1,1097)	1:409:A:LEU:HD11	1:409:A:LEU:HB2	49	0.12
(1,1049)	1:435:A:ILE:HG13	1:431:A:GLU:HA	25	0.12
(1,1017)	1:398:A:ILE:HG12	1:436:A:LEU:HA	47	0.12
(1,999)	1:412:A:LEU:HB3	1:412:A:LEU:HA	14	0.12
(1,999)	1:442:A:LYS:HB2	1:442:A:LYS:HA	19	0.12
(1,988)	1:406:A:GLU:HB2	1:403:A:ARG:HA	16	0.12
(1,947)	1:399:A:LYS:HE3	1:398:A:ILE:HG13	42	0.12
(1,924)	1:412:A:LEU:HB2	1:429:A:LEU:HD21	50	0.12
(1,923)	1:413:A:HIS:HB2	1:412:A:LEU:HG	49	0.12
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	24	0.12
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	46	0.12
(1,910)	1:399:A:LYS:HG2	1:398:A:ILE:HD12	30	0.12
(1,910)	1:399:A:LYS:HG3	1:402:A:ILE:HG23	38	0.12
(1,907)	1:405:A:GLN:HG3	1:408:A:LEU:HD21	34	0.12
(1,907)	1:405:A:GLN:HG3	1:408:A:LEU:HD23	43	0.12
(1,856)	1:409:A:LEU:HA	1:409:A:LEU:HG	41	0.12
(1,805)	1:428:A:ARG:HA	1:428:A:ARG:HD2	1	0.12
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	11	0.12
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	15	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	1	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	3	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	5	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	8	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	14	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	16	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	17	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	19	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	21	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	22	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	23	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	24	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	26	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	30	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	32	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	33	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	34	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	36	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	38	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	40	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	42	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	43	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	44	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	46	0.12
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	47	0.12
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	30	0.12
(1,776)	1:444:A:ARG:H	1:443:A:LEU:HB2	40	0.12
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	19	0.12
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	44	0.12
(1,765)	1:405:A:GLN:H	1:405:A:GLN:HG3	28	0.12
(1,758)	1:442:A:LYS:H	1:442:A:LYS:HB2	9	0.12
(1,758)	1:442:A:LYS:H	1:442:A:LYS:HB2	37	0.12
(1,753)	1:434:A:ARG:H	1:433:A:GLN:HG2	36	0.12
(1,751)	1:398:A:ILE:HA	1:439:A:LEU:HD21	25	0.12
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	31	0.12
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG22	5	0.12
(1,739)	1:439:A:LEU:H	1:439:A:LEU:HD11	15	0.12
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD11	39	0.12
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD12	39	0.12
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD13	39	0.12
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	48	0.12
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD2	8	0.12
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	25	0.12
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD21	4	0.12
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD22	4	0.12
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD23	4	0.12
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG21	36	0.12
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG22	36	0.12
(1,526)	1:429:A:LEU:HD11	1:432:A:VAL:HG23	36	0.12
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG21	36	0.12
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG22	36	0.12
(1,526)	1:429:A:LEU:HD12	1:432:A:VAL:HG23	36	0.12
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG21	36	0.12
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG22	36	0.12
(1,526)	1:429:A:LEU:HD13	1:432:A:VAL:HG23	36	0.12
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD21	29	0.12
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD22	29	0.12
(1,488)	1:413:A:HIS:HB2	1:429:A:LEU:HD23	29	0.12
(1,391)	1:417:A:GLN:H	1:417:A:GLN:HB3	42	0.12
(1,359)	1:414:A:ARG:H	1:413:A:HIS:HB2	50	0.12
(1,342)	1:422:A:ASP:H	1:421:A:LYS:HB3	34	0.12
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD21	17	0.12
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD22	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD23	17	0.12
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD21	43	0.12
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD22	43	0.12
(1,332)	1:413:A:HIS:H	1:429:A:LEU:HD23	43	0.12
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	39	0.12
(1,303)	1:430:A:TRP:HE1	1:433:A:GLN:HB2	17	0.12
(1,303)	1:430:A:TRP:HE1	1:433:A:GLN:HB2	19	0.12
(1,303)	1:430:A:TRP:HE1	1:433:A:GLN:HB2	25	0.12
(1,278)	1:429:A:LEU:H	1:428:A:ARG:H	3	0.12
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	12	0.12
(1,258)	1:394:A:THR:H	1:394:A:THR:HB	19	0.12
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	26	0.12
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	5	0.12
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	27	0.12
(1,242)	1:435:A:ILE:H	1:434:A:ARG:HB3	31	0.12
(1,193)	1:434:A:ARG:H	1:433:A:GLN:H	1	0.12
(1,143)	1:441:A:ARG:H	1:440:A:LYS:HA	2	0.12
(1,120)	1:408:A:LEU:HD11	1:410:A:ASN:HB3	19	0.12
(1,120)	1:408:A:LEU:HD12	1:410:A:ASN:HB3	19	0.12
(1,120)	1:408:A:LEU:HD13	1:410:A:ASN:HB3	19	0.12
(1,117)	1:398:A:ILE:HG13	1:399:A:LYS:HE3	33	0.12
(1,117)	1:398:A:ILE:HG13	1:399:A:LYS:HE3	47	0.12
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	11	0.12
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	21	0.12
(1,89)	1:394:A:THR:HG23	1:394:A:THR:HB	2	0.12
(1,89)	1:394:A:THR:HG23	1:394:A:THR:HB	13	0.12
(1,89)	1:394:A:THR:HG22	1:394:A:THR:HA	19	0.12
(1,89)	1:394:A:THR:HG21	1:394:A:THR:HA	26	0.12
(1,89)	1:394:A:THR:HG23	1:394:A:THR:HA	50	0.12
(1,72)	1:440:A:LYS:HE2	1:441:A:ARG:HG2	9	0.12
(1,46)	1:436:A:LEU:HA	1:398:A:ILE:HG12	47	0.12
(1,21)	1:430:A:TRP:HD1	1:434:A:ARG:HB3	50	0.12
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD11	36	0.12
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD12	36	0.12
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD13	36	0.12
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD11	46	0.12
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD12	46	0.12
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD13	46	0.12
(1,5)	1:394:A:THR:H	1:393:A:GLU:HB3	28	0.12
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	5	0.11
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	22	0.11
(2,10)	1:413:A:HIS:HD2	1:410:A:ASN:HA	41	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:406:A:GLU:HB3	1:410:A:ASN:HA	2	0.11
(2,3)	1:406:A:GLU:HB3	1:410:A:ASN:HA	11	0.11
(1,1206)	1:398:A:ILE:H	1:399:A:LYS:HD2	25	0.11
(1,1199)	1:428:A:ARG:HB3	1:428:A:ARG:HG2	8	0.11
(1,1199)	1:441:A:ARG:HB2	1:441:A:ARG:HG3	14	0.11
(1,1199)	1:414:A:ARG:HB3	1:414:A:ARG:HG2	20	0.11
(1,1199)	1:403:A:ARG:HB3	1:403:A:ARG:HG2	44	0.11
(1,1165)	1:446:A:ALA:HB2	1:445:A:GLU:HB2	33	0.11
(1,1160)	1:441:A:ARG:HG3	1:441:A:ARG:HB2	14	0.11
(1,1160)	1:414:A:ARG:HG2	1:414:A:ARG:HB3	20	0.11
(1,1160)	1:403:A:ARG:HG2	1:403:A:ARG:HB3	44	0.11
(1,1159)	1:399:A:LYS:HG2	1:399:A:LYS:HD3	16	0.11
(1,1159)	1:399:A:LYS:HG2	1:399:A:LYS:HD3	20	0.11
(1,1159)	1:399:A:LYS:HG2	1:399:A:LYS:HD3	38	0.11
(1,1159)	1:421:A:LYS:HG2	1:421:A:LYS:HD3	45	0.11
(1,1157)	1:396:A:ALA:HB2	1:400:A:GLU:HB2	31	0.11
(1,1150)	1:442:A:LYS:HD3	1:442:A:LYS:HB3	8	0.11
(1,1150)	1:442:A:LYS:HD2	1:442:A:LYS:HB3	10	0.11
(1,1150)	1:442:A:LYS:HD2	1:442:A:LYS:HB3	47	0.11
(1,1137)	1:412:A:LEU:HD21	1:432:A:VAL:HB	8	0.11
(1,1132)	1:408:A:LEU:HD12	1:405:A:GLN:HB3	26	0.11
(1,1132)	1:408:A:LEU:HD23	1:404:A:ARG:HB3	32	0.11
(1,1132)	1:408:A:LEU:HD12	1:405:A:GLN:HB3	42	0.11
(1,1116)	1:435:A:ILE:HD11	1:431:A:GLU:HG2	27	0.11
(1,1116)	1:435:A:ILE:HD12	1:431:A:GLU:HG2	30	0.11
(1,1113)	1:436:A:LEU:HD23	1:432:A:VAL:HB	14	0.11
(1,1112)	1:436:A:LEU:HD23	1:432:A:VAL:HB	14	0.11
(1,1109)	1:409:A:LEU:HD23	1:406:A:GLU:HB3	25	0.11
(1,1101)	1:436:A:LEU:HD21	1:436:A:LEU:HB3	2	0.11
(1,1101)	1:436:A:LEU:HD23	1:436:A:LEU:HB3	9	0.11
(1,1101)	1:436:A:LEU:HD23	1:436:A:LEU:HB3	16	0.11
(1,1101)	1:436:A:LEU:HD21	1:436:A:LEU:HB3	29	0.11
(1,1101)	1:398:A:ILE:HG21	1:440:A:LYS:HB3	43	0.11
(1,1100)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	3	0.11
(1,1100)	1:443:A:LEU:HD23	1:443:A:LEU:HB3	33	0.11
(1,1100)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	47	0.11
(1,1097)	1:409:A:LEU:HD12	1:409:A:LEU:HB2	3	0.11
(1,1097)	1:443:A:LEU:HD12	1:443:A:LEU:HB2	33	0.11
(1,1097)	1:409:A:LEU:HD13	1:409:A:LEU:HB2	47	0.11
(1,1049)	1:435:A:ILE:HG13	1:431:A:GLU:HA	50	0.11
(1,1045)	1:435:A:ILE:HG13	1:431:A:GLU:HA	13	0.11
(1,1045)	1:435:A:ILE:HG13	1:431:A:GLU:HA	35	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	1:412:A:LEU:HD13	1:413:A:HIS:HA	44	0.11
(1,1000)	1:420:A:ILE:HG22	1:420:A:ILE:HA	19	0.11
(1,1000)	1:420:A:ILE:HG22	1:420:A:ILE:HA	26	0.11
(1,999)	1:412:A:LEU:HB3	1:412:A:LEU:HA	50	0.11
(1,988)	1:406:A:GLU:HB2	1:403:A:ARG:HA	13	0.11
(1,963)	1:422:A:ASP:HB3	1:425:A:LYS:HB2	39	0.11
(1,957)	1:445:A:GLU:HG2	1:445:A:GLU:HB3	3	0.11
(1,957)	1:445:A:GLU:HG2	1:445:A:GLU:HB3	6	0.11
(1,957)	1:445:A:GLU:HG2	1:445:A:GLU:HB3	8	0.11
(1,937)	1:440:A:LYS:HE3	1:402:A:ILE:HD11	37	0.11
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD23	6	0.11
(1,919)	1:405:A:GLN:HG2	1:436:A:LEU:HD21	50	0.11
(1,913)	1:402:A:ILE:HA	1:398:A:ILE:HG12	44	0.11
(1,911)	1:405:A:GLN:HG3	1:436:A:LEU:HD21	2	0.11
(1,902)	1:406:A:GLU:HB2	1:402:A:ILE:HG12	42	0.11
(1,874)	1:426:A:GLU:HA	1:416:A:LEU:HD23	41	0.11
(1,873)	1:425:A:LYS:HA	1:412:A:LEU:HD23	34	0.11
(1,856)	1:409:A:LEU:HA	1:409:A:LEU:HG	16	0.11
(1,846)	1:443:A:LEU:HA	1:446:A:ALA:HB2	41	0.11
(1,813)	1:406:A:GLU:HA	1:405:A:GLN:HB3	10	0.11
(1,808)	1:416:A:LEU:HA	1:417:A:GLN:HG3	12	0.11
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	27	0.11
(1,802)	1:397:A:GLY:HA2	1:394:A:THR:HB	39	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	2	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	4	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	6	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	7	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	9	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	10	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	11	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	12	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	13	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	15	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	18	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	20	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	25	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	27	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	28	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	29	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	31	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	35	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	37	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	39	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	41	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	45	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	48	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	49	0.11
(1,801)	1:437:A:THR:HA	1:437:A:THR:HB	50	0.11
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	18	0.11
(1,783)	1:407:A:PHE:HD2	1:404:A:ARG:HG3	48	0.11
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	38	0.11
(1,758)	1:442:A:LYS:H	1:442:A:LYS:HB2	2	0.11
(1,753)	1:434:A:ARG:H	1:433:A:GLN:HG2	7	0.11
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	9	0.11
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	26	0.11
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	27	0.11
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	28	0.11
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	29	0.11
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	32	0.11
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	44	0.11
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	45	0.11
(1,748)	1:396:A:ALA:H	1:396:A:ALA:HA	47	0.11
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG23	26	0.11
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG21	29	0.11
(1,730)	1:441:A:ARG:H	1:398:A:ILE:HG21	28	0.11
(1,726)	1:446:A:ALA:H	1:445:A:GLU:HA	41	0.11
(1,726)	1:446:A:ALA:H	1:445:A:GLU:HA	49	0.11
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD21	16	0.11
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD22	16	0.11
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD23	16	0.11
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD11	34	0.11
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD12	34	0.11
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD13	34	0.11
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD21	43	0.11
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD22	43	0.11
(1,675)	1:444:A:ARG:H	1:443:A:LEU:HD23	43	0.11
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD2	20	0.11
(1,656)	1:399:A:LYS:H	1:399:A:LYS:HD2	21	0.11
(1,642)	1:416:A:LEU:H	1:412:A:LEU:HB3	41	0.11
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	6	0.11
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	37	0.11
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD3	3	0.11
(1,559)	1:430:A:TRP:HE1	1:434:A:ARG:HD2	12	0.11
(1,555)	1:395:A:GLN:HE21	1:395:A:GLN:HA	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	1:395:A:GLN:HE21	1:395:A:GLN:HA	33	0.11
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD21	1	0.11
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD22	1	0.11
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD23	1	0.11
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD21	45	0.11
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD22	45	0.11
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD23	45	0.11
(1,472)	1:410:A:ASN:HD22	1:414:A:ARG:HB2	5	0.11
(1,472)	1:410:A:ASN:HD22	1:414:A:ARG:HB2	40	0.11
(1,404)	1:444:A:ARG:H	1:444:A:ARG:HB3	20	0.11
(1,370)	1:419:A:GLY:H	1:419:A:GLY:HA2	3	0.11
(1,343)	1:418:A:GLY:H	1:417:A:GLN:HA	30	0.11
(1,342)	1:422:A:ASP:H	1:421:A:LYS:HB3	16	0.11
(1,325)	1:413:A:HIS:H	1:412:A:LEU:HB2	20	0.11
(1,320)	1:405:A:GLN:H	1:405:A:GLN:HG3	44	0.11
(1,277)	1:420:A:ILE:H	1:419:A:GLY:H	23	0.11
(1,260)	1:394:A:THR:H	1:394:A:THR:HG21	9	0.11
(1,260)	1:394:A:THR:H	1:394:A:THR:HG22	9	0.11
(1,260)	1:394:A:THR:H	1:394:A:THR:HG23	9	0.11
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	5	0.11
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	7	0.11
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	18	0.11
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	22	0.11
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	37	0.11
(1,249)	1:401:A:GLU:HA	1:401:A:GLU:HB3	21	0.11
(1,249)	1:401:A:GLU:HA	1:401:A:GLU:HB3	27	0.11
(1,249)	1:401:A:GLU:HA	1:401:A:GLU:HB3	44	0.11
(1,238)	1:411:A:SER:H	1:411:A:SER:HB3	23	0.11
(1,233)	1:398:A:ILE:HA	1:398:A:ILE:HB	28	0.11
(1,229)	1:396:A:ALA:H	1:394:A:THR:HA	30	0.11
(1,211)	1:430:A:TRP:H	1:427:A:GLU:HA	20	0.11
(1,193)	1:434:A:ARG:H	1:433:A:GLN:H	15	0.11
(1,117)	1:398:A:ILE:HG13	1:399:A:LYS:HE3	36	0.11
(1,117)	1:398:A:ILE:HG12	1:399:A:LYS:HE3	46	0.11
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	1	0.11
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	5	0.11
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	28	0.11
(1,98)	1:446:A:ALA:HB1	1:443:A:LEU:HA	14	0.11
(1,98)	1:446:A:ALA:HB2	1:443:A:LEU:HA	14	0.11
(1,98)	1:446:A:ALA:HB3	1:443:A:LEU:HA	14	0.11
(1,89)	1:394:A:THR:HG23	1:394:A:THR:HA	7	0.11
(1,89)	1:394:A:THR:HG23	1:394:A:THR:HA	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:394:A:THR:HG22	1:394:A:THR:HA	20	0.11
(1,89)	1:394:A:THR:HG23	1:394:A:THR:HA	21	0.11
(1,89)	1:394:A:THR:HG21	1:394:A:THR:HA	24	0.11
(1,89)	1:394:A:THR:HG23	1:394:A:THR:HA	30	0.11
(1,89)	1:394:A:THR:HG23	1:394:A:THR:HA	41	0.11
(1,79)	1:430:A:TRP:HB3	1:427:A:GLU:HA	40	0.11
(1,55)	1:417:A:GLN:HE21	1:414:A:ARG:HB3	49	0.11
(1,38)	1:425:A:LYS:HA	1:425:A:LYS:HG2	2	0.11
(1,38)	1:425:A:LYS:HA	1:425:A:LYS:HG2	18	0.11
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB2	25	0.11
(1,11)	1:424:A:SER:H	1:427:A:GLU:HB2	32	0.11
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD11	18	0.11
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD12	18	0.11
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD13	18	0.11
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD11	24	0.11
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD12	24	0.11
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD13	24	0.11
(2,3)	1:406:A:GLU:HB3	1:410:A:ASN:HA	20	0.1
(2,3)	1:406:A:GLU:HB3	1:410:A:ASN:HA	31	0.1
(2,2)	1:415:A:ASP:HB3	1:420:A:ILE:HG13	14	0.1
(1,1236)	1:430:A:TRP:HE1	1:434:A:ARG:HA	24	0.1
(1,1225)	1:427:A:GLU:H	1:412:A:LEU:HD13	3	0.1
(1,1199)	1:403:A:ARG:HB3	1:403:A:ARG:HG2	37	0.1
(1,1199)	1:414:A:ARG:HB3	1:414:A:ARG:HG2	43	0.1
(1,1160)	1:403:A:ARG:HG2	1:403:A:ARG:HB3	37	0.1
(1,1160)	1:414:A:ARG:HG2	1:414:A:ARG:HB3	43	0.1
(1,1159)	1:399:A:LYS:HG2	1:399:A:LYS:HD3	42	0.1
(1,1104)	1:412:A:LEU:HD11	1:412:A:LEU:HB2	23	0.1
(1,1104)	1:398:A:ILE:HG21	1:440:A:LYS:HB3	30	0.1
(1,1101)	1:436:A:LEU:HD11	1:436:A:LEU:HB2	20	0.1
(1,1045)	1:435:A:ILE:HG13	1:431:A:GLU:HA	18	0.1
(1,999)	1:412:A:LEU:HB3	1:412:A:LEU:HA	7	0.1
(1,999)	1:412:A:LEU:HB3	1:412:A:LEU:HA	48	0.1
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	2	0.1
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	10	0.1
(1,995)	1:422:A:ASP:HB3	1:415:A:ASP:HA	26	0.1
(1,963)	1:410:A:ASN:HB2	1:409:A:LEU:HB3	36	0.1
(1,957)	1:406:A:GLU:HB3	1:406:A:GLU:HG2	35	0.1
(1,938)	1:409:A:LEU:HG	1:408:A:LEU:HD13	48	0.1
(1,937)	1:440:A:LYS:HE3	1:402:A:ILE:HD12	39	0.1
(1,911)	1:406:A:GLU:HB3	1:409:A:LEU:HD22	9	0.1
(1,910)	1:399:A:LYS:HG3	1:402:A:ILE:HG21	28	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,907)	1:405:A:GLN:HG3	1:408:A:LEU:HD21	18	0.1
(1,805)	1:428:A:ARG:HA	1:428:A:ARG:HD3	26	0.1
(1,794)	1:430:A:TRP:HD1	1:434:A:ARG:HA	10	0.1
(1,768)	1:427:A:GLU:H	1:424:A:SER:HA	24	0.1
(1,766)	1:424:A:SER:H	1:423:A:LEU:HB2	26	0.1
(1,758)	1:428:A:ARG:H	1:428:A:ARG:HB2	19	0.1
(1,758)	1:442:A:LYS:H	1:442:A:LYS:HB2	24	0.1
(1,753)	1:434:A:ARG:H	1:433:A:GLN:HG2	42	0.1
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG22	11	0.1
(1,739)	1:439:A:LEU:H	1:435:A:ILE:HG22	16	0.1
(1,738)	1:440:A:LYS:HA	1:443:A:LEU:HB3	34	0.1
(1,733)	1:399:A:LYS:H	1:399:A:LYS:HB2	11	0.1
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD21	22	0.1
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD22	22	0.1
(1,713)	1:446:A:ALA:H	1:443:A:LEU:HD23	22	0.1
(1,678)	1:433:A:GLN:H	1:436:A:LEU:HB3	38	0.1
(1,640)	1:428:A:ARG:H	1:428:A:ARG:HG3	35	0.1
(1,569)	1:423:A:LEU:H	1:422:A:ASP:HA	3	0.1
(1,551)	1:410:A:ASN:HD22	1:407:A:PHE:HA	40	0.1
(1,544)	1:444:A:ARG:H	1:395:A:GLN:HE21	16	0.1
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD21	43	0.1
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD22	43	0.1
(1,531)	1:422:A:ASP:H	1:423:A:LEU:HD23	43	0.1
(1,469)	1:394:A:THR:HA	1:396:A:ALA:HB1	27	0.1
(1,469)	1:394:A:THR:HA	1:396:A:ALA:HB2	27	0.1
(1,469)	1:394:A:THR:HA	1:396:A:ALA:HB3	27	0.1
(1,465)	1:395:A:GLN:HE21	1:443:A:LEU:HB3	7	0.1
(1,366)	1:429:A:LEU:H	1:429:A:LEU:HB3	47	0.1
(1,364)	1:427:A:GLU:H	1:427:A:GLU:HG2	49	0.1
(1,342)	1:422:A:ASP:H	1:421:A:LYS:HB3	29	0.1
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	31	0.1
(1,258)	1:394:A:THR:H	1:394:A:THR:HA	48	0.1
(1,238)	1:411:A:SER:H	1:411:A:SER:HB3	35	0.1
(1,230)	1:398:A:ILE:H	1:399:A:LYS:H	26	0.1
(1,228)	1:397:A:GLY:H	1:398:A:ILE:H	4	0.1
(1,193)	1:434:A:ARG:H	1:433:A:GLN:H	50	0.1
(1,143)	1:441:A:ARG:H	1:440:A:LYS:HA	26	0.1
(1,143)	1:441:A:ARG:H	1:440:A:LYS:HA	44	0.1
(1,116)	1:439:A:LEU:HG	1:443:A:LEU:HG	20	0.1
(1,89)	1:394:A:THR:HG21	1:394:A:THR:HA	14	0.1
(1,89)	1:394:A:THR:HG21	1:394:A:THR:HA	27	0.1
(1,89)	1:394:A:THR:HG21	1:394:A:THR:HA	42	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:394:A:THR:HG22	1:394:A:THR:HA	45	0.1
(1,89)	1:394:A:THR:HG23	1:394:A:THR:HA	46	0.1
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD21	39	0.1
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD22	39	0.1
(1,81)	1:432:A:VAL:HG21	1:412:A:LEU:HD23	39	0.1
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD21	39	0.1
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD22	39	0.1
(1,81)	1:432:A:VAL:HG22	1:412:A:LEU:HD23	39	0.1
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD21	39	0.1
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD22	39	0.1
(1,81)	1:432:A:VAL:HG23	1:412:A:LEU:HD23	39	0.1
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD11	35	0.1
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD12	35	0.1
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD13	35	0.1
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD11	43	0.1
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD12	43	0.1
(1,6)	1:430:A:TRP:HE1	1:429:A:LEU:HD13	43	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found