Full wwPDB NMR Structure Validation Report (i)

Dec 25, 2024 – 03:57 PM EST

PDB ID	:	6V4T
BMRB ID	:	30503
Title	:	MPER-TMD of HIV-1 Env bound with the entry inhibitor S2C3
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Deposited on	:	2019-11-30

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

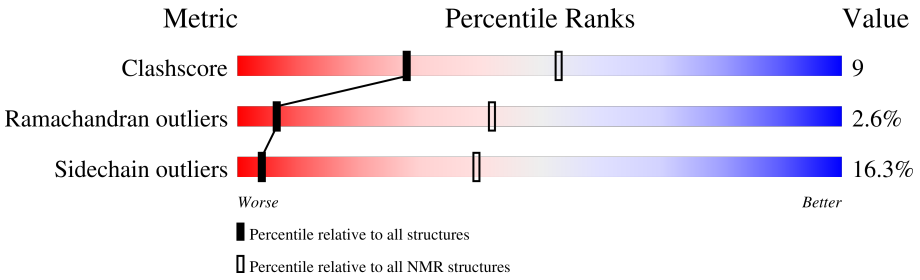
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 4%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain
1	A	51	73% 27%
1	B	51	76% 24%
1	C	51	67% 31% .

2 Ensemble composition and analysis

This entry contains 14 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:660-A:710, B:660-B:710, C:660-C:709 (152)	1.83	1

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

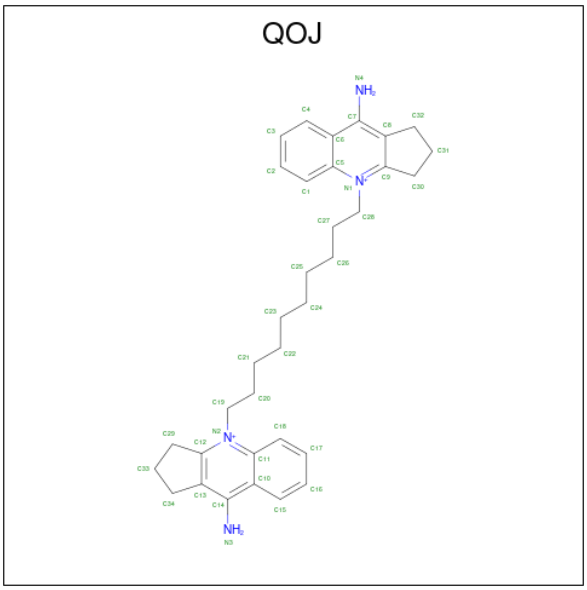
3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2958 atoms, of which 1521 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					Trace
1	A	51	Total	C	H	N	O	0
			904	301	463	73	67	
1	B	51	Total	C	H	N	O	0
			904	301	463	73	67	
1	C	51	Total	C	H	N	O	0
			904	301	463	73	67	

- Molecule 2 is 4,4'-(decane-1,10-diyl)bis(9-amino-2,3-dihydro-1H-cyclopenta[b]quinolin -4-ium) (three-letter code: QOJ) (formula: $C_{34}H_{44}N_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			
2	A	1	Total	C	H	N
			82	34	44	4
2	B	1	Total	C	H	N
			82	34	44	4
2	C	1	Total	C	H	N
			82	34	44	4

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: Envelope glycoprotein gp160

Chain A:

• Molecule 1: Envelope glycoprotein gp160

Chain B:

• Molecule 1: Envelope glycoprotein gp160

Chain C:

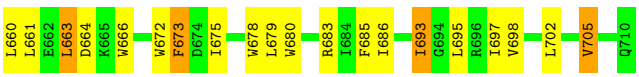
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

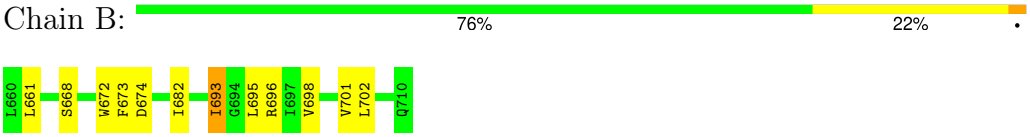
• Molecule 1: Envelope glycoprotein gp160

Chain A:



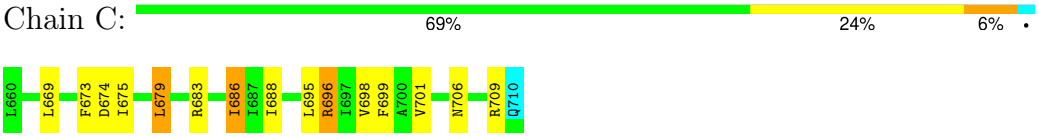
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

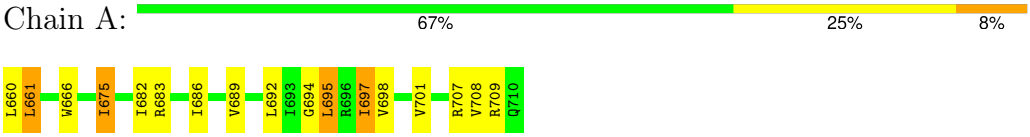
Chain C:



4.2.2 Score per residue for model 2

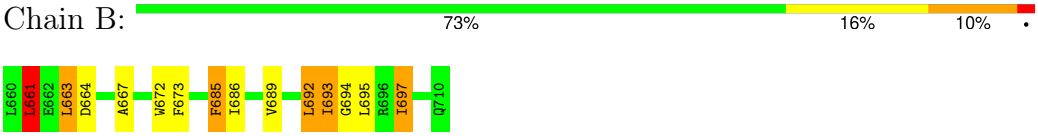
• Molecule 1: Envelope glycoprotein gp160

Chain A:



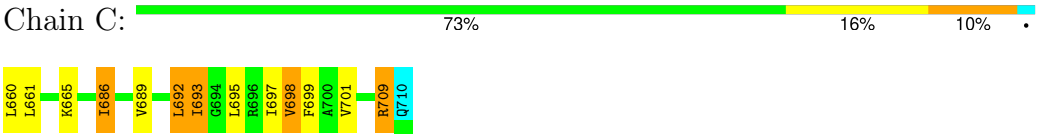
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

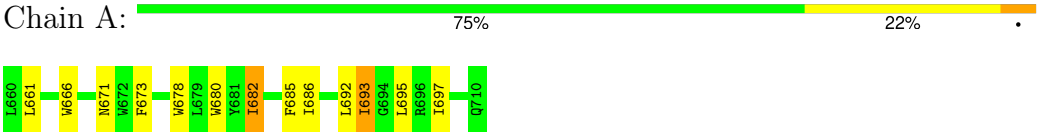
Chain C:



4.2.3 Score per residue for model 3

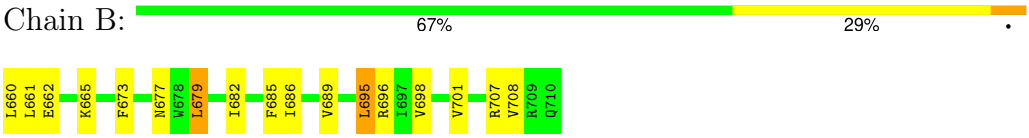
• Molecule 1: Envelope glycoprotein gp160

Chain A:



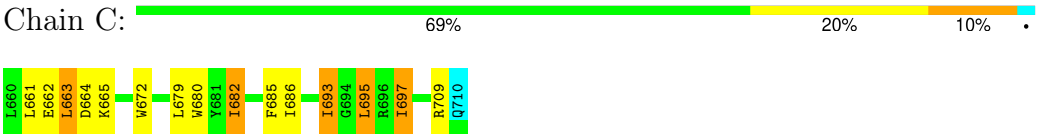
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

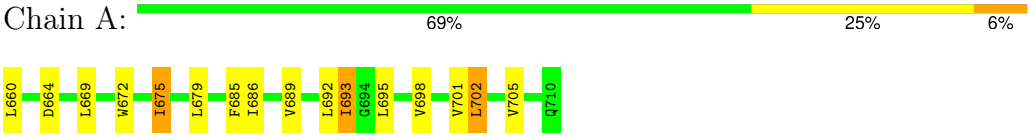
Chain C:



4.2.4 Score per residue for model 4

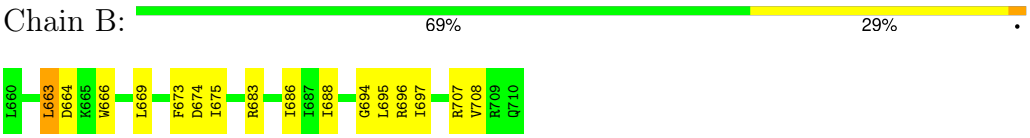
• Molecule 1: Envelope glycoprotein gp160

Chain A:



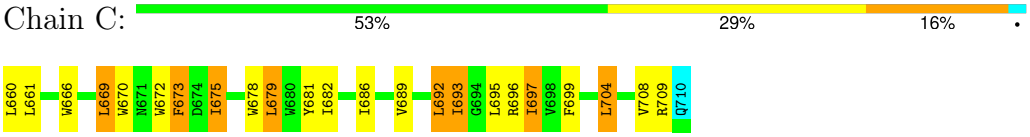
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

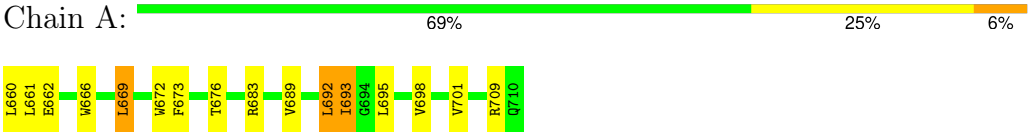
Chain C:



4.2.5 Score per residue for model 5

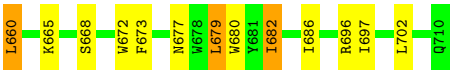
• Molecule 1: Envelope glycoprotein gp160

Chain A:

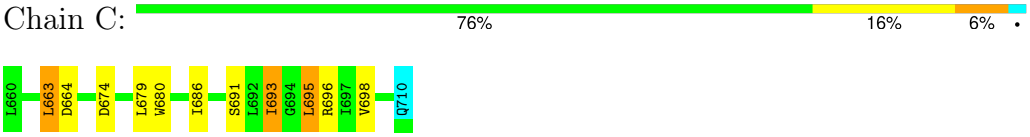


• Molecule 1: Envelope glycoprotein gp160

Chain B:

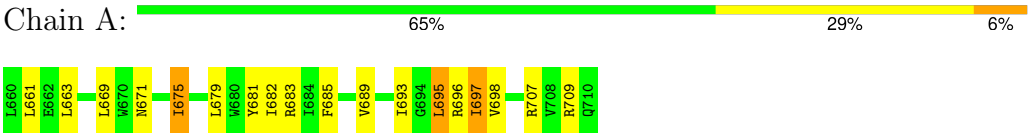


• Molecule 1: Envelope glycoprotein gp160

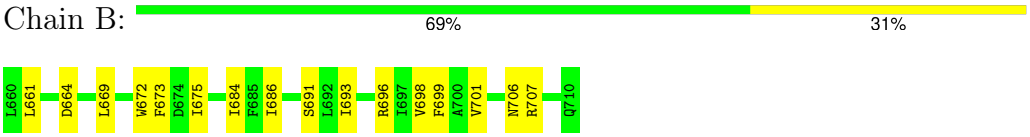


4.2.6 Score per residue for model 6

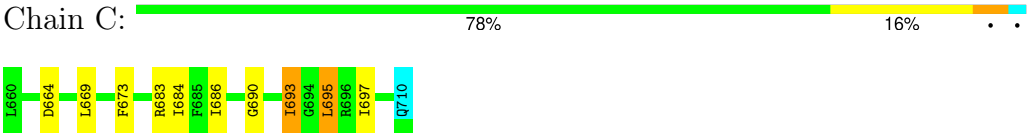
• Molecule 1: Envelope glycoprotein gp160



• Molecule 1: Envelope glycoprotein gp160

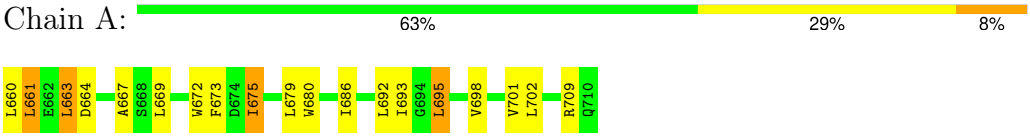


• Molecule 1: Envelope glycoprotein gp160

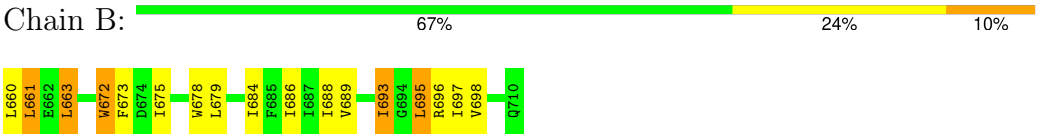


4.2.7 Score per residue for model 7

• Molecule 1: Envelope glycoprotein gp160

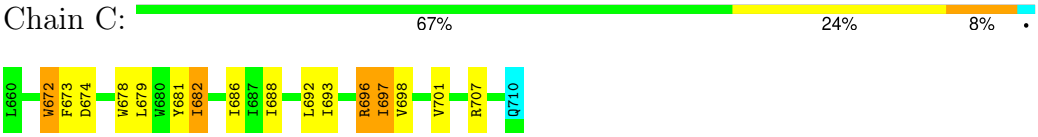


• Molecule 1: Envelope glycoprotein gp160



• Molecule 1: Envelope glycoprotein gp160

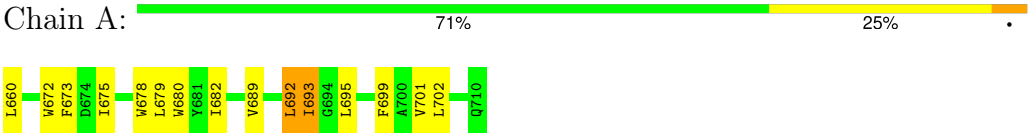
Chain C:



4.2.8 Score per residue for model 8

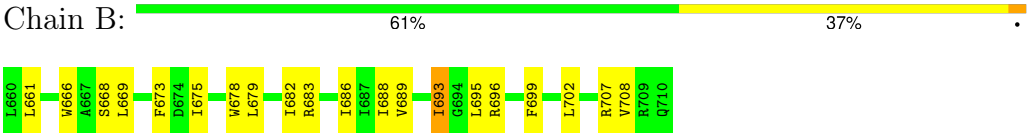
• Molecule 1: Envelope glycoprotein gp160

Chain A:



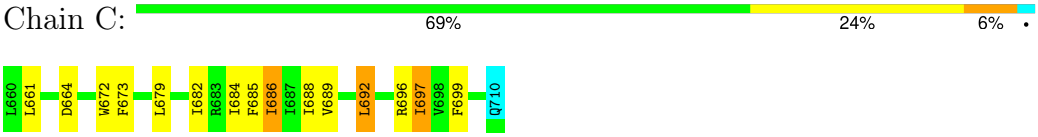
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

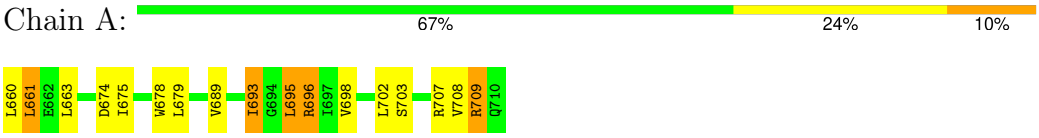
Chain C:



4.2.9 Score per residue for model 9

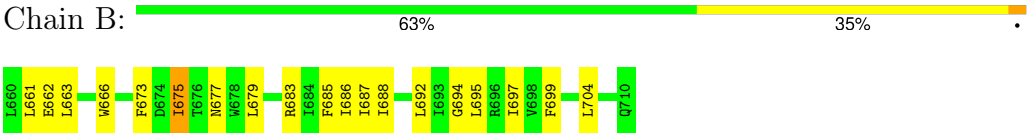
• Molecule 1: Envelope glycoprotein gp160

Chain A:



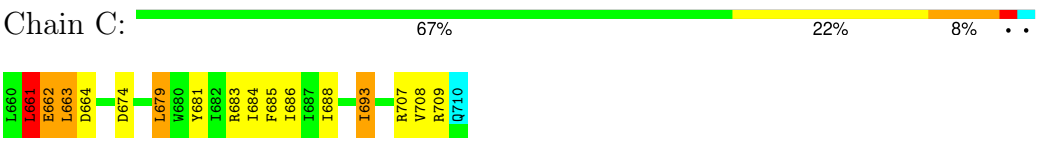
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

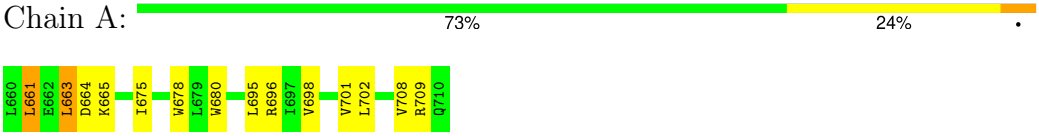
Chain C:



4.2.10 Score per residue for model 10

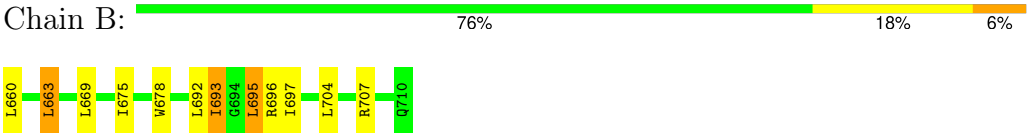
• Molecule 1: Envelope glycoprotein gp160

Chain A:



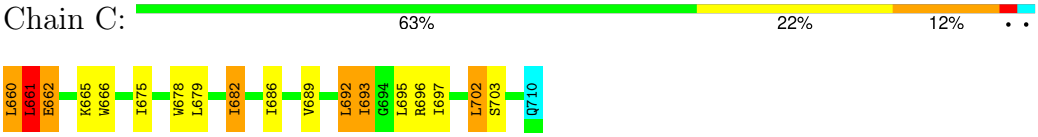
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

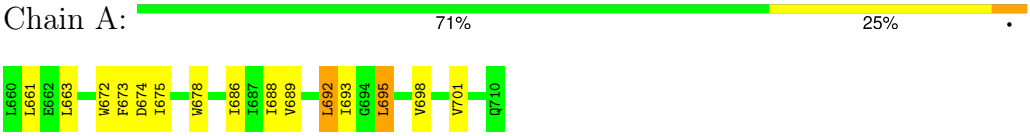
Chain C:



4.2.11 Score per residue for model 11

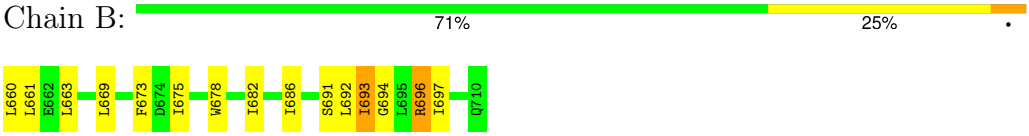
• Molecule 1: Envelope glycoprotein gp160

Chain A:



• Molecule 1: Envelope glycoprotein gp160

Chain B:



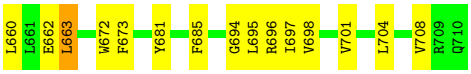
• Molecule 1: Envelope glycoprotein gp160

Chain C:

4.2.12 Score per residue for model 12

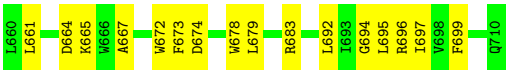
• Molecule 1: Envelope glycoprotein gp160

Chain A:



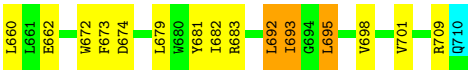
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

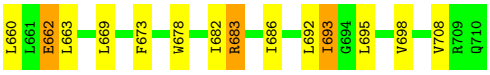
Chain C:



4.2.13 Score per residue for model 13

• Molecule 1: Envelope glycoprotein gp160

Chain A:



• Molecule 1: Envelope glycoprotein gp160

Chain B:

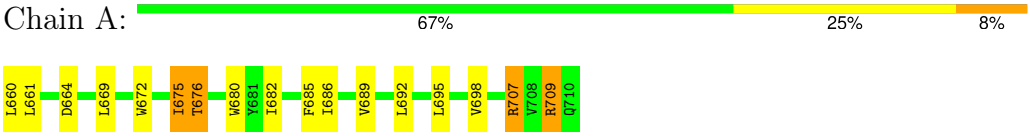
• Molecule 1: Envelope glycoprotein gp160

Chain C:

4.2.14 Score per residue for model 14

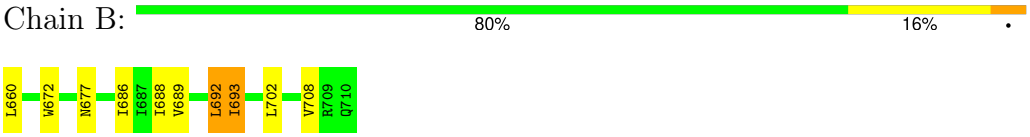
• Molecule 1: Envelope glycoprotein gp160

Chain A:



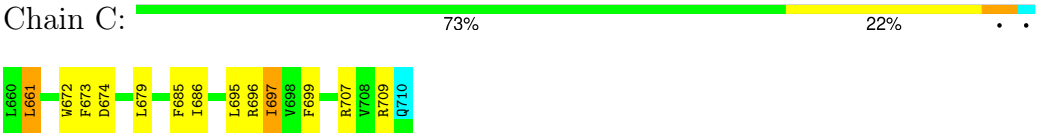
• Molecule 1: Envelope glycoprotein gp160

Chain B:



• Molecule 1: Envelope glycoprotein gp160

Chain C:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 14 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
X-PLOR NIH	refinement	
X-PLOR NIH	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	96
Number of shifts mapped to atoms	96
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	4%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QOJ

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	441	463	460	10±3
1	B	441	463	460	10±3
1	C	431	455	452	12±3
2	A	38	44	0	0±1
2	C	38	44	0	0±1
All	All	19978	21182	19208	370

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:692:LEU:HD13	1:C:693:ILE:N	0.79	1.92	4	4
1:B:686:ILE:HG21	1:C:686:ILE:HD11	0.75	1.58	5	2
1:B:686:ILE:HG21	1:C:686:ILE:HD12	0.75	1.56	11	5
1:A:661:LEU:HD13	1:C:666:TRP:NE1	0.72	2.00	10	1
1:A:698:VAL:O	1:A:701:VAL:HG22	0.71	1.84	10	2
1:A:663:LEU:HD13	1:A:664:ASP:N	0.71	2.00	1	3
1:B:669:LEU:HD21	1:B:675:ILE:HG23	0.70	1.63	6	1
1:A:695:LEU:O	1:A:698:VAL:HG12	0.69	1.87	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:682:ILE:HD12	1:C:683:ARG:N	0.68	2.03	12	1
1:A:661:LEU:HD11	1:A:666:TRP:CZ2	0.68	2.24	1	1
1:A:702:LEU:O	1:A:705:VAL:HG12	0.68	1.89	4	2
1:C:666:TRP:O	1:C:669:LEU:HD12	0.68	1.88	4	1
1:A:695:LEU:O	1:A:698:VAL:HG22	0.68	1.89	2	6
1:B:678:TRP:O	1:B:682:ILE:HG23	0.68	1.89	11	3
1:C:695:LEU:HD22	1:C:695:LEU:O	0.67	1.90	3	2
1:C:693:ILE:O	1:C:693:ILE:HD13	0.67	1.89	5	2
1:A:693:ILE:O	1:A:693:ILE:HD13	0.67	1.89	13	6
1:C:663:LEU:HD22	1:C:663:LEU:O	0.67	1.90	9	1
1:A:689:VAL:O	1:A:692:LEU:HD11	0.66	1.91	8	3
1:C:698:VAL:O	1:C:701:VAL:HG12	0.66	1.91	7	4
1:C:689:VAL:O	1:C:692:LEU:HD12	0.66	1.90	2	4
1:C:663:LEU:HD13	1:C:664:ASP:N	0.66	2.06	9	2
1:C:669:LEU:HD13	1:C:670:TRP:N	0.65	2.07	4	1
1:B:693:ILE:HD13	1:B:693:ILE:O	0.64	1.92	2	3
1:B:695:LEU:C	1:B:695:LEU:HD22	0.64	2.12	3	1
1:A:663:LEU:HD13	1:A:664:ASP:H	0.63	1.53	10	1
1:A:686:ILE:HG21	1:B:686:ILE:HD11	0.63	1.68	7	1
1:C:682:ILE:HD13	1:C:682:ILE:O	0.63	1.93	7	1
1:C:697:ILE:HD13	1:C:697:ILE:O	0.63	1.94	3	5
1:A:686:ILE:CG2	1:B:686:ILE:HD11	0.63	2.23	7	1
1:C:693:ILE:HD13	1:C:693:ILE:O	0.63	1.92	11	6
1:B:669:LEU:HD11	1:B:675:ILE:HG23	0.63	1.70	8	2
1:B:666:TRP:CG	1:C:661:LEU:HD12	0.62	2.30	9	1
1:A:693:ILE:HD13	1:A:693:ILE:O	0.61	1.94	5	1
1:B:697:ILE:HD13	1:C:696:ARG:NH1	0.61	2.10	10	1
1:A:660:LEU:CD1	1:C:667:ALA:HB2	0.61	2.26	13	1
1:C:669:LEU:O	1:C:669:LEU:HD22	0.61	1.95	4	1
1:C:681:TYR:HB2	1:C:684:ILE:HD12	0.61	1.73	9	1
1:B:669:LEU:HD21	1:B:675:ILE:CG2	0.60	2.26	6	1
1:C:698:VAL:O	1:C:701:VAL:HG22	0.60	1.96	2	2
1:A:686:ILE:HD11	1:C:686:ILE:CG2	0.60	2.26	1	2
1:C:692:LEU:HD13	1:C:693:ILE:H	0.60	1.56	2	4
1:B:694:GLY:O	1:B:697:ILE:HG22	0.60	1.97	4	6
1:A:686:ILE:CD1	1:C:686:ILE:HG21	0.59	2.27	14	1
1:B:697:ILE:O	1:B:697:ILE:HD13	0.59	1.97	2	1
1:C:663:LEU:HD22	1:C:664:ASP:N	0.59	2.13	3	1
1:A:695:LEU:C	1:A:695:LEU:HD22	0.59	2.18	7	1
1:A:661:LEU:HD11	2:A:801:QOJ:C9	0.59	2.27	14	1
1:A:697:ILE:O	1:A:697:ILE:HD13	0.59	1.97	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:686:ILE:HG23	1:C:686:ILE:HG12	0.59	1.75	3	1
1:B:693:ILE:HD11	1:C:696:ARG:HG3	0.59	1.75	14	2
1:B:669:LEU:HD22	1:B:675:ILE:HG21	0.59	1.74	11	1
1:A:698:VAL:O	1:A:701:VAL:HG12	0.59	1.98	5	5
1:A:666:TRP:CD1	1:B:661:LEU:HD21	0.58	2.32	1	1
1:C:695:LEU:O	1:C:698:VAL:HG22	0.58	1.97	12	3
1:B:685:PHE:HA	1:B:688:ILE:HD12	0.58	1.74	13	1
1:A:663:LEU:HD22	1:A:663:LEU:O	0.58	1.98	7	1
1:A:667:ALA:HB2	1:B:660:LEU:CD1	0.58	2.29	7	1
1:B:693:ILE:HD12	1:B:693:ILE:O	0.58	1.98	10	4
1:A:694:GLY:O	1:A:697:ILE:HG22	0.57	1.98	2	2
1:A:695:LEU:HD23	1:A:695:LEU:O	0.57	2.00	3	4
1:A:661:LEU:O	1:C:663:LEU:HD23	0.56	2.00	9	1
1:B:695:LEU:O	1:B:698:VAL:HG22	0.56	2.00	3	2
1:B:697:ILE:HD11	1:C:696:ARG:HD3	0.56	1.77	5	1
1:B:689:VAL:O	1:B:692:LEU:HD11	0.56	2.01	2	2
1:A:672:TRP:O	1:A:674:ASP:N	0.56	2.38	11	1
1:C:695:LEU:O	1:C:695:LEU:HD23	0.55	2.01	14	3
1:A:696:ARG:HG3	1:C:693:ILE:HD11	0.55	1.78	6	1
1:A:678:TRP:CD1	1:A:682:ILE:HG21	0.55	2.37	8	1
1:A:666:TRP:CD1	1:B:661:LEU:HD13	0.55	2.37	3	1
1:A:663:LEU:HD22	1:A:663:LEU:C	0.55	2.22	10	3
1:C:663:LEU:C	1:C:663:LEU:HD22	0.55	2.21	5	1
1:B:698:VAL:O	1:B:701:VAL:HG22	0.54	2.02	1	4
1:B:693:ILE:HG21	1:C:692:LEU:HD23	0.54	1.77	7	1
1:A:660:LEU:CG	1:C:663:LEU:HD23	0.54	2.33	5	1
1:A:682:ILE:HD12	1:A:683:ARG:N	0.54	2.18	2	3
1:A:697:ILE:HD11	1:B:699:PHE:CB	0.54	2.33	12	1
1:C:681:TYR:CB	1:C:684:ILE:HD12	0.53	2.33	9	1
1:A:661:LEU:HD23	1:A:666:TRP:CZ2	0.53	2.38	5	1
1:B:695:LEU:HD22	1:B:696:ARG:N	0.53	2.18	10	1
1:B:693:ILE:HD11	1:C:696:ARG:HD3	0.53	1.78	11	1
1:B:663:LEU:HD12	1:B:664:ASP:N	0.53	2.19	4	1
1:B:663:LEU:C	1:B:663:LEU:HD22	0.53	2.24	2	3
1:B:679:LEU:HD22	1:B:682:ILE:HG13	0.53	1.81	3	1
1:A:669:LEU:HD21	1:A:675:ILE:HG22	0.53	1.81	14	1
1:B:695:LEU:HD22	1:B:695:LEU:C	0.52	2.23	10	1
1:A:697:ILE:HD11	1:B:699:PHE:HB3	0.52	1.81	12	1
1:C:689:VAL:O	1:C:692:LEU:HD11	0.52	2.05	8	1
1:A:693:ILE:HD11	1:B:696:ARG:HG3	0.52	1.82	13	1
1:A:675:ILE:HD13	1:A:675:ILE:O	0.51	2.06	6	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:672:TRP:CZ3	1:B:675:ILE:HG22	0.51	2.40	7	1
1:B:669:LEU:CD1	1:B:675:ILE:HG23	0.51	2.35	13	2
1:B:663:LEU:HD23	1:B:663:LEU:O	0.51	2.05	9	1
1:A:675:ILE:HD12	1:A:679:LEU:CD1	0.51	2.36	6	1
1:A:661:LEU:HD23	1:A:666:TRP:CE2	0.51	2.41	5	1
1:A:678:TRP:O	1:A:682:ILE:HG23	0.51	2.06	13	1
1:A:686:ILE:HD11	1:C:686:ILE:HG23	0.50	1.83	1	2
1:C:663:LEU:HD22	1:C:663:LEU:C	0.50	2.26	3	2
1:C:690:GLY:O	1:C:693:ILE:HG22	0.50	2.06	6	1
1:B:693:ILE:HD11	1:C:696:ARG:CD	0.50	2.37	11	1
1:C:682:ILE:O	1:C:686:ILE:HD13	0.50	2.06	13	1
1:C:661:LEU:HD11	2:C:801:QOJ:C7	0.50	2.36	9	1
1:A:686:ILE:HD11	1:C:686:ILE:HG21	0.49	1.82	7	1
1:C:663:LEU:HD13	1:C:664:ASP:H	0.49	1.66	5	1
1:A:696:ARG:HG2	1:C:693:ILE:HD11	0.49	1.85	9	1
1:C:702:LEU:H	1:C:702:LEU:HD13	0.49	1.66	10	1
1:C:702:LEU:HD22	1:C:703:SER:N	0.49	2.22	10	1
1:A:692:LEU:HD23	1:C:693:ILE:HD11	0.49	1.84	7	1
1:A:686:ILE:HD12	1:C:686:ILE:HG21	0.49	1.84	14	1
1:A:685:PHE:O	1:A:689:VAL:HG23	0.49	2.08	14	1
1:C:679:LEU:HD13	1:C:679:LEU:O	0.49	2.06	9	2
1:B:667:ALA:HB2	1:C:660:LEU:HG	0.49	1.83	13	1
1:C:682:ILE:C	1:C:682:ILE:HD13	0.49	2.28	3	1
1:C:704:LEU:HD13	1:C:704:LEU:O	0.48	2.08	4	1
1:A:686:ILE:HG13	1:B:686:ILE:HD12	0.48	1.84	2	2
1:A:689:VAL:HG13	1:C:693:ILE:HG21	0.48	1.84	6	1
1:B:697:ILE:HD11	1:C:696:ARG:NH2	0.48	2.23	7	1
1:B:686:ILE:HG21	1:C:686:ILE:CD1	0.48	2.38	14	3
1:A:660:LEU:HG	1:C:663:LEU:HD23	0.48	1.84	5	1
1:B:675:ILE:HD12	1:B:678:TRP:CE3	0.48	2.43	7	3
1:C:685:PHE:HA	1:C:688:ILE:HD12	0.48	1.84	13	2
1:B:667:ALA:HB2	1:C:660:LEU:HD23	0.48	1.84	2	1
1:A:675:ILE:HD12	1:A:679:LEU:HD12	0.48	1.85	6	1
1:A:696:ARG:NH2	1:C:697:ILE:HD13	0.47	2.24	6	1
1:A:663:LEU:HD21	1:B:660:LEU:CD2	0.47	2.39	11	1
1:C:695:LEU:C	1:C:695:LEU:HD13	0.47	2.30	1	2
1:A:669:LEU:HD22	1:A:669:LEU:N	0.47	2.24	4	1
1:C:669:LEU:HD13	1:C:669:LEU:C	0.47	2.28	4	1
1:B:682:ILE:O	1:B:686:ILE:HD13	0.47	2.09	5	1
1:A:693:ILE:HD11	1:B:696:ARG:CG	0.47	2.39	6	1
1:C:684:ILE:O	1:C:688:ILE:HD12	0.47	2.10	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:661:LEU:HD23	1:B:661:LEU:N	0.47	2.23	1	1
1:B:660:LEU:O	1:B:661:LEU:HD22	0.47	2.09	7	1
1:C:693:ILE:HD12	1:C:693:ILE:O	0.47	2.10	9	1
1:A:675:ILE:HD11	1:A:678:TRP:CE3	0.47	2.44	8	4
1:A:689:VAL:O	1:A:689:VAL:HG12	0.47	2.10	8	4
1:A:669:LEU:C	1:A:669:LEU:HD12	0.47	2.31	6	1
1:A:708:VAL:HG12	1:A:708:VAL:O	0.47	2.10	2	4
1:A:661:LEU:HD11	2:A:801:QOJ:C30	0.46	2.39	14	1
1:A:682:ILE:O	1:A:682:ILE:HD13	0.46	2.11	3	1
1:C:708:VAL:HG12	1:C:708:VAL:O	0.46	2.11	4	3
1:B:708:VAL:HG12	1:B:708:VAL:O	0.46	2.10	8	3
1:A:686:ILE:CG1	1:C:686:ILE:HG21	0.46	2.40	11	1
1:B:688:ILE:HD12	1:B:688:ILE:N	0.46	2.26	4	4
1:A:683:ARG:NH2	1:B:679:LEU:HD22	0.46	2.26	5	1
1:A:708:VAL:O	1:A:708:VAL:HG12	0.46	2.11	12	1
1:A:660:LEU:HD22	1:A:660:LEU:N	0.46	2.26	9	1
1:A:688:ILE:HD12	1:A:688:ILE:H	0.45	1.71	11	1
1:C:675:ILE:HG23	1:C:679:LEU:HD23	0.45	1.88	1	1
1:A:663:LEU:HD13	1:A:663:LEU:C	0.45	2.32	7	1
1:B:688:ILE:HD12	1:B:688:ILE:H	0.45	1.71	9	2
1:B:693:ILE:HD13	1:B:693:ILE:C	0.45	2.31	2	1
1:A:669:LEU:CD2	1:A:675:ILE:HG22	0.45	2.42	14	1
1:B:695:LEU:HD22	1:B:695:LEU:O	0.45	2.12	3	1
1:A:696:ARG:NE	1:C:697:ILE:HD13	0.45	2.27	10	1
1:C:692:LEU:HD12	1:C:693:ILE:H	0.45	1.70	12	1
1:B:704:LEU:HD12	1:B:704:LEU:N	0.45	2.26	10	1
1:A:667:ALA:HB2	1:B:660:LEU:HD13	0.45	1.88	7	1
1:A:660:LEU:O	1:A:661:LEU:O	0.44	2.36	7	1
1:B:697:ILE:HD11	1:C:696:ARG:CZ	0.44	2.42	7	1
1:C:688:ILE:H	1:C:688:ILE:HD12	0.44	1.72	7	1
1:A:686:ILE:CG2	1:B:686:ILE:HD12	0.44	2.42	14	1
1:A:663:LEU:C	1:A:663:LEU:HD23	0.44	2.32	6	1
1:A:660:LEU:N	1:A:660:LEU:HD23	0.44	2.27	8	1
1:C:661:LEU:HD23	1:C:665:LYS:CG	0.44	2.43	10	1
1:B:675:ILE:HD13	1:B:675:ILE:O	0.44	2.13	9	1
1:A:707:ARG:CZ	1:C:707:ARG:CZ	0.44	2.96	14	1
1:C:697:ILE:HD12	1:C:698:VAL:N	0.44	2.27	2	1
1:C:679:LEU:N	1:C:679:LEU:HD12	0.44	2.27	5	1
1:B:708:VAL:HG22	1:B:708:VAL:O	0.44	2.12	3	2
1:B:663:LEU:HD13	1:B:664:ASP:N	0.44	2.28	2	1
1:C:693:ILE:HD13	1:C:693:ILE:C	0.44	2.33	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:663:LEU:HD13	1:C:663:LEU:C	0.44	2.33	9	1
1:C:660:LEU:HD23	1:C:660:LEU:N	0.44	2.28	10	1
1:A:697:ILE:HD12	1:A:698:VAL:N	0.43	2.28	1	1
1:C:669:LEU:HD11	1:C:675:ILE:HG22	0.43	1.90	1	1
1:C:672:TRP:CZ3	1:C:675:ILE:HG22	0.43	2.48	4	1
1:C:693:ILE:HD12	1:C:697:ILE:HD11	0.43	1.90	10	1
1:C:669:LEU:HD11	2:C:801:QOJ:C19	0.43	2.43	6	1
1:B:684:ILE:HD12	1:B:684:ILE:N	0.43	2.28	7	2
1:B:686:ILE:HG21	1:C:686:ILE:HG13	0.43	1.91	8	1
1:A:669:LEU:HD11	1:A:675:ILE:HG22	0.43	1.91	7	1
1:B:693:ILE:HD11	1:C:696:ARG:HG2	0.43	1.90	1	1
1:B:685:PHE:O	1:B:689:VAL:HG23	0.43	2.13	2	1
1:B:689:VAL:O	1:B:689:VAL:HG12	0.43	2.13	14	5
1:A:661:LEU:HD12	2:A:801:QOJ:C31	0.43	2.44	10	1
1:C:675:ILE:HD12	1:C:678:TRP:CE3	0.43	2.48	11	1
1:C:661:LEU:HD11	2:C:801:QOJ:C8	0.43	2.44	9	1
1:B:695:LEU:C	1:B:695:LEU:CD2	0.43	2.86	3	1
1:C:672:TRP:O	1:C:674:ASP:N	0.43	2.52	14	4
1:A:669:LEU:HD11	1:A:676:THR:OG1	0.43	2.14	14	1
1:B:667:ALA:HB2	1:C:660:LEU:CD2	0.42	2.44	12	1
1:B:672:TRP:O	1:B:674:ASP:N	0.42	2.52	1	2
1:C:663:LEU:C	1:C:663:LEU:HD23	0.42	2.35	11	1
1:C:695:LEU:O	1:C:698:VAL:HG23	0.42	2.15	2	1
1:A:693:ILE:HD11	1:B:696:ARG:HG2	0.42	1.89	11	1
1:C:678:TRP:CD1	1:C:678:TRP:C	0.42	2.92	13	1
1:A:682:ILE:CD1	1:A:686:ILE:HD11	0.42	2.44	3	1
1:A:693:ILE:HD12	1:B:696:ARG:HG3	0.42	1.90	1	1
1:C:688:ILE:HD12	1:C:688:ILE:H	0.42	1.75	1	1
1:B:686:ILE:CG2	1:C:686:ILE:HD11	0.42	2.44	3	1
1:C:695:LEU:C	1:C:695:LEU:HD23	0.42	2.35	10	1
1:B:702:LEU:C	1:B:702:LEU:HD23	0.42	2.34	1	1
1:C:678:TRP:O	1:C:682:ILE:HG23	0.42	2.14	10	2
1:A:675:ILE:HD12	1:A:678:TRP:CE3	0.42	2.50	10	1
1:B:692:LEU:HD12	1:B:693:ILE:H	0.42	1.75	14	1
1:A:661:LEU:O	1:C:663:LEU:HD12	0.41	2.15	11	1
1:A:704:LEU:O	1:A:704:LEU:HD23	0.41	2.15	12	1
1:A:686:ILE:HG21	1:B:686:ILE:CD1	0.41	2.45	14	1
1:C:692:LEU:C	1:C:692:LEU:HD22	0.41	2.34	2	1
1:B:686:ILE:HD12	1:B:686:ILE:N	0.41	2.30	7	1
1:A:689:VAL:HG12	1:A:689:VAL:O	0.41	2.16	2	1
1:C:678:TRP:O	1:C:682:ILE:HG22	0.41	2.15	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:660:LEU:O	1:C:661:LEU:HD12	0.41	2.15	10	1
1:B:660:LEU:N	1:B:660:LEU:HD23	0.41	2.31	5	1
1:A:696:ARG:HD3	1:C:693:ILE:HD11	0.41	1.90	9	1
1:B:687:ILE:HD12	1:B:687:ILE:H	0.41	1.76	9	1
1:B:686:ILE:HG21	1:C:686:ILE:CG1	0.41	2.45	13	1
1:A:669:LEU:HD22	1:A:676:THR:OG1	0.41	2.15	5	1
1:A:663:LEU:O	1:A:663:LEU:HD23	0.41	2.15	9	1
1:A:661:LEU:N	1:A:661:LEU:HD12	0.41	2.30	2	1
1:B:661:LEU:HD22	1:B:666:TRP:CZ2	0.41	2.50	8	1
1:A:688:ILE:HD12	1:A:688:ILE:N	0.41	2.30	11	1
1:B:678:TRP:CZ3	1:B:679:LEU:HD21	0.41	2.51	12	1
1:C:661:LEU:HD12	1:C:661:LEU:O	0.41	2.15	8	1
1:A:666:TRP:NE1	1:B:661:LEU:HD22	0.41	2.30	2	1
1:C:692:LEU:HD12	1:C:693:ILE:N	0.41	2.31	12	1
1:A:669:LEU:O	1:A:669:LEU:HD13	0.41	2.15	14	1
1:A:666:TRP:HE1	1:B:661:LEU:HD22	0.41	1.76	2	1
1:B:666:TRP:CD1	1:C:661:LEU:HD12	0.41	2.52	4	1
1:C:688:ILE:HD12	1:C:688:ILE:N	0.41	2.31	7	1
1:A:678:TRP:O	1:A:682:ILE:HG22	0.40	2.16	3	1
1:B:663:LEU:HD13	1:B:664:ASP:H	0.40	1.76	2	1
1:B:663:LEU:HD23	1:B:663:LEU:C	0.40	2.36	9	1
1:B:667:ALA:HB2	1:C:660:LEU:HD22	0.40	1.92	12	1
1:C:682:ILE:HD13	1:C:682:ILE:C	0.40	2.37	7	1
1:C:675:ILE:HG13	1:C:679:LEU:HD23	0.40	1.93	10	1
1:B:666:TRP:CD1	1:C:661:LEU:HD21	0.40	2.52	8	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	49/51 (96%)	45±1 (91±3%)	3±1 (6±2%)	1±1 (3±1%)	6	42
1	B	49/51 (96%)	46±1 (94±3%)	2±1 (4±2%)	1±1 (2±2%)	8	50
1	C	49/51 (96%)	46±1 (93±3%)	2±1 (3±2%)	2±1 (3±2%)	5	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2058/2142 (96%)	1913 (93%)	92 (4%)	53 (3%)	6 42

All 13 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	673	PHE	9
1	A	673	PHE	8
1	C	673	PHE	7
1	A	661	LEU	5
1	C	709	ARG	5
1	B	661	LEU	4
1	C	681	TYR	3
1	C	661	LEU	3
1	C	662	GLU	3
1	A	662	GLU	2
1	A	709	ARG	2
1	A	681	TYR	1
1	B	662	GLU	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	47/47 (100%)	39±2 (84±5%)	8±2 (16±5%)	4 40
1	B	47/47 (100%)	39±2 (84±3%)	8±2 (16±3%)	4 40
1	C	46/47 (98%)	38±2 (83±4%)	8±2 (17±4%)	4 39
All	All	1960/1974 (99%)	1641 (84%)	319 (16%)	4 39

All 94 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	B	695	LEU	10
1	B	693	ILE	9
1	C	693	ILE	9

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Mol	Chain	Res	Type	Models (Total)
1	A	693	ILE	8
1	C	679	LEU	8
1	A	692	LEU	8
1	A	695	LEU	8
1	A	672	TRP	7
1	A	709	ARG	7
1	B	692	LEU	7
1	B	696	ARG	7
1	A	680	TRP	6
1	C	699	PHE	6
1	C	661	LEU	6
1	C	692	LEU	6
1	B	679	LEU	6
1	A	660	LEU	5
1	A	663	LEU	5
1	A	679	LEU	5
1	A	685	PHE	5
1	C	696	ARG	5
1	A	675	ILE	5
1	B	663	LEU	5
1	B	672	TRP	5
1	B	707	ARG	5
1	C	662	GLU	5
1	C	695	LEU	5
1	C	697	ILE	5
1	A	702	LEU	5
1	C	674	ASP	4
1	C	686	ILE	4
1	A	707	ARG	4
1	B	661	LEU	4
1	B	660	LEU	4
1	B	677	ASN	4
1	C	663	LEU	4
1	C	672	TRP	4
1	C	682	ILE	4
1	B	683	ARG	4
1	B	668	SER	3
1	C	683	ARG	3
1	C	709	ARG	3
1	A	697	ILE	3
1	B	685	PHE	3
1	B	665	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	C	685	PHE	3
1	B	669	LEU	3
1	C	660	LEU	3
1	B	702	LEU	3
1	B	699	PHE	3
1	C	664	ASP	3
1	B	673	PHE	3
1	A	683	ARG	2
1	B	682	ILE	2
1	C	665	LYS	2
1	A	671	ASN	2
1	A	682	ILE	2
1	C	680	TRP	2
1	A	664	ASP	2
1	B	675	ILE	2
1	C	673	PHE	2
1	A	669	LEU	2
1	B	664	ASP	2
1	B	691	SER	2
1	C	707	ARG	2
1	A	696	ARG	2
1	A	662	GLU	2
1	A	673	PHE	1
1	A	705	VAL	1
1	C	706	ASN	1
1	B	697	ILE	1
1	C	698	VAL	1
1	A	661	LEU	1
1	B	662	GLU	1
1	A	686	ILE	1
1	B	674	ASP	1
1	C	669	LEU	1
1	C	675	ILE	1
1	C	704	LEU	1
1	B	680	TRP	1
1	C	691	SER	1
1	B	706	ASN	1
1	C	684	ILE	1
1	A	699	PHE	1
1	A	701	VAL	1
1	A	674	ASP	1
1	A	703	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	B	704	LEU	1
1	A	665	LYS	1
1	C	702	LEU	1
1	A	681	TYR	1
1	B	710	GLN	1
1	C	678	TRP	1
1	A	676	THR	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	QOJ	C	801	-	41,43,43	3.78±0.01	28±0 (68±0%)
2	QOJ	A	801	-	41,43,43	3.79±0.01	28±0 (68±0%)
2	QOJ	B	801	-	41,43,43	3.78±0.02	28±0 (68±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles

that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	QOJ	C	801	-	50,60,60	2.60±0.05	13±1 (26±1%)
2	QOJ	A	801	-	50,60,60	2.61±0.05	13±1 (26±2%)
2	QOJ	B	801	-	50,60,60	2.60±0.06	13±1 (26±1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	QOJ	B	801	-	-	0±0,13,25,25	0±0,6,6,6
2	QOJ	C	801	-	-	0±0,13,25,25	0±0,6,6,6
2	QOJ	A	801	-	-	0±0,13,25,25	0±0,6,6,6

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	801	QOJ	C6-C5	10.28	1.58	1.42	3	14
2	A	801	QOJ	C6-C5	10.27	1.58	1.42	10	14
2	B	801	QOJ	C10-C11	10.25	1.58	1.42	8	14
2	C	801	QOJ	C6-C5	10.24	1.58	1.42	10	14
2	C	801	QOJ	C10-C11	10.23	1.58	1.42	10	14
2	A	801	QOJ	C10-C11	10.21	1.58	1.42	11	14
2	A	801	QOJ	C4-C6	6.65	1.55	1.42	12	14
2	B	801	QOJ	C4-C6	6.53	1.55	1.42	12	14
2	C	801	QOJ	C4-C6	6.51	1.55	1.42	5	14
2	C	801	QOJ	C15-C10	6.50	1.55	1.42	7	14
2	B	801	QOJ	C15-C10	6.50	1.55	1.42	1	14
2	A	801	QOJ	C15-C10	6.48	1.55	1.42	5	14
2	A	801	QOJ	C7-C6	5.64	1.51	1.44	12	14
2	C	801	QOJ	C7-C6	5.57	1.51	1.44	13	14
2	B	801	QOJ	C14-C10	5.50	1.51	1.44	2	14
2	A	801	QOJ	C14-C10	5.48	1.51	1.44	1	14
2	B	801	QOJ	C7-C6	5.48	1.51	1.44	13	14

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	801	QOJ	C14-C10	5.46	1.51	1.44	11	14
2	C	801	QOJ	C12-N2	5.25	1.49	1.36	1	14
2	A	801	QOJ	C9-N1	5.15	1.48	1.36	5	14
2	C	801	QOJ	C9-N1	5.15	1.48	1.36	9	14
2	A	801	QOJ	C12-N2	5.11	1.48	1.36	2	14
2	B	801	QOJ	C9-N1	5.11	1.48	1.36	12	14
2	B	801	QOJ	C12-N2	5.10	1.48	1.36	1	14
2	B	801	QOJ	C14-N3	4.75	1.49	1.36	3	14
2	A	801	QOJ	C7-N4	4.75	1.49	1.36	6	14
2	C	801	QOJ	C7-N4	4.74	1.49	1.36	7	14
2	B	801	QOJ	C7-N4	4.74	1.49	1.36	8	14
2	A	801	QOJ	C14-N3	4.73	1.49	1.36	5	14
2	C	801	QOJ	C14-N3	4.72	1.49	1.36	7	14
2	C	801	QOJ	C17-C18	4.09	1.45	1.36	9	14
2	B	801	QOJ	C2-C1	4.01	1.45	1.36	5	14
2	C	801	QOJ	C2-C1	3.99	1.45	1.36	9	14
2	A	801	QOJ	C17-C18	3.97	1.45	1.36	3	14
2	A	801	QOJ	C2-C1	3.95	1.45	1.36	9	14
2	B	801	QOJ	C17-C18	3.87	1.44	1.36	8	14
2	A	801	QOJ	C32-C8	3.64	1.44	1.51	9	14
2	C	801	QOJ	C32-C8	3.59	1.44	1.51	13	14
2	C	801	QOJ	C34-C13	3.48	1.45	1.51	9	14
2	B	801	QOJ	C32-C8	3.47	1.45	1.51	12	14
2	A	801	QOJ	C34-C13	3.44	1.45	1.51	14	14
2	B	801	QOJ	C34-C13	3.43	1.45	1.51	11	14
2	A	801	QOJ	C5-N1	3.18	1.44	1.40	5	14
2	C	801	QOJ	C11-N2	3.12	1.44	1.40	9	14
2	C	801	QOJ	C5-N1	3.04	1.44	1.40	10	14
2	B	801	QOJ	C7-C8	3.02	1.52	1.41	12	14
2	A	801	QOJ	C14-C13	2.98	1.52	1.41	1	14
2	A	801	QOJ	C7-C8	2.98	1.52	1.41	3	14
2	C	801	QOJ	C14-C13	2.98	1.52	1.41	3	14
2	C	801	QOJ	C7-C8	2.97	1.52	1.41	8	14
2	B	801	QOJ	C14-C13	2.97	1.52	1.41	1	14
2	B	801	QOJ	C5-N1	2.96	1.44	1.40	3	14
2	C	801	QOJ	C29-C12	2.94	1.45	1.49	5	14
2	B	801	QOJ	C11-N2	2.92	1.44	1.40	7	14
2	A	801	QOJ	C11-N2	2.91	1.44	1.40	8	14
2	A	801	QOJ	C30-C9	2.90	1.45	1.49	13	14
2	A	801	QOJ	C29-C12	2.89	1.45	1.49	3	14
2	B	801	QOJ	C29-C12	2.85	1.45	1.49	4	14

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	801	QOJ	C30-C9	2.81	1.45	1.49	14	14
2	B	801	QOJ	C30-C9	2.78	1.45	1.49	9	14
2	C	801	QOJ	C18-C11	2.70	1.46	1.41	1	13
2	A	801	QOJ	C17-C16	2.68	1.44	1.38	3	14
2	A	801	QOJ	C1-C5	2.66	1.46	1.41	12	14
2	B	801	QOJ	C18-C11	2.66	1.46	1.41	7	13
2	B	801	QOJ	C16-C15	2.66	1.42	1.36	6	14
2	C	801	QOJ	C3-C4	2.65	1.42	1.36	12	14
2	B	801	QOJ	C3-C4	2.64	1.42	1.36	3	14
2	C	801	QOJ	C3-C2	2.63	1.44	1.38	4	14
2	A	801	QOJ	C3-C4	2.63	1.42	1.36	6	14
2	B	801	QOJ	C3-C2	2.63	1.44	1.38	8	14
2	A	801	QOJ	C3-C2	2.62	1.44	1.38	8	14
2	A	801	QOJ	C16-C15	2.61	1.42	1.36	1	14
2	C	801	QOJ	C16-C15	2.61	1.42	1.36	3	14
2	B	801	QOJ	C17-C16	2.59	1.43	1.38	1	14
2	A	801	QOJ	C18-C11	2.57	1.46	1.41	9	14
2	C	801	QOJ	C17-C16	2.57	1.43	1.38	11	14
2	B	801	QOJ	C1-C5	2.55	1.46	1.41	8	14
2	C	801	QOJ	C1-C5	2.48	1.45	1.41	6	14
2	C	801	QOJ	C9-C8	2.36	1.44	1.38	9	14
2	C	801	QOJ	C12-C13	2.36	1.44	1.38	4	14
2	A	801	QOJ	C12-C13	2.35	1.44	1.38	14	14
2	B	801	QOJ	C12-C13	2.35	1.44	1.38	4	14
2	B	801	QOJ	C9-C8	2.32	1.44	1.38	4	14
2	A	801	QOJ	C9-C8	2.30	1.44	1.38	7	14

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	801	QOJ	C18-C11-N2	8.49	129.11	121.43	1	14
2	C	801	QOJ	C1-C5-N1	8.45	129.07	121.43	10	14
2	B	801	QOJ	C18-C11-N2	8.41	129.03	121.43	7	14
2	B	801	QOJ	C1-C5-N1	8.40	129.03	121.43	8	14
2	A	801	QOJ	C1-C5-N1	8.31	128.95	121.43	5	14
2	A	801	QOJ	C18-C11-N2	8.22	128.86	121.43	9	14
2	A	801	QOJ	C31-C30-C9	5.78	108.07	102.49	13	14
2	B	801	QOJ	C31-C30-C9	5.64	107.93	102.49	13	14
2	C	801	QOJ	C31-C30-C9	5.63	107.92	102.49	10	14
2	A	801	QOJ	C33-C29-C12	5.62	107.91	102.49	2	14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	801	QOJ	C33-C29-C12	5.61	107.91	102.49	2	14
2	B	801	QOJ	C33-C29-C12	5.56	107.86	102.49	1	14
2	C	801	QOJ	C10-C11-N2	5.24	116.14	119.61	1	14
2	B	801	QOJ	C6-C5-N1	5.24	116.14	119.61	8	14
2	B	801	QOJ	C10-C11-N2	5.19	116.18	119.61	7	14
2	A	801	QOJ	C6-C5-N1	5.18	116.18	119.61	1	14
2	A	801	QOJ	C10-C11-N2	5.13	116.21	119.61	9	14
2	C	801	QOJ	C6-C5-N1	5.13	116.22	119.61	10	14
2	A	801	QOJ	C28-N1-C9	3.87	116.70	119.26	10	12
2	B	801	QOJ	C18-C11-C10	3.85	114.69	119.43	11	14
2	C	801	QOJ	C1-C5-C6	3.82	114.72	119.43	10	14
2	C	801	QOJ	C18-C11-C10	3.79	114.75	119.43	1	14
2	B	801	QOJ	C1-C5-C6	3.73	114.83	119.43	8	14
2	A	801	QOJ	C1-C5-C6	3.71	114.85	119.43	9	14
2	C	801	QOJ	C28-N1-C9	3.66	116.84	119.26	1	11
2	A	801	QOJ	C18-C11-C10	3.65	114.92	119.43	9	14
2	B	801	QOJ	C28-N1-C9	3.55	116.91	119.26	8	8
2	B	801	QOJ	C19-N2-C12	3.51	116.94	119.26	11	10
2	A	801	QOJ	C19-N2-C12	3.41	117.01	119.26	9	11
2	C	801	QOJ	C31-C32-C8	3.37	107.81	103.57	1	14
2	A	801	QOJ	C31-C32-C8	3.36	107.80	103.57	4	14
2	B	801	QOJ	C31-C32-C8	3.33	107.76	103.57	11	14
2	B	801	QOJ	C33-C34-C13	3.17	107.56	103.57	14	14
2	A	801	QOJ	C33-C34-C13	3.17	107.55	103.57	5	14
2	C	801	QOJ	C33-C34-C13	3.16	107.54	103.57	1	14
2	C	801	QOJ	C19-N2-C12	3.04	117.25	119.26	14	9
2	C	801	QOJ	C9-N1-C5	2.35	123.82	121.97	3	12
2	B	801	QOJ	C9-N1-C5	2.29	123.77	121.97	7	11
2	A	801	QOJ	C9-N1-C5	2.28	123.77	121.97	8	10
2	C	801	QOJ	C12-N2-C11	2.27	123.76	121.97	8	9
2	B	801	QOJ	C12-N2-C11	2.25	123.74	121.97	5	7
2	B	801	QOJ	C17-C18-C11	2.22	123.56	119.50	11	6
2	A	801	QOJ	C12-N2-C11	2.22	123.72	121.97	7	12
2	C	801	QOJ	C17-C18-C11	2.04	123.22	119.50	4	2
2	B	801	QOJ	C2-C1-C5	2.03	123.20	119.50	13	1
2	A	801	QOJ	C17-C18-C11	2.01	123.17	119.50	5	2
2	C	801	QOJ	C2-C1-C5	2.01	123.17	119.50	5	1
2	A	801	QOJ	C2-C1-C5	2.01	123.16	119.50	3	1

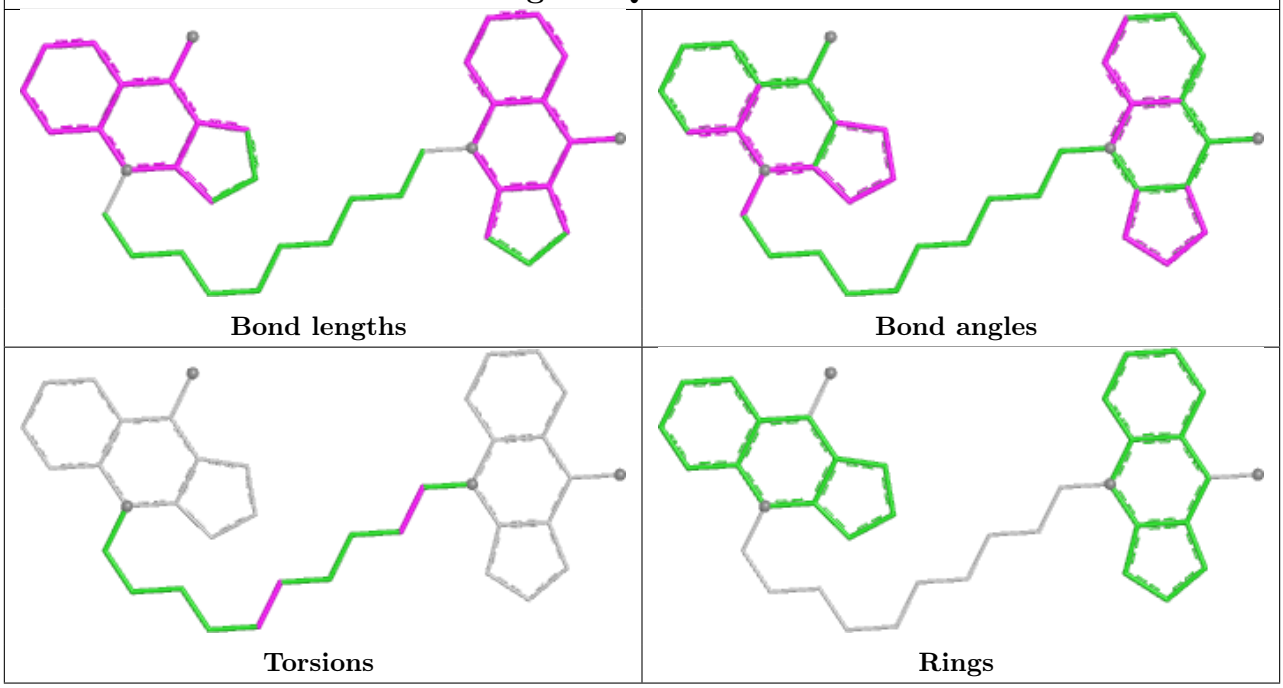
There are no chirality outliers.

There are no torsion outliers.

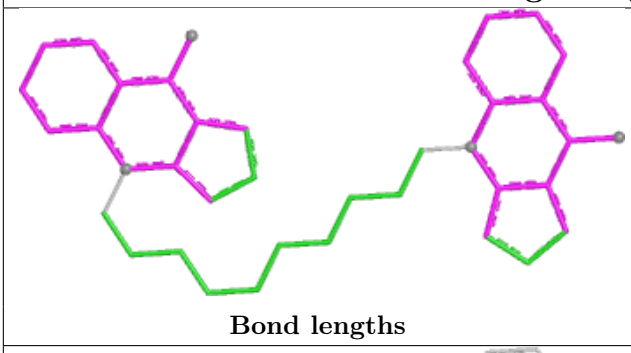
There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

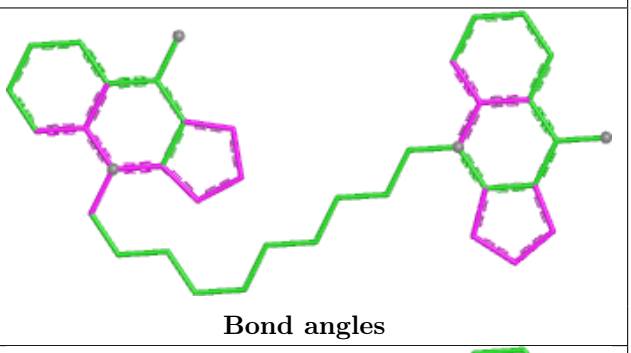
Ligand QOJ B 801



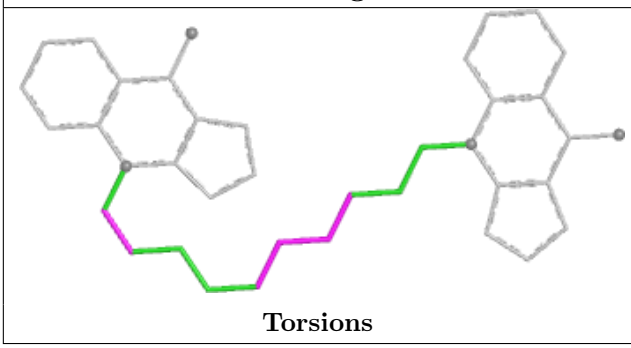
Ligand QOJ C 801



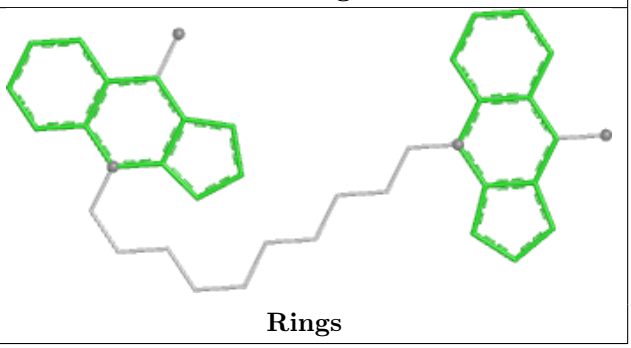
Bond lengths



Bond angles

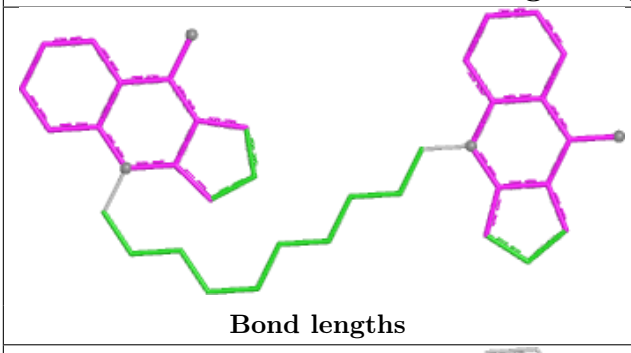


Torsions

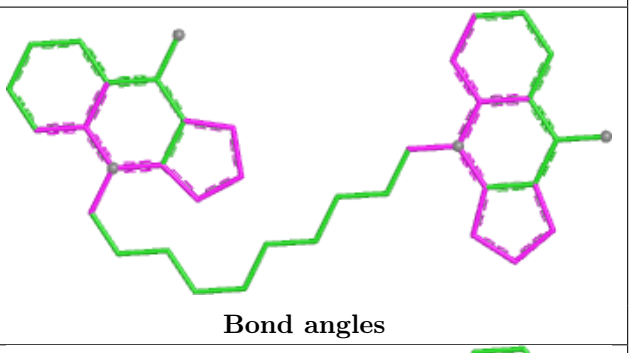


Rings

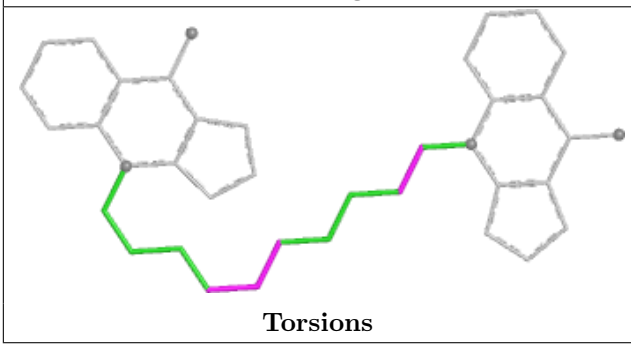
Ligand QOJ A 801



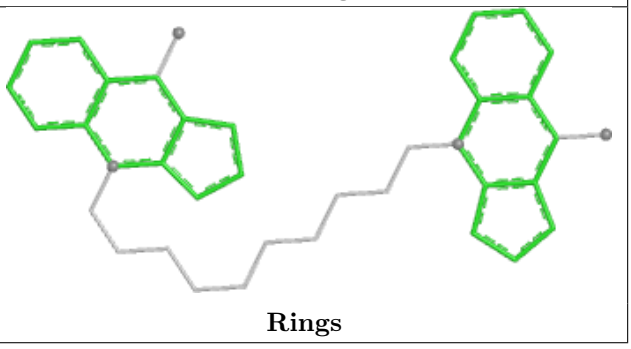
Bond lengths



Bond angles



Torsions



Rings

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 4% for the well-defined parts and 4% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *BMRB.txt*

7.1.1 Bookkeeping

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

Total number of shifts	96
Number of shifts mapped to atoms	96
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	None (insufficient data)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	48	1.54 ± 0.51	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 4%, i.e. 96 atoms were assigned a chemical shift out of a possible 2409. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	96/766 (13%)	48/310 (15%)	0/304 (0%)	48/152 (32%)
Sidechain	0/1346 (0%)	0/894 (0%)	0/402 (0%)	0/50 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/297 (0%)	0/147 (0%)	0/135 (0%)	0/15 (0%)
Overall	96/2409 (4%)	48/1351 (4%)	0/841 (0%)	48/217 (22%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 96 atoms were assigned a chemical shift out of a possible 2424. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	96/771 (12%)	48/312 (15%)	0/306 (0%)	48/153 (31%)
Sidechain	0/1356 (0%)	0/900 (0%)	0/405 (0%)	0/51 (0%)
Aromatic	0/297 (0%)	0/147 (0%)	0/135 (0%)	0/15 (0%)
Overall	96/2424 (4%)	48/1359 (4%)	0/846 (0%)	48/219 (22%)

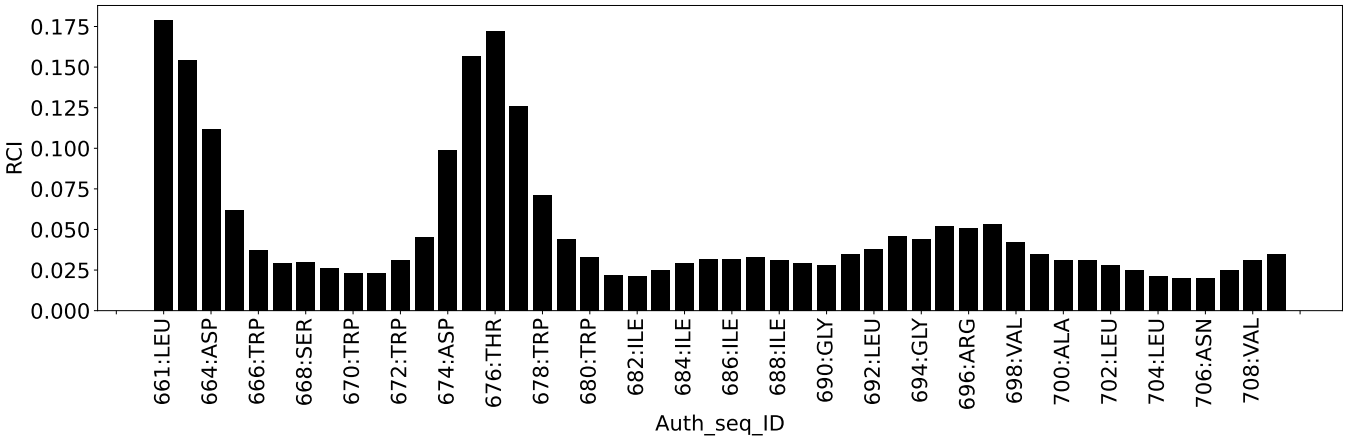
7.1.4 Statistically unusual chemical shifts (i)

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	729
Intra-residue (|i-j|=0)	96
Sequential (|i-j|=1)	294
Medium range (|i-j|>1 and |i-j|<5)	285
Long range (|i-j|≥5)	33
Inter-chain	21
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	84
Number of unmapped restraints	0
Number of restraints per residue	5.2
Number of long range restraints per residue[1]	0.2

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	38.4	0.2
0.2-0.5 (Medium)	26.8	0.5
>0.5 (Large)	67.2	28.51

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	7.9	4.01
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

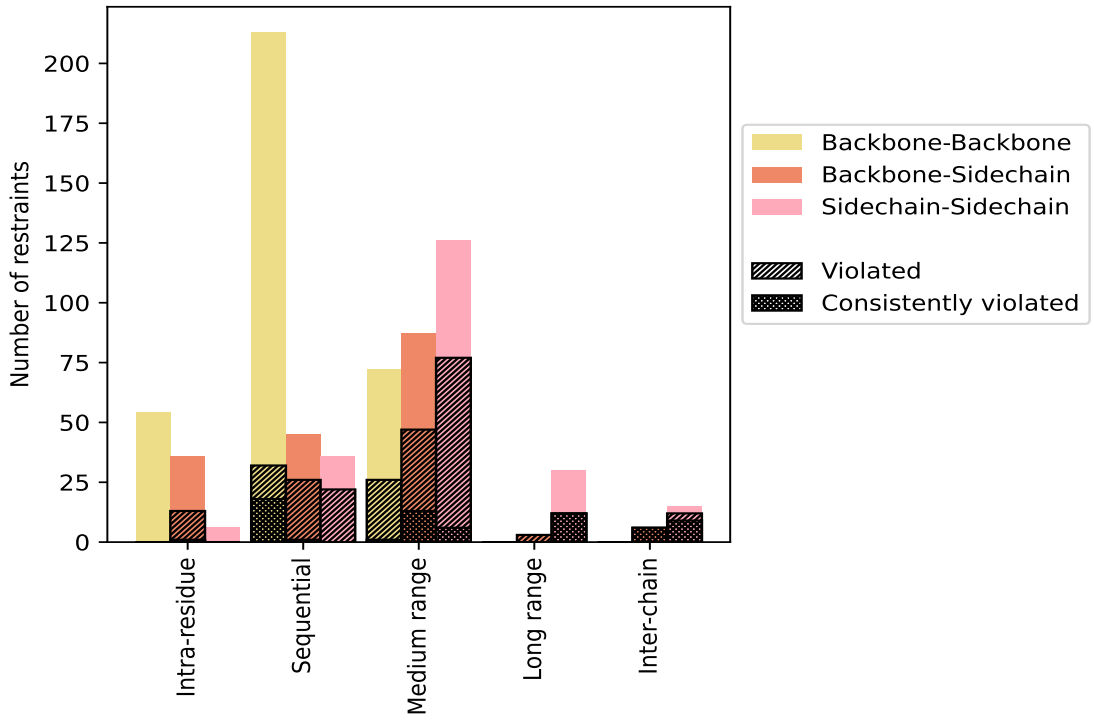
9.1 Summary of distance violations (i)

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)	96	13.2	13	13.5	1.8	1	1.0	0.1
Backbone-Backbone	54	7.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	36	4.9	13	36.1	1.8	1	2.8	0.1
Sidechain-Sidechain	6	0.8	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	294	40.3	80	27.2	11.0	19	6.5	2.6
Backbone-Backbone	213	29.2	32	15.0	4.4	18	8.5	2.5
Backbone-Sidechain	45	6.2	26	57.8	3.6	1	2.2	0.1
Sidechain-Sidechain	36	4.9	22	61.1	3.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	285	39.1	150	52.6	20.6	20	7.0	2.7
Backbone-Backbone	72	9.9	26	36.1	3.6	1	1.4	0.1
Backbone-Sidechain	87	11.9	47	54.0	6.4	13	14.9	1.8
Sidechain-Sidechain	126	17.3	77	61.1	10.6	6	4.8	0.8
Long range (|i-j|≥5)	33	4.5	15	45.5	2.1	12	36.4	1.6
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	3	0.4	3	100.0	0.4	0	0.0	0.0
Sidechain-Sidechain	30	4.1	12	40.0	1.6	12	40.0	1.6
Inter-chain	21	2.9	18	85.7	2.5	15	71.4	2.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	6	0.8	6	100.0	0.8	6	100.0	0.8
Sidechain-Sidechain	15	2.1	12	80.0	1.6	9	60.0	1.2
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	729	100.0	276	37.9	37.9	67	9.2	9.2
Backbone-Backbone	339	46.5	58	17.1	8.0	19	5.6	2.6
Backbone-Sidechain	177	24.3	95	53.7	13.0	21	11.9	2.9
Sidechain-Sidechain	213	29.2	123	57.7	16.9	27	12.7	3.7

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	1	41	54	12	15	123	3.79	27.09	7.32	0.55
2	9	34	58	12	18	131	3.54	24.44	6.51	0.56
3	2	47	55	12	18	134	3.25	24.28	6.39	0.5
4	4	37	62	12	18	133	3.31	22.93	6.03	0.61
5	3	47	60	12	18	140	3.36	26.54	6.75	0.47
6	7	44	60	12	18	141	2.92	20.2	5.42	0.46
7	5	34	55	12	18	124	4.0	28.44	7.71	0.5
8	8	44	63	12	18	145	3.17	26.45	6.58	0.35
9	1	43	60	12	18	134	3.75	28.51	7.46	0.58
10	4	39	53	12	18	126	3.71	26.08	6.92	0.54

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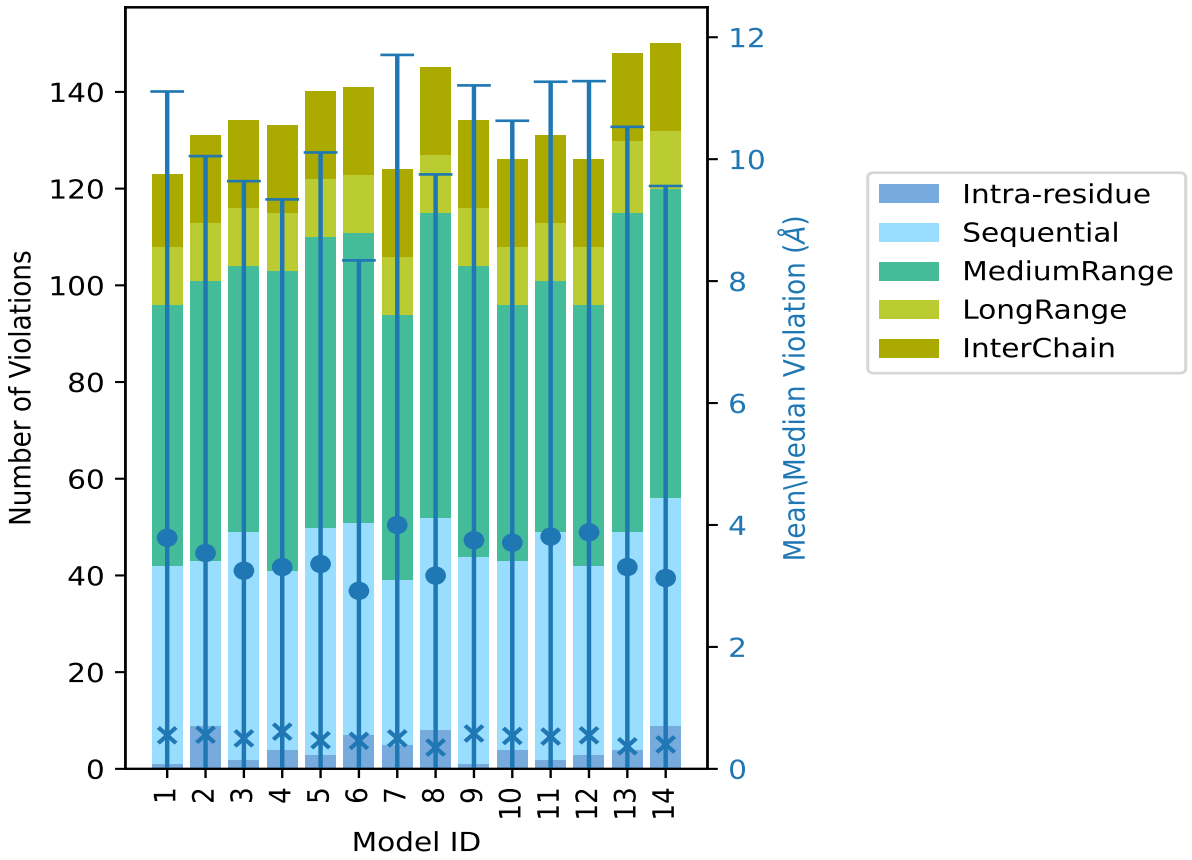
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	2	47	52	12	18	131	3.81	28.38	7.46	0.53
12	3	39	54	12	18	126	3.88	27.91	7.4	0.55
13	4	45	66	15	18	148	3.31	28.51	7.22	0.37
14	9	47	64	12	18	150	3.13	25.86	6.43	0.4

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

9.3 Distance violation statistics for the ensemble

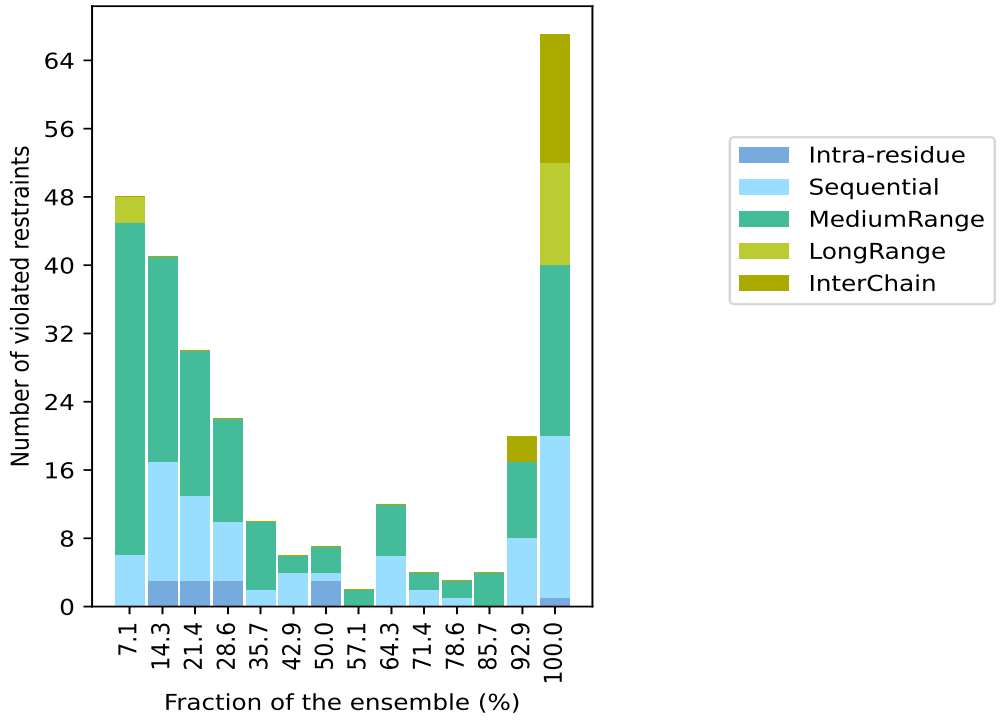
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints

for a given fraction of the ensemble. In total, 453(IR:83, SQ:214, MR:135, LR:18, IC:3) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	6	39	3	0	48	1	7.1
3	14	24	0	0	41	2	14.3
3	10	17	0	0	30	3	21.4
3	7	12	0	0	22	4	28.6
0	2	8	0	0	10	5	35.7
0	4	2	0	0	6	6	42.9
3	1	3	0	0	7	7	50.0
0	0	2	0	0	2	8	57.1
0	6	6	0	0	12	9	64.3
0	2	2	0	0	4	10	71.4
0	1	2	0	0	3	11	78.6
0	0	4	0	0	4	12	85.7
0	8	9	0	3	20	13	92.9
1	19	20	12	15	67	14	100.0

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

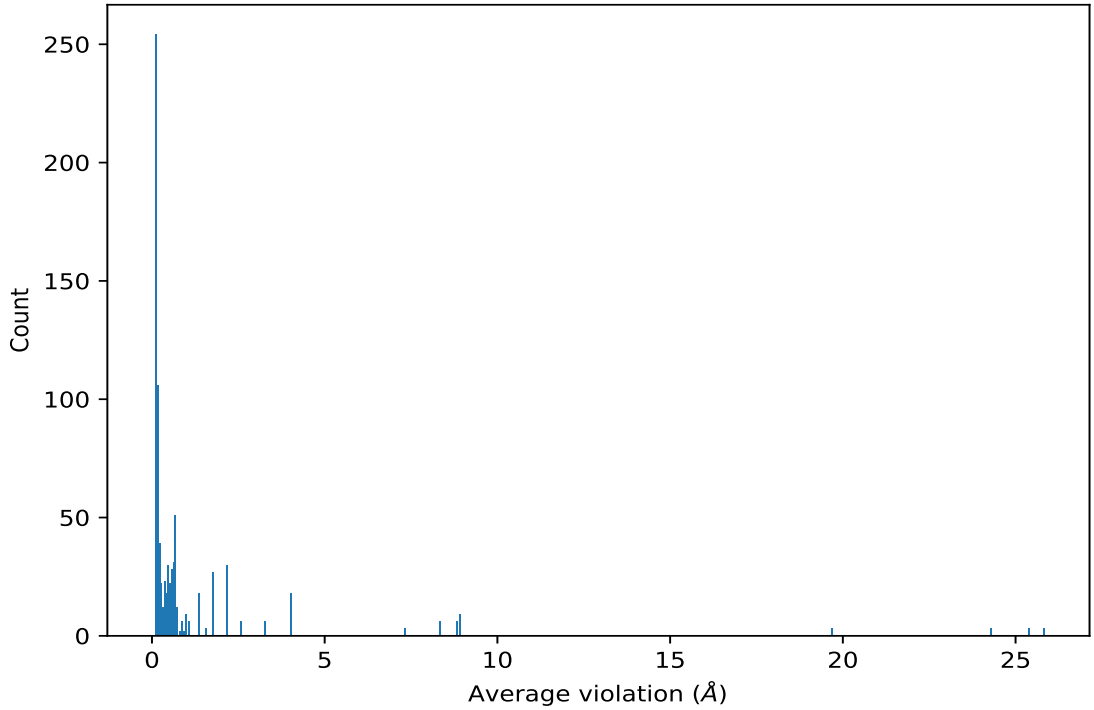
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	14	25.8	2.82	26.49
(1,5)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	14	25.8	2.82	26.49
(1,6)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	14	25.8	2.82	26.49
(1,7)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	14	25.36	2.03	25.52
(1,8)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	14	25.36	2.03	25.52
(1,9)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	14	25.36	2.03	25.52
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	14	24.29	2.67	24.7
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	14	24.29	2.67	24.7
(1,3)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	14	24.29	2.67	24.7

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,13)	1:675:A:ILE:H	2:801:B:QOJ:H181	14	19.68	1.48	19.28
(1,14)	1:675:A:ILE:H	2:801:B:QOJ:H181	14	19.68	1.48	19.28
(1,15)	1:675:A:ILE:H	2:801:B:QOJ:H181	14	19.68	1.48	19.28
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	8.9	0.56	8.8
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	8.9	0.56	8.8
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	8.9	0.56	8.8
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	8.9	0.56	8.8
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	8.9	0.56	8.8
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	8.9	0.56	8.8
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	8.9	0.56	8.8
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	8.9	0.56	8.8
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	8.9	0.56	8.8
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	8.83	0.78	8.78
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	8.83	0.78	8.78
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	8.83	0.78	8.78
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	8.83	0.78	8.78
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	8.83	0.78	8.78
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	8.83	0.78	8.78
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H271	14	8.34	0.67	8.4
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H272	14	8.34	0.67	8.4
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H271	14	8.34	0.67	8.4
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H272	14	8.34	0.67	8.4
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H271	14	8.34	0.67	8.4
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H272	14	8.34	0.67	8.4
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	7.33	1.09	7.41
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	7.33	1.09	7.41
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	7.33	1.09	7.41
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	14	4.04	1.52	4.1
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	14	4.04	1.52	4.1
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	14	4.04	1.52	4.1
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	14	4.04	1.52	4.1
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	14	4.04	1.52	4.1
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	14	4.04	1.52	4.1
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	14	4.04	1.52	4.1
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	14	4.04	1.52	4.1
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	14	4.04	1.52	4.1
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	14	4.04	1.52	4.1
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	14	4.04	1.52	4.1
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	14	4.04	1.52	4.1
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	14	4.04	1.52	4.1
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	14	4.04	1.52	4.1
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	14	4.04	1.52	4.1

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	14	4.04	1.52	4.1
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	14	4.04	1.52	4.1
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	14	4.04	1.52	4.1
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	3.28	0.65	3.22
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	3.28	0.65	3.22
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	3.28	0.65	3.22
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	3.28	0.65	3.22
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	3.28	0.65	3.22
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	3.28	0.65	3.22
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA2	14	2.58	0.76	2.88
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA3	14	2.58	0.76	2.88
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA2	14	2.58	0.76	2.88
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA3	14	2.58	0.76	2.88
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA2	14	2.58	0.76	2.88
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA3	14	2.58	0.76	2.88
(2,52)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	2.17	1.15	1.89
(2,52)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	14	2.17	1.15	1.89
(2,52)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	14	2.17	1.15	1.89
(2,52)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	14	2.17	1.15	1.89
(2,52)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	14	2.17	1.15	1.89
(2,52)	1:693:A:ILE:HD12	1:696:A:ARG:HH12	14	2.17	1.15	1.89
(2,52)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	14	2.17	1.15	1.89
(2,52)	1:693:A:ILE:HD13	1:696:A:ARG:HH12	14	2.17	1.15	1.89
(2,52)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	14	2.17	1.15	1.89
(2,52)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	14	2.17	1.15	1.89
(2,53)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	2.17	1.15	1.89
(2,53)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	14	2.17	1.15	1.89
(2,53)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	14	2.17	1.15	1.89
(2,53)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	14	2.17	1.15	1.89
(2,53)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	14	2.17	1.15	1.89
(2,53)	1:693:A:ILE:HD12	1:696:A:ARG:HH12	14	2.17	1.15	1.89
(2,53)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	14	2.17	1.15	1.89
(2,53)	1:693:A:ILE:HD13	1:696:A:ARG:HH12	14	2.17	1.15	1.89
(2,53)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	14	2.17	1.15	1.89
(2,53)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	14	2.17	1.15	1.89
(2,54)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	2.17	1.15	1.89
(2,54)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	14	2.17	1.15	1.89
(2,54)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	14	2.17	1.15	1.89
(2,54)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	14	2.17	1.15	1.89
(2,54)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	14	2.17	1.15	1.89
(2,54)	1:693:A:ILE:HD12	1:696:A:ARG:HH12	14	2.17	1.15	1.89
(2,54)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	14	2.17	1.15	1.89

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,54)	1:693:A:ILE:HD13	1:696:A:ARG:HH12	14	2.17	1.15	1.89
(2,54)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	14	2.17	1.15	1.89
(2,54)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	14	2.17	1.15	1.89
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	14	1.79	0.51	1.91
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	14	1.79	0.51	1.91
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	14	1.79	0.51	1.91
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	14	1.79	0.51	1.91
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	14	1.79	0.51	1.91
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	14	1.79	0.51	1.91
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	14	1.79	0.51	1.91
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	14	1.79	0.51	1.91
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	14	1.79	0.51	1.91
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	14	1.79	0.51	1.91
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	14	1.79	0.51	1.91
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	14	1.79	0.51	1.91
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	14	1.79	0.51	1.91
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	14	1.79	0.51	1.91
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	14	1.79	0.51	1.91
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	14	1.79	0.51	1.91
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	14	1.79	0.51	1.91
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	14	1.79	0.51	1.91
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	14	1.79	0.51	1.91
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	14	1.79	0.51	1.91
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	14	1.79	0.51	1.91
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	14	1.79	0.51	1.91
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	14	1.79	0.51	1.91
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	14	1.79	0.51	1.91
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	14	1.79	0.51	1.91
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	14	1.79	0.51	1.91
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	14	1.79	0.51	1.91
(2,43)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	1.39	0.11	1.39
(2,43)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	1.39	0.11	1.39
(2,43)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	1.39	0.11	1.39
(2,44)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	1.39	0.11	1.39
(2,44)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	1.39	0.11	1.39
(2,44)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	1.39	0.11	1.39
(2,45)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	1.39	0.11	1.39
(2,45)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	1.39	0.11	1.39
(2,45)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	1.39	0.11	1.39
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	1.39	0.11	1.39
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	1.39	0.11	1.39
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	1.39	0.11	1.39

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	1.39	0.11	1.39
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	1.39	0.11	1.39
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	1.39	0.11	1.39
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	1.39	0.11	1.39
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	1.39	0.11	1.39
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	1.39	0.11	1.39
(3,483)	1:672:A:TRP:H	1:673:A:PHE:H	14	0.81	0.16	0.88
(3,486)	1:673:A:PHE:H	1:672:A:TRP:H	14	0.81	0.16	0.88
(3,567)	1:706:A:ASN:H	1:703:A:SER:HA	14	0.56	0.36	0.45
(3,422)	1:700:A:ALA:HB1	1:697:A:ILE:HA	14	0.51	0.09	0.54
(3,422)	1:700:A:ALA:HB2	1:697:A:ILE:HA	14	0.51	0.09	0.54
(3,422)	1:700:A:ALA:HB3	1:697:A:ILE:HA	14	0.51	0.09	0.54
(3,348)	1:705:A:VAL:HG11	1:706:A:ASN:HA	14	0.32	0.21	0.24
(3,348)	1:705:A:VAL:HG12	1:706:A:ASN:HA	14	0.32	0.21	0.24
(3,348)	1:705:A:VAL:HG13	1:706:A:ASN:HA	14	0.32	0.21	0.24
(3,337)	1:704:A:LEU:H	1:704:A:LEU:HB2	14	0.3	0.08	0.29
(3,191)	1:696:A:ARG:H	1:695:A:LEU:H	14	0.23	0.03	0.23
(3,405)	1:696:A:ARG:H	1:695:A:LEU:H	14	0.23	0.03	0.23
(3,619)	1:696:A:ARG:H	1:695:A:LEU:H	14	0.23	0.03	0.23
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	14	0.22	0.05	0.21
(3,204)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.21	0.01	0.21
(3,418)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.21	0.01	0.21
(3,632)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.21	0.01	0.21
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	14	0.19	0.06	0.19
(3,482)	1:672:A:TRP:H	1:671:A:ASN:H	14	0.19	0.06	0.19
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.19	0.03	0.18
(3,230)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.19	0.03	0.18
(3,444)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.19	0.03	0.18
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	14	0.19	0.02	0.19
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.18	0.04	0.2
(3,225)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.18	0.04	0.2
(3,439)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.18	0.04	0.2
(1,19)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	13	1.59	0.68	1.82
(1,20)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	13	1.59	0.68	1.82
(1,21)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	13	1.59	0.68	1.82
(3,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	13	0.69	0.16	0.65
(3,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	13	0.69	0.16	0.65
(3,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	13	0.69	0.16	0.65
(3,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	13	0.69	0.16	0.65
(3,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	13	0.69	0.16	0.65
(3,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	13	0.69	0.16	0.65
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	13	0.63	0.07	0.61

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	13	0.63	0.07	0.61
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	13	0.63	0.07	0.61
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	13	0.63	0.07	0.61
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	13	0.63	0.07	0.61
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	13	0.63	0.07	0.61
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	13	0.63	0.07	0.61
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	13	0.63	0.07	0.61
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	13	0.63	0.07	0.61
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	13	0.63	0.07	0.61
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	13	0.63	0.07	0.61
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	13	0.63	0.07	0.61
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	13	0.63	0.07	0.61
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	13	0.63	0.07	0.61
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	13	0.63	0.07	0.61
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	13	0.63	0.07	0.61
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	13	0.63	0.07	0.61
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	13	0.63	0.07	0.61
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	13	0.63	0.07	0.61
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	13	0.63	0.07	0.61
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	13	0.63	0.07	0.61
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	13	0.63	0.07	0.61
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	13	0.63	0.07	0.61
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	13	0.63	0.07	0.61
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	13	0.63	0.07	0.61
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	13	0.63	0.07	0.61
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	13	0.63	0.07	0.61
(3,599)	1:690:A:GLY:H	1:691:A:SER:H	13	0.61	0.19	0.58
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	13	0.58	0.25	0.47
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	13	0.58	0.25	0.47
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	13	0.58	0.25	0.47
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	13	0.58	0.25	0.47
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	13	0.58	0.25	0.47
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	13	0.58	0.25	0.47
(3,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	13	0.56	0.08	0.58
(3,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	13	0.56	0.08	0.58
(3,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	13	0.56	0.08	0.58
(3,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	13	0.56	0.08	0.58
(3,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	13	0.56	0.08	0.58
(3,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	13	0.56	0.08	0.58
(3,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	13	0.56	0.08	0.57
(3,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	13	0.56	0.08	0.57
(3,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	13	0.56	0.08	0.57

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	13	0.56	0.08	0.57
(3,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	13	0.56	0.08	0.57
(3,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	13	0.56	0.08	0.57
(3,573)	1:707:A:ARG:H	1:704:A:LEU:HA	13	0.51	0.15	0.49
(3,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	13	0.46	0.08	0.48
(3,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	13	0.46	0.08	0.48
(3,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	13	0.46	0.08	0.48
(3,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	13	0.46	0.08	0.48
(3,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	13	0.46	0.08	0.48
(3,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	13	0.46	0.08	0.48
(3,612)	1:695:A:LEU:H	1:694:A:GLY:H	13	0.42	0.11	0.43
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	13	0.18	0.05	0.17
(3,384)	1:690:A:GLY:H	1:689:A:VAL:H	13	0.18	0.05	0.17
(3,531)	1:689:A:VAL:H	1:690:A:GLY:H	13	0.18	0.05	0.17
(3,598)	1:690:A:GLY:H	1:689:A:VAL:H	13	0.18	0.05	0.17
(3,378)	1:687:A:ILE:HG21	1:691:A:SER:HG	12	0.7	0.25	0.74
(3,378)	1:687:A:ILE:HG22	1:691:A:SER:HG	12	0.7	0.25	0.74
(3,378)	1:687:A:ILE:HG23	1:691:A:SER:HG	12	0.7	0.25	0.74
(3,592)	1:687:A:ILE:HG21	1:691:A:SER:HG	12	0.7	0.25	0.74
(3,592)	1:687:A:ILE:HG22	1:691:A:SER:HG	12	0.7	0.25	0.74
(3,592)	1:687:A:ILE:HG23	1:691:A:SER:HG	12	0.7	0.25	0.74
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	12	0.68	0.25	0.7
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	12	0.68	0.25	0.7
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	12	0.68	0.25	0.7
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	12	0.68	0.25	0.7
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	12	0.68	0.25	0.7
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	12	0.68	0.25	0.7
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	12	0.68	0.25	0.7
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	12	0.68	0.25	0.7
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	12	0.68	0.25	0.7
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	12	0.68	0.25	0.7
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	12	0.68	0.25	0.7
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	12	0.68	0.25	0.7
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	12	0.68	0.25	0.7
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	12	0.68	0.25	0.7
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	12	0.68	0.25	0.7
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	12	0.68	0.25	0.7
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	12	0.68	0.25	0.7
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	12	0.68	0.25	0.7
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	11	0.18	0.05	0.19
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	11	0.18	0.05	0.19
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	11	0.18	0.05	0.19

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	11	0.18	0.05	0.19
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	11	0.18	0.05	0.19
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	11	0.18	0.05	0.19
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	11	0.14	0.03	0.13
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	11	0.14	0.03	0.13
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	11	0.14	0.03	0.13
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	11	0.14	0.03	0.13
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	11	0.14	0.03	0.13
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	11	0.14	0.03	0.13
(3,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	10	0.44	0.15	0.52
(3,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	10	0.44	0.15	0.52
(3,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	10	0.44	0.15	0.52
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	10	0.19	0.06	0.19
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	10	0.19	0.06	0.19
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	10	0.19	0.06	0.19
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	10	0.19	0.06	0.19
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	10	0.19	0.06	0.19
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	10	0.19	0.06	0.19
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	10	0.16	0.03	0.16
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	10	0.15	0.03	0.14
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	10	0.15	0.03	0.14
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	10	0.15	0.03	0.14
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	10	0.15	0.03	0.14
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	10	0.15	0.03	0.14
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	10	0.15	0.03	0.14
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	9	0.65	0.3	0.83
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	9	0.65	0.3	0.83
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	9	0.65	0.3	0.83
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	9	0.65	0.3	0.83
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	9	0.65	0.3	0.83
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	9	0.65	0.3	0.83
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	9	0.65	0.3	0.83
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	9	0.65	0.3	0.83
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	9	0.65	0.3	0.83
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	9	0.65	0.3	0.83
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	9	0.65	0.3	0.83
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	9	0.65	0.3	0.83
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	9	0.55	0.24	0.52
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	9	0.55	0.24	0.52
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	9	0.55	0.24	0.52
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	9	0.55	0.24	0.52
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	9	0.55	0.24	0.52

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	9	0.55	0.24	0.52
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	9	0.51	0.16	0.55
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	9	0.51	0.16	0.55
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	9	0.51	0.16	0.55
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	9	0.51	0.16	0.55
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	9	0.51	0.16	0.55
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	9	0.51	0.16	0.55
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	9	0.5	0.03	0.51
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	9	0.5	0.03	0.51
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	9	0.5	0.03	0.51
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	9	0.5	0.03	0.51
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	9	0.5	0.03	0.51
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	9	0.5	0.03	0.51
(3,545)	1:704:A:LEU:H	1:701:A:VAL:HA	9	0.19	0.05	0.18
(3,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	9	0.14	0.03	0.13
(3,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	9	0.14	0.03	0.13
(3,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	9	0.14	0.03	0.13
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	9	0.14	0.03	0.13
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	9	0.13	0.03	0.12
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	9	0.13	0.03	0.12
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	9	0.13	0.03	0.12
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	9	0.13	0.03	0.12
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	9	0.13	0.03	0.12
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	9	0.13	0.03	0.12
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	9	0.13	0.03	0.12
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	9	0.13	0.03	0.12
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	9	0.13	0.03	0.12
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	9	0.13	0.03	0.12
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	9	0.13	0.03	0.12
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	9	0.13	0.03	0.12
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	8	0.51	0.08	0.52
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	8	0.51	0.08	0.52
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	8	0.51	0.08	0.52

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	8	0.51	0.08	0.52
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	8	0.51	0.08	0.52
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	8	0.51	0.08	0.52
(3,175)	1:692:A:LEU:HD11	1:696:A:ARG:HH21	8	0.38	0.13	0.38
(3,175)	1:692:A:LEU:HD11	1:696:A:ARG:HH22	8	0.38	0.13	0.38
(3,175)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	8	0.38	0.13	0.38
(3,175)	1:692:A:LEU:HD11	1:696:A:ARG:HH12	8	0.38	0.13	0.38
(3,175)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	8	0.38	0.13	0.38
(3,175)	1:692:A:LEU:HD13	1:696:A:ARG:HH12	8	0.38	0.13	0.38
(3,175)	1:692:A:LEU:HD12	1:696:A:ARG:HH21	8	0.38	0.13	0.38
(3,175)	1:692:A:LEU:HD12	1:696:A:ARG:HH22	8	0.38	0.13	0.38
(3,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	7	0.23	0.02	0.23
(3,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	7	0.23	0.02	0.23
(3,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	7	0.23	0.02	0.23
(3,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	7	0.23	0.02	0.23
(3,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	7	0.23	0.02	0.23
(3,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	7	0.23	0.02	0.23
(3,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	7	0.22	0.05	0.22
(3,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	7	0.22	0.05	0.22
(3,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	7	0.19	0.04	0.17
(3,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	7	0.19	0.04	0.17
(3,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	7	0.19	0.04	0.17
(3,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	7	0.19	0.04	0.17
(3,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	7	0.19	0.04	0.17
(3,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	7	0.19	0.04	0.17
(3,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	7	0.18	0.07	0.16
(3,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	7	0.18	0.07	0.16
(3,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	7	0.18	0.07	0.16
(3,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	7	0.18	0.07	0.16
(3,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	7	0.18	0.07	0.16
(3,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	7	0.18	0.07	0.16
(3,351)	1:705:A:VAL:HG21	1:702:A:LEU:HG	6	0.44	0.32	0.29
(3,351)	1:705:A:VAL:HG22	1:702:A:LEU:HG	6	0.44	0.32	0.29
(3,351)	1:705:A:VAL:HG23	1:702:A:LEU:HG	6	0.44	0.32	0.29
(3,554)	1:704:A:LEU:HD11	1:707:A:ARG:HE	6	0.43	0.12	0.48
(3,554)	1:704:A:LEU:HD12	1:707:A:ARG:HE	6	0.43	0.12	0.48
(3,554)	1:704:A:LEU:HD13	1:707:A:ARG:HE	6	0.43	0.12	0.48
(3,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	6	0.26	0.03	0.24
(3,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	6	0.26	0.03	0.24
(3,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	6	0.26	0.03	0.24
(3,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	6	0.26	0.03	0.24
(3,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	6	0.26	0.03	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	6	0.26	0.03	0.24
(3,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	6	0.26	0.03	0.24
(3,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	6	0.26	0.03	0.24
(3,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	6	0.26	0.03	0.24
(3,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	6	0.26	0.03	0.24
(3,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	6	0.26	0.03	0.24
(3,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	6	0.26	0.03	0.24
(3,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	6	0.16	0.03	0.16
(3,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	6	0.16	0.03	0.16
(3,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	6	0.16	0.03	0.16
(3,641)	1:701:A:VAL:HG11	1:698:A:VAL:HA	5	0.97	0.59	1.44
(3,641)	1:701:A:VAL:HG12	1:698:A:VAL:HA	5	0.97	0.59	1.44
(3,641)	1:701:A:VAL:HG13	1:698:A:VAL:HA	5	0.97	0.59	1.44
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	5	0.66	0.19	0.73
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	5	0.66	0.19	0.73
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	5	0.66	0.19	0.73
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	5	0.66	0.19	0.73
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	5	0.66	0.19	0.73
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	5	0.66	0.19	0.73
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	5	0.66	0.19	0.73
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	5	0.66	0.19	0.73
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	5	0.66	0.19	0.73
(3,642)	1:701:A:VAL:HG21	1:698:A:VAL:HA	5	0.64	0.33	0.44
(3,642)	1:701:A:VAL:HG22	1:698:A:VAL:HA	5	0.64	0.33	0.44
(3,642)	1:701:A:VAL:HG23	1:698:A:VAL:HA	5	0.64	0.33	0.44
(3,597)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	5	0.42	0.31	0.25
(3,597)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	5	0.42	0.31	0.25
(3,597)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	5	0.42	0.31	0.25
(3,597)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	5	0.42	0.31	0.25
(3,597)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	5	0.42	0.31	0.25
(3,597)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	5	0.42	0.31	0.25
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG21	5	0.38	0.13	0.39
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG22	5	0.38	0.13	0.39
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG23	5	0.38	0.13	0.39
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG21	5	0.38	0.13	0.39
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG22	5	0.38	0.13	0.39
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG23	5	0.38	0.13	0.39
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG21	5	0.38	0.13	0.39
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG22	5	0.38	0.13	0.39
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG23	5	0.38	0.13	0.39
(3,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	5	0.15	0.02	0.15
(3,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	5	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	5	0.15	0.02	0.15
(3,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	5	0.15	0.02	0.15
(3,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	5	0.15	0.02	0.15
(3,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	5	0.15	0.02	0.15
(3,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	5	0.14	0.02	0.14
(3,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	5	0.14	0.02	0.14
(3,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	5	0.14	0.02	0.14
(3,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	5	0.14	0.02	0.14
(3,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	5	0.14	0.02	0.14
(3,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	5	0.14	0.02	0.14
(3,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	5	0.14	0.02	0.14
(3,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	5	0.14	0.02	0.14
(3,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	5	0.14	0.02	0.14
(3,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	5	0.14	0.02	0.14
(3,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	5	0.14	0.02	0.14
(3,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	5	0.14	0.02	0.14
(3,83)	1:682:A:ILE:HD11	1:681:A:TYR:H	5	0.13	0.03	0.12
(3,83)	1:682:A:ILE:HD12	1:681:A:TYR:H	5	0.13	0.03	0.12
(3,83)	1:682:A:ILE:HD13	1:681:A:TYR:H	5	0.13	0.03	0.12
(3,403)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	5	0.13	0.01	0.13
(3,403)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	5	0.13	0.01	0.13
(3,403)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	5	0.13	0.01	0.13
(3,403)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	5	0.13	0.01	0.13
(3,403)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	5	0.13	0.01	0.13
(3,403)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	5	0.13	0.01	0.13
(3,564)	1:705:A:VAL:HG21	1:701:A:VAL:HA	4	0.6	0.06	0.6
(3,564)	1:705:A:VAL:HG22	1:701:A:VAL:HA	4	0.6	0.06	0.6
(3,564)	1:705:A:VAL:HG23	1:701:A:VAL:HA	4	0.6	0.06	0.6
(2,59)	1:696:A:ARG:H	1:693:A:ILE:HD11	4	0.48	0.04	0.48
(2,59)	1:696:A:ARG:H	1:693:A:ILE:HD12	4	0.48	0.04	0.48
(2,59)	1:696:A:ARG:H	1:693:A:ILE:HD13	4	0.48	0.04	0.48
(2,60)	1:696:A:ARG:H	1:693:A:ILE:HD11	4	0.48	0.04	0.48
(2,60)	1:696:A:ARG:H	1:693:A:ILE:HD12	4	0.48	0.04	0.48
(2,60)	1:696:A:ARG:H	1:693:A:ILE:HD13	4	0.48	0.04	0.48
(3,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	4	0.4	0.24	0.3
(3,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	4	0.4	0.24	0.3
(3,194)	1:697:A:ILE:HG21	1:698:A:VAL:HA	4	0.34	0.01	0.34
(3,194)	1:697:A:ILE:HG22	1:698:A:VAL:HA	4	0.34	0.01	0.34
(3,194)	1:697:A:ILE:HG23	1:698:A:VAL:HA	4	0.34	0.01	0.34
(3,408)	1:697:A:ILE:HG21	1:698:A:VAL:HA	4	0.34	0.01	0.34
(3,408)	1:697:A:ILE:HG22	1:698:A:VAL:HA	4	0.34	0.01	0.34
(3,408)	1:697:A:ILE:HG23	1:698:A:VAL:HA	4	0.34	0.01	0.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,622)	1:697:A:ILE:HG21	1:698:A:VAL:HA	4	0.34	0.01	0.34
(3,622)	1:697:A:ILE:HG22	1:698:A:VAL:HA	4	0.34	0.01	0.34
(3,622)	1:697:A:ILE:HG23	1:698:A:VAL:HA	4	0.34	0.01	0.34
(3,15)	1:665:A:LYS:H	1:662:A:GLU:HA	4	0.22	0.09	0.2
(3,229)	1:665:A:LYS:H	1:662:A:GLU:HA	4	0.22	0.09	0.2
(3,443)	1:665:A:LYS:H	1:662:A:GLU:HA	4	0.22	0.09	0.2
(3,174)	1:692:A:LEU:HD11	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,174)	1:692:A:LEU:HD11	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,174)	1:692:A:LEU:HD12	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,174)	1:692:A:LEU:HD12	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,174)	1:692:A:LEU:HD13	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,174)	1:692:A:LEU:HD13	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,388)	1:692:A:LEU:HD11	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,388)	1:692:A:LEU:HD11	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,388)	1:692:A:LEU:HD12	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,388)	1:692:A:LEU:HD12	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,388)	1:692:A:LEU:HD13	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,388)	1:692:A:LEU:HD13	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,602)	1:692:A:LEU:HD11	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,602)	1:692:A:LEU:HD11	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,602)	1:692:A:LEU:HD12	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,602)	1:692:A:LEU:HD12	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,602)	1:692:A:LEU:HD13	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,602)	1:692:A:LEU:HD13	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,46)	1:670:A:TRP:H	1:667:A:ALA:HA	4	0.16	0.01	0.16
(3,260)	1:670:A:TRP:H	1:667:A:ALA:HA	4	0.16	0.01	0.16
(3,406)	1:696:A:ARG:H	1:696:A:ARG:HE	4	0.16	0.03	0.15
(3,620)	1:696:A:ARG:H	1:696:A:ARG:HE	4	0.16	0.03	0.15
(3,88)	1:684:A:ILE:HD11	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,88)	1:684:A:ILE:HD12	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,88)	1:684:A:ILE:HD13	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,302)	1:684:A:ILE:HD11	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,302)	1:684:A:ILE:HD12	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,302)	1:684:A:ILE:HD13	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,516)	1:684:A:ILE:HD11	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,516)	1:684:A:ILE:HD12	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,516)	1:684:A:ILE:HD13	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	4	0.13	0.02	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	4	0.13	0.02	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	4	0.13	0.02	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	4	0.13	0.02	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	4	0.13	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	4	0.13	0.02	0.14
(3,336)	1:704:A:LEU:H	1:704:A:LEU:HB3	4	0.12	0.02	0.12
(2,46)	1:693:A:ILE:H	1:693:A:ILE:HG12	3	1.07	0.03	1.08
(2,46)	1:693:A:ILE:H	1:693:A:ILE:HG13	3	1.07	0.03	1.08
(2,47)	1:693:A:ILE:H	1:693:A:ILE:HG12	3	1.07	0.03	1.08
(2,47)	1:693:A:ILE:H	1:693:A:ILE:HG13	3	1.07	0.03	1.08
(2,48)	1:693:A:ILE:H	1:693:A:ILE:HG12	3	1.07	0.03	1.08
(2,48)	1:693:A:ILE:H	1:693:A:ILE:HG13	3	1.07	0.03	1.08
(3,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	3	0.96	0.09	0.99
(3,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	3	0.96	0.09	0.99
(3,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	3	0.96	0.09	0.99
(3,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	3	0.96	0.09	0.99
(3,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	3	0.96	0.09	0.99
(3,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	3	0.96	0.09	0.99
(3,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	3	0.95	0.06	0.95
(3,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	3	0.95	0.06	0.95
(3,391)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	3	0.71	0.03	0.7
(3,391)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	3	0.71	0.03	0.7
(3,391)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	3	0.71	0.03	0.7
(3,391)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	3	0.71	0.03	0.7
(3,391)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	3	0.71	0.03	0.7
(3,391)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	3	0.71	0.03	0.7
(3,605)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	3	0.71	0.03	0.7
(3,605)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	3	0.71	0.03	0.7
(3,605)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	3	0.71	0.03	0.7
(3,605)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	3	0.71	0.03	0.7
(3,605)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	3	0.71	0.03	0.7
(3,605)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	3	0.71	0.03	0.7
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD11	3	0.38	0.14	0.45
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD12	3	0.38	0.14	0.45
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD13	3	0.38	0.14	0.45
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD21	3	0.38	0.14	0.45
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD22	3	0.38	0.14	0.45
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD23	3	0.38	0.14	0.45
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	3	0.16	0.04	0.14
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	3	0.16	0.04	0.14
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	3	0.16	0.04	0.14
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	3	0.16	0.04	0.14
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	3	0.16	0.04	0.14
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	3	0.16	0.04	0.14
(3,565)	1:705:A:VAL:HG21	1:702:A:LEU:HG	3	0.16	0.05	0.13
(3,565)	1:705:A:VAL:HG22	1:702:A:LEU:HG	3	0.16	0.05	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,565)	1:705:A:VAL:HG23	1:702:A:LEU:HG	3	0.16	0.05	0.13
(3,53)	1:671:A:ASN:H	1:672:A:TRP:HE1	3	0.15	0.04	0.13
(3,57)	1:672:A:TRP:HE1	1:671:A:ASN:H	3	0.15	0.04	0.13
(3,267)	1:671:A:ASN:H	1:672:A:TRP:HE1	3	0.15	0.04	0.13
(3,271)	1:672:A:TRP:HE1	1:671:A:ASN:H	3	0.15	0.04	0.13
(3,178)	1:693:A:ILE:HD11	1:697:A:ILE:H	3	0.15	0.02	0.14
(3,178)	1:693:A:ILE:HD12	1:697:A:ILE:H	3	0.15	0.02	0.14
(3,178)	1:693:A:ILE:HD13	1:697:A:ILE:H	3	0.15	0.02	0.14
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	3	0.14	0.05	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	3	0.14	0.05	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	3	0.14	0.05	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	3	0.14	0.05	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	3	0.14	0.05	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	3	0.14	0.05	0.1
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	3	0.13	0.01	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	3	0.13	0.01	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	3	0.13	0.01	0.14
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	3	0.13	0.01	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	3	0.13	0.01	0.14
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	3	0.13	0.01	0.14
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	3	0.13	0.01	0.14
(3,128)	1:705:A:VAL:H	1:702:A:LEU:HA	3	0.13	0.01	0.12
(3,342)	1:705:A:VAL:H	1:702:A:LEU:HA	3	0.13	0.01	0.12
(3,197)	1:698:A:VAL:HG11	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,197)	1:698:A:VAL:HG12	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,197)	1:698:A:VAL:HG13	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,411)	1:698:A:VAL:HG11	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,411)	1:698:A:VAL:HG12	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,411)	1:698:A:VAL:HG13	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,625)	1:698:A:VAL:HG11	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,625)	1:698:A:VAL:HG12	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,625)	1:698:A:VAL:HG13	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,79)	1:681:A:TYR:H	1:682:A:ILE:H	3	0.11	0.0	0.11
(3,187)	1:695:A:LEU:HD21	1:698:A:VAL:HB	3	0.11	0.01	0.1
(3,187)	1:695:A:LEU:HD22	1:698:A:VAL:HB	3	0.11	0.01	0.1
(3,187)	1:695:A:LEU:HD23	1:698:A:VAL:HB	3	0.11	0.01	0.1
(3,293)	1:681:A:TYR:H	1:682:A:ILE:H	3	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,401)	1:695:A:LEU:HD21	1:698:A:VAL:HB	3	0.11	0.01	0.1
(3,401)	1:695:A:LEU:HD22	1:698:A:VAL:HB	3	0.11	0.01	0.1
(3,401)	1:695:A:LEU:HD23	1:698:A:VAL:HB	3	0.11	0.01	0.1
(3,507)	1:681:A:TYR:H	1:682:A:ILE:H	3	0.11	0.0	0.11
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	2	0.88	0.18	0.88
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	2	0.88	0.18	0.88
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	2	0.88	0.18	0.88
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	2	0.88	0.18	0.88
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	2	0.88	0.18	0.88
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	2	0.88	0.18	0.88
(3,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	2	0.48	0.24	0.48
(3,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	2	0.48	0.24	0.48
(3,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	2	0.48	0.24	0.48
(3,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	2	0.48	0.24	0.48
(3,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	2	0.48	0.24	0.48
(3,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	2	0.48	0.24	0.48
(3,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	2	0.48	0.24	0.48
(3,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	2	0.48	0.24	0.48
(3,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	2	0.48	0.24	0.48
(3,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	2	0.48	0.24	0.48
(3,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	2	0.48	0.24	0.48
(3,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	2	0.48	0.24	0.48
(3,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	2	0.48	0.24	0.48
(3,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	2	0.48	0.24	0.48
(3,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	2	0.48	0.24	0.48
(3,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	2	0.48	0.24	0.48
(3,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	2	0.48	0.24	0.48
(3,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	2	0.48	0.24	0.48
(3,78)	1:681:A:TYR:H	1:680:A:TRP:H	2	0.29	0.01	0.29
(3,292)	1:681:A:TYR:H	1:680:A:TRP:H	2	0.29	0.01	0.29
(3,506)	1:681:A:TYR:H	1:680:A:TRP:H	2	0.29	0.01	0.29
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD11	2	0.29	0.06	0.29
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD12	2	0.29	0.06	0.29
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD13	2	0.29	0.06	0.29
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD21	2	0.29	0.06	0.29
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD22	2	0.29	0.06	0.29
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD23	2	0.29	0.06	0.29
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HG2	2	0.21	0.01	0.21
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HG3	2	0.21	0.01	0.21
(3,365)	1:707:A:ARG:H	1:707:A:ARG:HG2	2	0.21	0.01	0.21
(3,365)	1:707:A:ARG:H	1:707:A:ARG:HG3	2	0.21	0.01	0.21
(3,579)	1:707:A:ARG:H	1:707:A:ARG:HG2	2	0.21	0.01	0.21

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,579)	1:707:A:ARG:H	1:707:A:ARG:HG3	2	0.21	0.01	0.21
(3,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,80)	1:682:A:ILE:HG21	1:679:A:LEU:H	2	0.2	0.04	0.2
(3,80)	1:682:A:ILE:HG22	1:679:A:LEU:H	2	0.2	0.04	0.2
(3,80)	1:682:A:ILE:HG23	1:679:A:LEU:H	2	0.2	0.04	0.2
(3,289)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,289)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,289)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,289)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,289)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,289)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	2	0.18	0.01	0.18
(3,40)	1:669:A:LEU:H	1:666:A:TRP:HA	2	0.18	0.08	0.18
(3,234)	1:665:A:LYS:H	1:666:A:TRP:HD1	2	0.18	0.01	0.18
(3,254)	1:669:A:LEU:H	1:666:A:TRP:HA	2	0.18	0.08	0.18
(3,448)	1:665:A:LYS:H	1:666:A:TRP:HD1	2	0.18	0.01	0.18
(3,468)	1:669:A:LEU:H	1:666:A:TRP:HA	2	0.18	0.08	0.18
(2,64)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	2	0.16	0.02	0.16
(2,64)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	2	0.16	0.02	0.16
(2,64)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	2	0.16	0.02	0.16
(2,64)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	2	0.16	0.02	0.16
(2,64)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	2	0.16	0.02	0.16
(2,64)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	2	0.16	0.02	0.16
(2,65)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	2	0.16	0.02	0.16
(2,65)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	2	0.16	0.02	0.16
(2,65)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	2	0.16	0.02	0.16
(2,65)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	2	0.16	0.02	0.16
(2,65)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	2	0.16	0.02	0.16
(2,65)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	2	0.16	0.02	0.16
(2,66)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	2	0.16	0.02	0.16
(2,66)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	2	0.16	0.02	0.16
(2,66)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	2	0.16	0.02	0.16
(2,66)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	2	0.16	0.02	0.16
(2,66)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	2	0.16	0.02	0.16
(2,66)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	2	0.16	0.02	0.16
(3,166)	1:688:A:ILE:HG21	1:692:A:LEU:HG	2	0.15	0.01	0.15
(3,166)	1:688:A:ILE:HG22	1:692:A:LEU:HG	2	0.15	0.01	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,166)	1:688:A:ILE:HG23	1:692:A:LEU:HG	2	0.15	0.01	0.15
(3,380)	1:688:A:ILE:HG21	1:692:A:LEU:HG	2	0.15	0.01	0.15
(3,380)	1:688:A:ILE:HG22	1:692:A:LEU:HG	2	0.15	0.01	0.15
(3,380)	1:688:A:ILE:HG23	1:692:A:LEU:HG	2	0.15	0.01	0.15
(3,594)	1:688:A:ILE:HG21	1:692:A:LEU:HG	2	0.15	0.01	0.15
(3,594)	1:688:A:ILE:HG22	1:692:A:LEU:HG	2	0.15	0.01	0.15
(3,594)	1:688:A:ILE:HG23	1:692:A:LEU:HG	2	0.15	0.01	0.15
(3,136)	1:705:A:VAL:HG21	1:701:A:VAL:HA	2	0.14	0.03	0.14
(3,136)	1:705:A:VAL:HG22	1:701:A:VAL:HA	2	0.14	0.03	0.14
(3,136)	1:705:A:VAL:HG23	1:701:A:VAL:HA	2	0.14	0.03	0.14
(3,350)	1:705:A:VAL:HG21	1:701:A:VAL:HA	2	0.14	0.03	0.14
(3,350)	1:705:A:VAL:HG22	1:701:A:VAL:HA	2	0.14	0.03	0.14
(3,350)	1:705:A:VAL:HG23	1:701:A:VAL:HA	2	0.14	0.03	0.14
(3,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	2	0.14	0.01	0.14
(3,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	2	0.14	0.01	0.14
(3,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	2	0.14	0.01	0.14
(3,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	2	0.14	0.01	0.14
(3,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	2	0.14	0.01	0.14
(3,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	2	0.14	0.01	0.14
(3,193)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	2	0.14	0.02	0.14
(3,193)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	2	0.14	0.02	0.14
(3,193)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	2	0.14	0.02	0.14
(3,193)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	2	0.14	0.02	0.14
(3,193)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	2	0.14	0.02	0.14
(3,193)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	2	0.14	0.02	0.14
(3,517)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	2	0.14	0.01	0.14
(3,517)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	2	0.14	0.01	0.14
(3,517)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	2	0.14	0.01	0.14
(3,517)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	2	0.14	0.01	0.14
(3,517)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	2	0.14	0.01	0.14
(3,517)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	2	0.14	0.01	0.14
(3,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	2	0.12	0.02	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,177)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	2	0.12	0.02	0.12
(3,177)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	2	0.12	0.02	0.12
(3,177)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	2	0.12	0.02	0.12
(3,177)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	2	0.12	0.02	0.12
(3,177)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	2	0.12	0.02	0.12
(3,177)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	2	0.12	0.02	0.12
(3,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	2	0.12	0.02	0.12
(3,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	2	0.12	0.02	0.12
(3,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	2	0.12	0.02	0.12
(3,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	2	0.12	0.02	0.12
(3,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	2	0.12	0.02	0.12
(3,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	2	0.12	0.02	0.12
(3,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	2	0.12	0.02	0.12
(3,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	2	0.12	0.02	0.12
(3,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	2	0.12	0.02	0.12

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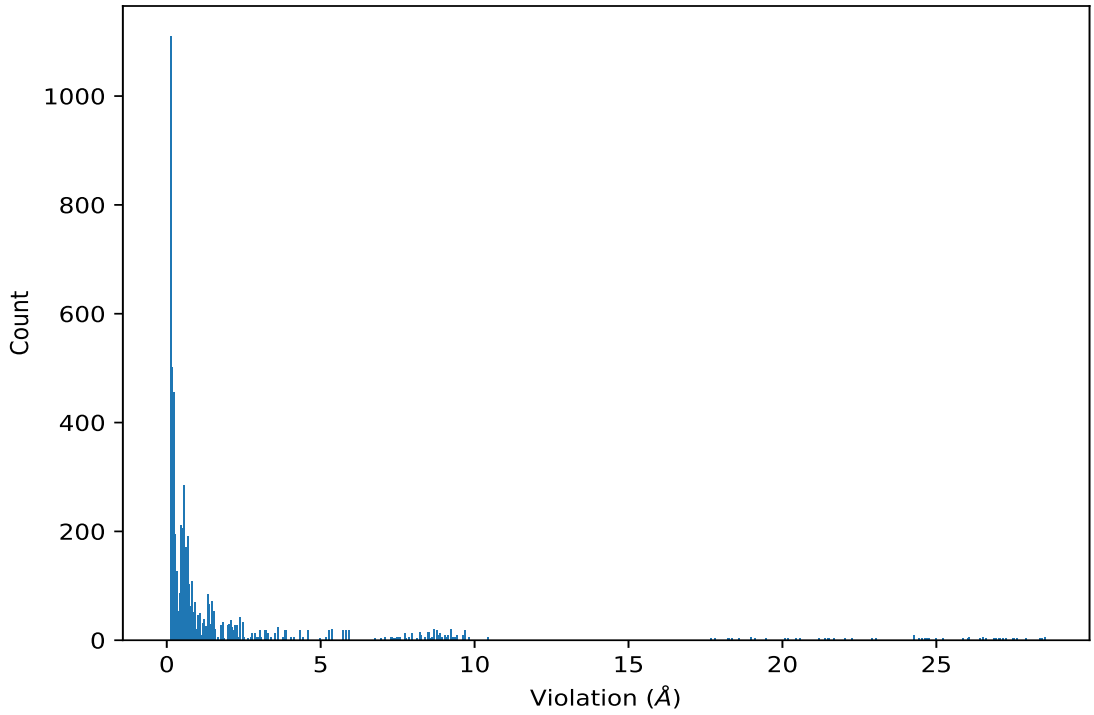
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	2	0.12	0.02	0.12
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	2	0.11	0.0	0.11
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	2	0.11	0.0	0.11
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	2	0.11	0.0	0.11
(3,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	2	0.11	0.0	0.11
(3,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	2	0.11	0.0	0.11
(3,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	2	0.11	0.0	0.11
(3,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	2	0.11	0.0	0.11
(3,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	2	0.11	0.0	0.11
(3,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	9	28.51
(1,6)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	13	28.51
(1,5)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	9	28.51
(1,5)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	13	28.51
(1,4)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	9	28.51
(1,4)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	13	28.51
(1,6)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	7	28.44
(1,5)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	7	28.44
(1,4)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	7	28.44
(1,6)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	11	28.38
(1,5)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	11	28.38
(1,4)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	11	28.38
(1,6)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	12	27.91
(1,5)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	12	27.91
(1,4)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	12	27.91
(1,9)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	7	27.64
(1,8)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	7	27.64
(1,7)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	7	27.64
(1,3)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	11	27.53
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	11	27.53
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	11	27.53
(1,9)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	13	27.47
(1,8)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	13	27.47
(1,7)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	13	27.47
(1,9)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	9	27.26
(1,8)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	9	27.26
(1,7)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	9	27.26
(1,9)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	12	27.16
(1,8)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	12	27.16
(1,7)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	12	27.16
(1,9)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	1	27.09
(1,8)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	1	27.09
(1,7)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	1	27.09
(1,3)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	9	27.01
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	9	27.01
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	9	27.01
(1,3)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	13	26.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	13	26.91
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	13	26.91
(1,6)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	1	26.86
(1,5)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	1	26.86
(1,4)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	1	26.86
(1,3)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	7	26.6
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	7	26.6
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	7	26.6
(1,6)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	5	26.54
(1,5)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	5	26.54
(1,4)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	5	26.54
(1,9)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	11	26.51
(1,8)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	11	26.51
(1,7)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	11	26.51
(1,6)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	8	26.45
(1,5)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	8	26.45
(1,4)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	8	26.45
(1,6)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	10	26.08
(1,5)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	10	26.08
(1,4)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	10	26.08
(1,9)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	5	26.07
(1,8)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	5	26.07
(1,7)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	5	26.07
(1,3)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	12	26.04
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	12	26.04
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	12	26.04
(1,6)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	14	25.86
(1,5)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	14	25.86
(1,4)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	14	25.86
(1,3)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	8	25.21
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	8	25.21
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	8	25.21
(1,9)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	8	24.96
(1,8)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	8	24.96
(1,7)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	8	24.96
(1,9)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	10	24.77
(1,8)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	10	24.77
(1,7)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	10	24.77
(1,3)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	14	24.73
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	14	24.73
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	14	24.73
(1,3)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	10	24.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	10	24.66
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	10	24.66
(1,3)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	5	24.63
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	5	24.63
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	5	24.63
(1,3)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	1	24.54
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	1	24.54
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	1	24.54
(1,9)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	2	24.44
(1,8)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	2	24.44
(1,7)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	2	24.44
(1,9)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	14	24.28
(1,8)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	14	24.28
(1,7)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	14	24.28
(1,6)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	3	24.28
(1,5)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	3	24.28
(1,4)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	3	24.28
(1,9)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	3	24.27
(1,8)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	3	24.27
(1,7)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	3	24.27
(1,6)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	2	23.0
(1,5)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	2	23.0
(1,4)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	2	23.0
(1,9)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	4	22.93
(1,8)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	4	22.93
(1,7)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	4	22.93
(1,15)	1:675:A:ILE:H	2:801:B:QOJ:H181	13	22.27
(1,14)	1:675:A:ILE:H	2:801:B:QOJ:H181	13	22.27
(1,13)	1:675:A:ILE:H	2:801:B:QOJ:H181	13	22.27
(1,3)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	3	22.03
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	3	22.03
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	3	22.03
(1,15)	1:675:A:ILE:H	2:801:B:QOJ:H181	7	21.67
(1,14)	1:675:A:ILE:H	2:801:B:QOJ:H181	7	21.67
(1,13)	1:675:A:ILE:H	2:801:B:QOJ:H181	7	21.67
(1,15)	1:675:A:ILE:H	2:801:B:QOJ:H181	9	21.52
(1,14)	1:675:A:ILE:H	2:801:B:QOJ:H181	9	21.52
(1,13)	1:675:A:ILE:H	2:801:B:QOJ:H181	9	21.52
(1,3)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	2	21.48
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	2	21.48
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	2	21.48
(1,6)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	4	21.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	4	21.36
(1,4)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	4	21.36
(1,15)	1:675:A:ILE:H	2:801:B:QOJ:H181	11	21.18
(1,14)	1:675:A:ILE:H	2:801:B:QOJ:H181	11	21.18
(1,13)	1:675:A:ILE:H	2:801:B:QOJ:H181	11	21.18
(1,15)	1:675:A:ILE:H	2:801:B:QOJ:H181	2	20.58
(1,14)	1:675:A:ILE:H	2:801:B:QOJ:H181	2	20.58
(1,13)	1:675:A:ILE:H	2:801:B:QOJ:H181	2	20.58
(1,3)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	4	20.42
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	4	20.42
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	4	20.42
(1,9)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	6	20.2
(1,8)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	6	20.2
(1,7)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	6	20.2
(1,15)	1:675:A:ILE:H	2:801:B:QOJ:H181	1	20.06
(1,14)	1:675:A:ILE:H	2:801:B:QOJ:H181	1	20.06
(1,13)	1:675:A:ILE:H	2:801:B:QOJ:H181	1	20.06
(1,15)	1:675:A:ILE:H	2:801:B:QOJ:H181	12	19.47
(1,14)	1:675:A:ILE:H	2:801:B:QOJ:H181	12	19.47
(1,13)	1:675:A:ILE:H	2:801:B:QOJ:H181	12	19.47
(1,15)	1:675:A:ILE:H	2:801:B:QOJ:H181	14	19.1
(1,14)	1:675:A:ILE:H	2:801:B:QOJ:H181	14	19.1
(1,13)	1:675:A:ILE:H	2:801:B:QOJ:H181	14	19.1
(1,15)	1:675:A:ILE:H	2:801:B:QOJ:H181	10	18.99
(1,14)	1:675:A:ILE:H	2:801:B:QOJ:H181	10	18.99
(1,13)	1:675:A:ILE:H	2:801:B:QOJ:H181	10	18.99
(1,6)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	6	18.96
(1,5)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	6	18.96
(1,4)	1:672:A:TRP:HE1	2:801:B:QOJ:H161	6	18.96
(1,15)	1:675:A:ILE:H	2:801:B:QOJ:H181	5	18.59
(1,14)	1:675:A:ILE:H	2:801:B:QOJ:H181	5	18.59
(1,13)	1:675:A:ILE:H	2:801:B:QOJ:H181	5	18.59
(1,15)	1:675:A:ILE:H	2:801:B:QOJ:H181	6	18.35
(1,14)	1:675:A:ILE:H	2:801:B:QOJ:H181	6	18.35
(1,13)	1:675:A:ILE:H	2:801:B:QOJ:H181	6	18.35
(1,15)	1:675:A:ILE:H	2:801:B:QOJ:H181	4	18.26
(1,14)	1:675:A:ILE:H	2:801:B:QOJ:H181	4	18.26
(1,13)	1:675:A:ILE:H	2:801:B:QOJ:H181	4	18.26
(1,3)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	6	18.2
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	6	18.2
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	6	18.2
(1,15)	1:675:A:ILE:H	2:801:B:QOJ:H181	3	17.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:675:A:ILE:H	2:801:B:QOJ:H181	3	17.8
(1,13)	1:675:A:ILE:H	2:801:B:QOJ:H181	3	17.8
(1,15)	1:675:A:ILE:H	2:801:B:QOJ:H181	8	17.67
(1,14)	1:675:A:ILE:H	2:801:B:QOJ:H181	8	17.67
(1,13)	1:675:A:ILE:H	2:801:B:QOJ:H181	8	17.67
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	6	10.41
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	6	10.41
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	6	10.41
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	6	10.41
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	6	10.41
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	6	10.41
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	2	9.85
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	2	9.85
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	2	9.85
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	2	9.85
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	2	9.85
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	2	9.85
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	1	9.67
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	1	9.67
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	1	9.67
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	1	9.67
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	1	9.67
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	1	9.67
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	1	9.67
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	1	9.67
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	1	9.67
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	7	9.66
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	7	9.66
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	7	9.66
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	7	9.66
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	7	9.66
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	7	9.66
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	7	9.66
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	7	9.66
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	7	9.66
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	3	9.63
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	3	9.63
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	3	9.63
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	3	9.63
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	3	9.63
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	3	9.63
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	3	9.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	3	9.63
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	3	9.63
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	13	9.44
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	13	9.44
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	13	9.44
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	13	9.44
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	13	9.44
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	13	9.44
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	13	9.44
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	13	9.44
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	13	9.44
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	7	9.39
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	7	9.39
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	7	9.39
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	7	9.39
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	7	9.39
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	7	9.39
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	8	9.31
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	8	9.31
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	8	9.31
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	8	9.31
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	8	9.31
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	8	9.31
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H271	6	9.25
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H272	6	9.25
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H271	6	9.25
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H272	6	9.25
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H271	6	9.25
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H272	6	9.25
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	11	9.23
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	11	9.23
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	11	9.23
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	11	9.23
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	11	9.23
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	11	9.23
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H271	9	9.22
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H272	9	9.22
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H271	9	9.22
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H272	9	9.22
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H271	9	9.22
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H272	9	9.22
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	2	9.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	2	9.21
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	2	9.21
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	2	9.21
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	2	9.21
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	2	9.21
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	2	9.21
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	2	9.21
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	2	9.21
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	13	9.12
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	13	9.12
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	13	9.12
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H271	4	9.12
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H272	4	9.12
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H271	4	9.12
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H272	4	9.12
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H271	4	9.12
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H272	4	9.12
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	4	9.06
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	4	9.06
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	4	9.06
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	4	9.06
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	4	9.06
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	4	9.06
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	12	9.0
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	12	9.0
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	12	9.0
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	12	9.0
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	12	9.0
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	12	9.0
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	12	9.0
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	12	9.0
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	12	9.0
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H271	8	8.94
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H272	8	8.94
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H271	8	8.94
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H272	8	8.94
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H271	8	8.94
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H272	8	8.94
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	10	8.88
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	10	8.88
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	10	8.88
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	10	8.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	10	8.88
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	10	8.88
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H271	7	8.88
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H272	7	8.88
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H271	7	8.88
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H272	7	8.88
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H271	7	8.88
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H272	7	8.88
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	4	8.82
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	4	8.82
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	4	8.82
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	4	8.82
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	4	8.82
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	4	8.82
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	4	8.82
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	4	8.82
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	4	8.82
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	8.78
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	8.78
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	8.78
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	8.78
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	8.78
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	8.78
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	8.78
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	8.78
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	8.78
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	5	8.75
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	5	8.75
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	5	8.75
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	5	8.75
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	5	8.75
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	5	8.75
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	5	8.75
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	5	8.75
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	5	8.75
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	12	8.69
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	12	8.69
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	12	8.69
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	12	8.69
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	12	8.69
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	12	8.69
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	6	8.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	6	8.66
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	6	8.66
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	6	8.66
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	6	8.66
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	6	8.66
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	6	8.66
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	6	8.66
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	6	8.66
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H271	3	8.65
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H272	3	8.65
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H271	3	8.65
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H272	3	8.65
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H271	3	8.65
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H272	3	8.65
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	9	8.6
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	9	8.6
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	9	8.6
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	9	8.6
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	9	8.6
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	9	8.6
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	2	8.55
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	2	8.55
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	2	8.55
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	9	8.54
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	9	8.54
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	9	8.54
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	9	8.54
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	9	8.54
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	9	8.54
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	9	8.54
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	9	8.54
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	9	8.54
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H271	2	8.54
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H272	2	8.54
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H271	2	8.54
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H272	2	8.54
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H271	2	8.54
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H272	2	8.54
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	11	8.49
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	11	8.49
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	11	8.49
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	11	8.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	11	8.49
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	11	8.49
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	11	8.49
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	11	8.49
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	11	8.49
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	5	8.48
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	5	8.48
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	5	8.48
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	5	8.48
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	5	8.48
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	5	8.48
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	1	8.39
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	1	8.39
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	1	8.39
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	1	8.39
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	1	8.39
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	1	8.39
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	9	8.26
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	9	8.26
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	9	8.26
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H271	12	8.25
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H272	12	8.25
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H271	12	8.25
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H272	12	8.25
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H271	12	8.25
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H272	12	8.25
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	8.24
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	8.24
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	8.24
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	8.24
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	8.24
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	8.24
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	10	8.23
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	10	8.23
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	10	8.23
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	10	8.23
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	10	8.23
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	10	8.23
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	10	8.23
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	10	8.23
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	10	8.23
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	1	8.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	1	8.12
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	1	8.12
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H271	11	7.98
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H272	11	7.98
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H271	11	7.98
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H272	11	7.98
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H271	11	7.98
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H272	11	7.98
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H271	13	7.95
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H272	13	7.95
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H271	13	7.95
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H272	13	7.95
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H271	13	7.95
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H272	13	7.95
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H271	1	7.86
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H272	1	7.86
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H271	1	7.86
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H272	1	7.86
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H271	1	7.86
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H272	1	7.86
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	7.79
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	7.79
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	7.79
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	8	7.71
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	8	7.71
(2,24)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	8	7.71
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	8	7.71
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	8	7.71
(2,23)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	8	7.71
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	8	7.71
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	8	7.71
(2,22)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	8	7.71
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	12	7.71
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	12	7.71
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	12	7.71
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	3	7.56
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	3	7.56
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	3	7.56
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	3	7.56
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	3	7.56
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	3	7.56
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H271	5	7.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H272	5	7.51
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H271	5	7.51
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H272	5	7.51
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H271	5	7.51
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H272	5	7.51
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	13	7.48
(2,18)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	13	7.48
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	13	7.48
(2,17)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	13	7.48
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	13	7.48
(2,16)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	13	7.48
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	11	7.43
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	11	7.43
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	11	7.43
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	3	7.39
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	3	7.39
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	3	7.39
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H271	14	7.35
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H272	14	7.35
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H271	14	7.35
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H272	14	7.35
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H271	14	7.35
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H272	14	7.35
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H271	10	7.27
(1,18)	1:661:A:LEU:H	2:801:B:QOJ:H272	10	7.27
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H271	10	7.27
(1,17)	1:661:A:LEU:H	2:801:B:QOJ:H272	10	7.27
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H271	10	7.27
(1,16)	1:661:A:LEU:H	2:801:B:QOJ:H272	10	7.27
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	7	7.09
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	7	7.09
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	7	7.09
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	10	7.08
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	10	7.08
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	10	7.08
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	4	6.98
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	4	6.98
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	4	6.98
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	5	6.75
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	5	6.75
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	5	6.75
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	4	5.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	4	5.92
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	4	5.92
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	4	5.92
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	4	5.92
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	4	5.92
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	4	5.92
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	4	5.92
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	4	5.92
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	4	5.92
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	4	5.92
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	4	5.92
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	4	5.92
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	4	5.92
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	4	5.92
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	4	5.92
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	4	5.92
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	4	5.92
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	12	5.81
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	12	5.81
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	12	5.81
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	12	5.81
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	12	5.81
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	12	5.81
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	12	5.81
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	12	5.81
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	12	5.81
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	12	5.81
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	12	5.81
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	12	5.81
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	12	5.81
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	12	5.81
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	12	5.81
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	12	5.81
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	12	5.81
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	12	5.81
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	9	5.74
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	9	5.74
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	9	5.74
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	9	5.74
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	9	5.74
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	9	5.74
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	9	5.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	9	5.74
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	9	5.74
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	9	5.74
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	9	5.74
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	9	5.74
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	9	5.74
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	9	5.74
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	9	5.74
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	9	5.74
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	9	5.74
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	9	5.74
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	5	5.38
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	5	5.38
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	5	5.38
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	5	5.38
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	5	5.38
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	5	5.38
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	5	5.38
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	5	5.38
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	5	5.38
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	5	5.38
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	5	5.38
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	5	5.38
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	5	5.38
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	5	5.38
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	5	5.38
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	5	5.38
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	5	5.38
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	5	5.38
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	6	5.36
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	6	5.36
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	6	5.36
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	11	5.3
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	11	5.3
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	11	5.3
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	11	5.3
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	11	5.3
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	11	5.3
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	11	5.3
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	11	5.3
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	11	5.3
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	11	5.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	11	5.3
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	11	5.3
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	11	5.3
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	11	5.3
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	11	5.3
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	11	5.3
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	11	5.3
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	11	5.3
(2,54)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	10	5.18
(2,54)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	10	5.18
(2,53)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	10	5.18
(2,53)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	10	5.18
(2,52)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	10	5.18
(2,52)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	10	5.18
(2,21)	1:678:A:TRP:HE1	1:683:A:ARG:HE	8	4.95
(2,20)	1:678:A:TRP:HE1	1:683:A:ARG:HE	8	4.95
(2,19)	1:678:A:TRP:HE1	1:683:A:ARG:HE	8	4.95
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	8	4.57
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	8	4.57
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	8	4.57
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	8	4.57
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	8	4.57
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	8	4.57
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	8	4.57
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	8	4.57
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	8	4.57
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	8	4.57
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	8	4.57
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	8	4.57
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	8	4.57
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	8	4.57
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	8	4.57
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	8	4.57
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	8	4.57
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	8	4.57
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	4	4.4
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	4	4.4
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	4	4.4
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	4	4.4
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	4	4.4
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	4	4.4
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	14	4.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	14	4.35
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	14	4.35
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	14	4.35
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	14	4.35
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	14	4.35
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	14	4.35
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	14	4.35
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	14	4.35
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	14	4.35
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	14	4.35
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	14	4.35
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	14	4.35
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	14	4.35
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	14	4.35
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	14	4.35
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	14	4.35
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	14	4.35
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	11	4.14
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	11	4.14
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	11	4.14
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	11	4.14
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	11	4.14
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	11	4.14
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	7	4.0
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	7	4.0
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	7	4.0
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	7	4.0
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	7	4.0
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	7	4.0
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	6	3.85
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	6	3.85
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	6	3.85
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	6	3.85
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	6	3.85
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	6	3.85
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	6	3.85
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	6	3.85
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	6	3.85
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	6	3.85
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	6	3.85
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	6	3.85
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	6	3.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	6	3.85
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	6	3.85
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	6	3.85
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	6	3.85
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	6	3.85
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	3	3.82
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	3	3.82
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	3	3.82
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	3	3.82
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	3	3.82
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	3	3.82
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	3	3.82
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	3	3.82
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	3	3.82
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	3	3.82
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	3	3.82
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	3	3.82
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	3	3.82
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	3	3.82
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	3	3.82
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	3	3.82
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	3	3.82
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	3	3.82
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	10	3.76
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	10	3.76
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	10	3.76
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	10	3.76
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	10	3.76
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	10	3.76
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	2	3.62
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	2	3.62
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	2	3.62
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	2	3.62
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	2	3.62
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	2	3.62
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	10	3.6
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	10	3.6
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	10	3.6
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	10	3.6
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	10	3.6
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	10	3.6
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	10	3.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	10	3.6
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	10	3.6
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	10	3.6
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	10	3.6
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	10	3.6
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	10	3.6
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	10	3.6
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	10	3.6
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	10	3.6
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	10	3.6
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	10	3.6
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	8	3.54
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	8	3.54
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	8	3.54
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	8	3.54
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	8	3.54
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	8	3.54
(2,54)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	7	3.53
(2,54)	1:693:A:ILE:HD13	1:696:A:ARG:HH12	7	3.53
(2,53)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	7	3.53
(2,53)	1:693:A:ILE:HD13	1:696:A:ARG:HH12	7	3.53
(2,52)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	7	3.53
(2,52)	1:693:A:ILE:HD13	1:696:A:ARG:HH12	7	3.53
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA2	14	3.39
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA3	14	3.39
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA2	14	3.39
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA3	14	3.39
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA2	14	3.39
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA3	14	3.39
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	5	3.28
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	5	3.28
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	5	3.28
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	5	3.28
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	5	3.28
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	5	3.28
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA2	2	3.26
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA3	2	3.26
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA2	2	3.26
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA3	2	3.26
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA2	2	3.26
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA3	2	3.26
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	7	3.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	7	3.24
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	7	3.24
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	7	3.24
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	7	3.24
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	7	3.24
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	7	3.24
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	7	3.24
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	7	3.24
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	7	3.24
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	7	3.24
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	7	3.24
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	7	3.24
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	7	3.24
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	7	3.24
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	7	3.24
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	7	3.24
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	7	3.24
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA2	12	3.17
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA3	12	3.17
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA2	12	3.17
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA3	12	3.17
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA2	12	3.17
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA3	12	3.17
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	9	3.17
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	9	3.17
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	9	3.17
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	9	3.17
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	9	3.17
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	9	3.17
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA2	10	3.16
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA3	10	3.16
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA2	10	3.16
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA3	10	3.16
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA2	10	3.16
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA3	10	3.16
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	3.09
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	3.09
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	3.09
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	3.09
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	3.09
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	3.09
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA2	8	3.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA3	8	3.03
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA2	8	3.03
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA3	8	3.03
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA2	8	3.03
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA3	8	3.03
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA2	9	3.02
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA3	9	3.02
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA2	9	3.02
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA3	9	3.02
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA2	9	3.02
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA3	9	3.02
(2,54)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	2	3.01
(2,54)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	2	3.01
(2,53)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	2	3.01
(2,53)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	2	3.01
(2,52)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	2	3.01
(2,52)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	2	3.01
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA2	5	2.99
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA3	5	2.99
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA2	5	2.99
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA3	5	2.99
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA2	5	2.99
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA3	5	2.99
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	12	2.94
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	12	2.94
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	12	2.94
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	12	2.94
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	12	2.94
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	12	2.94
(2,54)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	2.85
(2,54)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	14	2.85
(2,53)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	2.85
(2,53)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	14	2.85
(2,52)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	2.85
(2,52)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	14	2.85
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	13	2.85
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	13	2.85
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	13	2.85
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	13	2.85
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	13	2.85
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	13	2.85
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	1	2.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	1	2.8
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	1	2.8
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	1	2.8
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	1	2.8
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	1	2.8
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA2	6	2.78
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA3	6	2.78
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA2	6	2.78
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA3	6	2.78
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA2	6	2.78
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA3	6	2.78
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA2	1	2.7
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA3	1	2.7
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA2	1	2.7
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA3	1	2.7
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA2	1	2.7
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA3	1	2.7
(1,21)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	11	2.6
(1,20)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	11	2.6
(1,19)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	11	2.6
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA2	11	2.52
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA3	11	2.52
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA2	11	2.52
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA3	11	2.52
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA2	11	2.52
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA3	11	2.52
(2,54)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	6	2.48
(2,54)	1:693:A:ILE:HD12	1:696:A:ARG:HH12	6	2.48
(2,53)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	6	2.48
(2,53)	1:693:A:ILE:HD12	1:696:A:ARG:HH12	6	2.48
(2,52)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	6	2.48
(2,52)	1:693:A:ILE:HD12	1:696:A:ARG:HH12	6	2.48
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	6	2.45
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	6	2.45
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	6	2.45
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	6	2.45
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	6	2.45
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	6	2.45
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	6	2.45
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	6	2.45
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	6	2.45
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	6	2.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	6	2.45
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	6	2.45
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	6	2.45
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	6	2.45
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	6	2.45
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	6	2.45
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	6	2.45
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	6	2.45
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	6	2.45
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	6	2.45
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	6	2.45
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	6	2.45
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	6	2.45
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	6	2.45
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	6	2.45
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	6	2.45
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	6	2.45
(2,54)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	13	2.4
(2,54)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	13	2.4
(2,53)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	13	2.4
(2,53)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	13	2.4
(2,52)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	13	2.4
(2,52)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	13	2.4
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	11	2.38
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	11	2.38
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	11	2.38
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	11	2.38
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	11	2.38
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	11	2.38
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	11	2.38
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	11	2.38
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	11	2.38
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	11	2.38
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	11	2.38
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	11	2.38
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	11	2.38
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	11	2.38
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	11	2.38
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	11	2.38
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	11	2.38
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	11	2.38
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	11	2.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	11	2.38
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	11	2.38
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	11	2.38
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	11	2.38
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	11	2.38
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	11	2.38
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	11	2.38
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	11	2.38
(1,21)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	12	2.37
(1,20)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	12	2.37
(1,19)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	12	2.37
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA2	7	2.36
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA3	7	2.36
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA2	7	2.36
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA3	7	2.36
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA2	7	2.36
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA3	7	2.36
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	6	2.33
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	6	2.33
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	6	2.33
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	6	2.33
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	6	2.33
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	6	2.33
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	5	2.27
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	5	2.27
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	5	2.27
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	5	2.27
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	5	2.27
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	5	2.27
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	5	2.27
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	5	2.27
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	5	2.27
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	5	2.27
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	5	2.27
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	5	2.27
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	5	2.27
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	5	2.27
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	5	2.27
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	5	2.27
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	5	2.27
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	5	2.27
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	5	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	5	2.27
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	5	2.27
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	5	2.27
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	5	2.27
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	5	2.27
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	5	2.27
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	5	2.27
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	5	2.27
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	2	2.22
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	2	2.22
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	2	2.22
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	2	2.22
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	2	2.22
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	2	2.22
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	2	2.22
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	2	2.22
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	2	2.22
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	2	2.22
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	2	2.22
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	2	2.22
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	2	2.22
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	2	2.22
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	2	2.22
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	2	2.22
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	2	2.22
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	2	2.22
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	2	2.22
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	2	2.22
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	2	2.22
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	2	2.22
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	2	2.22
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	2	2.22
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	2	2.22
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	2	2.22
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	2	2.22
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	1	2.19
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	1	2.19
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	1	2.19
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	1	2.19
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	1	2.19
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	1	2.19
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	1	2.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	1	2.19
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	1	2.19
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	1	2.19
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	1	2.19
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	1	2.19
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	1	2.19
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	1	2.19
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	1	2.19
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	1	2.19
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	1	2.19
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	1	2.19
(2,54)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	8	2.12
(2,54)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	8	2.12
(2,53)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	8	2.12
(2,53)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	8	2.12
(2,52)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	8	2.12
(2,52)	1:693:A:ILE:HD12	1:696:A:ARG:HH22	8	2.12
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	2	2.11
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	2	2.11
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	2	2.11
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	2	2.11
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	2	2.11
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	2	2.11
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	2	2.11
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	2	2.11
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	2	2.11
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	2	2.11
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	2	2.11
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	2	2.11
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	2	2.11
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	2	2.11
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	2	2.11
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	2	2.11
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	2	2.11
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	2	2.11
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	1	2.06
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	1	2.06
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	1	2.06
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	1	2.06
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	1	2.06
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	1	2.06
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	1	2.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	1	2.06
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	1	2.06
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	1	2.06
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	1	2.06
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	1	2.06
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	1	2.06
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	1	2.06
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	1	2.06
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	1	2.06
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	1	2.06
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	1	2.06
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	1	2.06
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	1	2.06
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	1	2.06
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	1	2.06
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	1	2.06
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	1	2.06
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	1	2.06
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	1	2.06
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	1	2.06
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB2	3	2.06
(2,9)	1:664:A:ASP:H	1:660:A:LEU:HB3	3	2.06
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB2	3	2.06
(2,8)	1:664:A:ASP:H	1:660:A:LEU:HB3	3	2.06
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB2	3	2.06
(2,7)	1:664:A:ASP:H	1:660:A:LEU:HB3	3	2.06
(1,21)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	2	2.06
(1,20)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	2	2.06
(1,19)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	2	2.06
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	3	2.04
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	3	2.04
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	3	2.04
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	3	2.04
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	3	2.04
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	3	2.04
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	3	2.04
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	3	2.04
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	3	2.04
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	3	2.04
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	3	2.04
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	3	2.04
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	3	2.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	3	2.04
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	3	2.04
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	3	2.04
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	3	2.04
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	3	2.04
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	3	2.04
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	3	2.04
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	3	2.04
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	3	2.04
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	3	2.04
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	3	2.04
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	3	2.04
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	3	2.04
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	3	2.04
(1,21)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	6	2.02
(1,20)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	6	2.02
(1,19)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	6	2.02
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	12	1.98
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	12	1.98
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	12	1.98
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	12	1.98
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	12	1.98
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	12	1.98
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	12	1.98
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	12	1.98
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	12	1.98
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	12	1.98
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	12	1.98
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	12	1.98
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	12	1.98
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	12	1.98
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	12	1.98
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	12	1.98
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	12	1.98
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	12	1.98
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	12	1.98
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	12	1.98
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	12	1.98
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	12	1.98
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	12	1.98
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	12	1.98
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	12	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	12	1.98
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	12	1.98
(1,21)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	10	1.86
(1,20)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	10	1.86
(1,19)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	10	1.86
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	13	1.84
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	13	1.84
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	13	1.84
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	13	1.84
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	13	1.84
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	13	1.84
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	13	1.84
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	13	1.84
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	13	1.84
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	13	1.84
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	13	1.84
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	13	1.84
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	13	1.84
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	13	1.84
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	13	1.84
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	13	1.84
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	13	1.84
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	13	1.84
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	13	1.84
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	13	1.84
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	13	1.84
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	13	1.84
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	13	1.84
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	13	1.84
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	13	1.84
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	13	1.84
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	13	1.84
(1,21)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	4	1.82
(1,21)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	5	1.82
(1,20)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	4	1.82
(1,20)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	5	1.82
(1,19)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	4	1.82
(1,19)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	5	1.82
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	14	1.76
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	14	1.76
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	14	1.76
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	14	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	14	1.76
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	14	1.76
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	14	1.76
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	14	1.76
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	14	1.76
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	14	1.76
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	14	1.76
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	14	1.76
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	14	1.76
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	14	1.76
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	14	1.76
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	14	1.76
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	14	1.76
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	14	1.76
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	14	1.76
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	14	1.76
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	14	1.76
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	14	1.76
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	14	1.76
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	14	1.76
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	14	1.76
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	14	1.76
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	14	1.76
(2,54)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	12	1.66
(2,54)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	12	1.66
(2,53)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	12	1.66
(2,53)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	12	1.66
(2,52)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	12	1.66
(2,52)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	12	1.66
(1,21)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	13	1.59
(1,20)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	13	1.59
(1,19)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	13	1.59
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	1.57
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	1.57
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	1.57
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	1.57
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	1.57
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	1.57
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	1.57
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	1.57
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	1.57
(2,45)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,45)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	1.57
(2,45)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	1.57
(2,44)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	1.57
(2,44)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	1.57
(2,44)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	1.57
(2,43)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	1.57
(2,43)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	1.57
(2,43)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	1.57
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD21	4	1.53
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD22	4	1.53
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD23	4	1.53
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD21	7	1.53
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD22	7	1.53
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD23	7	1.53
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD21	4	1.53
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD22	4	1.53
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD23	4	1.53
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD21	7	1.53
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD22	7	1.53
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD23	7	1.53
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD21	4	1.53
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD22	4	1.53
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD23	4	1.53
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD21	7	1.53
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD22	7	1.53
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD23	7	1.53
(2,45)	1:692:A:LEU:HD21	1:694:A:GLY:H	4	1.53
(2,45)	1:692:A:LEU:HD22	1:694:A:GLY:H	4	1.53
(2,45)	1:692:A:LEU:HD23	1:694:A:GLY:H	4	1.53
(2,45)	1:692:A:LEU:HD21	1:694:A:GLY:H	7	1.53
(2,45)	1:692:A:LEU:HD22	1:694:A:GLY:H	7	1.53
(2,45)	1:692:A:LEU:HD23	1:694:A:GLY:H	7	1.53
(2,44)	1:692:A:LEU:HD21	1:694:A:GLY:H	4	1.53
(2,44)	1:692:A:LEU:HD22	1:694:A:GLY:H	4	1.53
(2,44)	1:692:A:LEU:HD23	1:694:A:GLY:H	4	1.53
(2,44)	1:692:A:LEU:HD21	1:694:A:GLY:H	7	1.53
(2,44)	1:692:A:LEU:HD22	1:694:A:GLY:H	7	1.53
(2,44)	1:692:A:LEU:HD23	1:694:A:GLY:H	7	1.53
(2,43)	1:692:A:LEU:HD21	1:694:A:GLY:H	4	1.53
(2,43)	1:692:A:LEU:HD22	1:694:A:GLY:H	4	1.53
(2,43)	1:692:A:LEU:HD23	1:694:A:GLY:H	4	1.53
(2,43)	1:692:A:LEU:HD21	1:694:A:GLY:H	7	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,43)	1:692:A:LEU:HD22	1:694:A:GLY:H	7	1.53
(2,43)	1:692:A:LEU:HD23	1:694:A:GLY:H	7	1.53
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD21	1	1.51
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD22	1	1.51
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD23	1	1.51
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD21	1	1.51
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD22	1	1.51
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD23	1	1.51
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD21	1	1.51
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD22	1	1.51
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD23	1	1.51
(2,45)	1:692:A:LEU:HD21	1:694:A:GLY:H	1	1.51
(2,45)	1:692:A:LEU:HD22	1:694:A:GLY:H	1	1.51
(2,45)	1:692:A:LEU:HD23	1:694:A:GLY:H	1	1.51
(2,44)	1:692:A:LEU:HD21	1:694:A:GLY:H	1	1.51
(2,44)	1:692:A:LEU:HD22	1:694:A:GLY:H	1	1.51
(2,44)	1:692:A:LEU:HD23	1:694:A:GLY:H	1	1.51
(2,43)	1:692:A:LEU:HD21	1:694:A:GLY:H	1	1.51
(2,43)	1:692:A:LEU:HD22	1:694:A:GLY:H	1	1.51
(2,43)	1:692:A:LEU:HD23	1:694:A:GLY:H	1	1.51
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	9	1.49
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	9	1.49
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	9	1.49
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	9	1.49
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	9	1.49
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	9	1.49
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	9	1.49
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	9	1.49
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	9	1.49
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	9	1.49
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	9	1.49
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	9	1.49
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	9	1.49
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	9	1.49
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	9	1.49
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	9	1.49
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	9	1.49
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	9	1.49
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	9	1.49
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	9	1.49
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	9	1.49
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	9	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	9	1.49
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	9	1.49
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	9	1.49
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	9	1.49
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	9	1.49
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD21	13	1.48
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD22	13	1.48
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD23	13	1.48
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD21	13	1.48
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD22	13	1.48
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD23	13	1.48
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD21	13	1.48
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD22	13	1.48
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD23	13	1.48
(2,45)	1:692:A:LEU:HD21	1:694:A:GLY:H	13	1.48
(2,45)	1:692:A:LEU:HD22	1:694:A:GLY:H	13	1.48
(2,45)	1:692:A:LEU:HD23	1:694:A:GLY:H	13	1.48
(2,44)	1:692:A:LEU:HD21	1:694:A:GLY:H	13	1.48
(2,44)	1:692:A:LEU:HD22	1:694:A:GLY:H	13	1.48
(2,44)	1:692:A:LEU:HD23	1:694:A:GLY:H	13	1.48
(2,43)	1:692:A:LEU:HD21	1:694:A:GLY:H	13	1.48
(2,43)	1:692:A:LEU:HD22	1:694:A:GLY:H	13	1.48
(2,43)	1:692:A:LEU:HD23	1:694:A:GLY:H	13	1.48
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	4	1.48
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	4	1.48
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	4	1.48
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	4	1.48
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	4	1.48
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	4	1.48
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	4	1.48
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	4	1.48
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	4	1.48
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	4	1.48
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	4	1.48
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	4	1.48
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	4	1.48
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	4	1.48
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	4	1.48
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	4	1.48
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	4	1.48
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	4	1.48
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	4	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	4	1.48
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	4	1.48
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	4	1.48
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	4	1.48
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	4	1.48
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	4	1.48
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	4	1.48
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	4	1.48
(3,641)	1:701:A:VAL:HG11	1:698:A:VAL:HA	4	1.45
(3,641)	1:701:A:VAL:HG12	1:698:A:VAL:HA	4	1.45
(3,641)	1:701:A:VAL:HG13	1:698:A:VAL:HA	4	1.45
(3,641)	1:701:A:VAL:HG11	1:698:A:VAL:HA	14	1.45
(3,641)	1:701:A:VAL:HG12	1:698:A:VAL:HA	14	1.45
(3,641)	1:701:A:VAL:HG13	1:698:A:VAL:HA	14	1.45
(3,641)	1:701:A:VAL:HG11	1:698:A:VAL:HA	2	1.44
(3,641)	1:701:A:VAL:HG12	1:698:A:VAL:HA	2	1.44
(3,641)	1:701:A:VAL:HG13	1:698:A:VAL:HA	2	1.44
(1,21)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	9	1.44
(1,20)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	9	1.44
(1,19)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	9	1.44
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD21	10	1.41
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD22	10	1.41
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD23	10	1.41
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD21	10	1.41
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD22	10	1.41
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD23	10	1.41
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD21	10	1.41
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD22	10	1.41
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD23	10	1.41
(2,45)	1:692:A:LEU:HD21	1:694:A:GLY:H	10	1.41
(2,45)	1:692:A:LEU:HD22	1:694:A:GLY:H	10	1.41
(2,45)	1:692:A:LEU:HD23	1:694:A:GLY:H	10	1.41
(2,44)	1:692:A:LEU:HD21	1:694:A:GLY:H	10	1.41
(2,44)	1:692:A:LEU:HD22	1:694:A:GLY:H	10	1.41
(2,44)	1:692:A:LEU:HD23	1:694:A:GLY:H	10	1.41
(2,43)	1:692:A:LEU:HD21	1:694:A:GLY:H	10	1.41
(2,43)	1:692:A:LEU:HD22	1:694:A:GLY:H	10	1.41
(2,43)	1:692:A:LEU:HD23	1:694:A:GLY:H	10	1.41
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD21	3	1.4
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD22	3	1.4
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD23	3	1.4
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD21	3	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD22	3	1.4
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD23	3	1.4
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD21	3	1.4
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD22	3	1.4
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD23	3	1.4
(2,45)	1:692:A:LEU:HD21	1:694:A:GLY:H	3	1.4
(2,45)	1:692:A:LEU:HD22	1:694:A:GLY:H	3	1.4
(2,45)	1:692:A:LEU:HD23	1:694:A:GLY:H	3	1.4
(2,44)	1:692:A:LEU:HD21	1:694:A:GLY:H	3	1.4
(2,44)	1:692:A:LEU:HD22	1:694:A:GLY:H	3	1.4
(2,44)	1:692:A:LEU:HD23	1:694:A:GLY:H	3	1.4
(2,43)	1:692:A:LEU:HD21	1:694:A:GLY:H	3	1.4
(2,43)	1:692:A:LEU:HD22	1:694:A:GLY:H	3	1.4
(2,43)	1:692:A:LEU:HD23	1:694:A:GLY:H	3	1.4
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD21	11	1.38
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD22	11	1.38
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD23	11	1.38
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD21	11	1.38
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD22	11	1.38
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD23	11	1.38
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD21	11	1.38
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD22	11	1.38
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD23	11	1.38
(2,45)	1:692:A:LEU:HD21	1:694:A:GLY:H	11	1.38
(2,45)	1:692:A:LEU:HD22	1:694:A:GLY:H	11	1.38
(2,45)	1:692:A:LEU:HD23	1:694:A:GLY:H	11	1.38
(2,44)	1:692:A:LEU:HD21	1:694:A:GLY:H	11	1.38
(2,44)	1:692:A:LEU:HD22	1:694:A:GLY:H	11	1.38
(2,44)	1:692:A:LEU:HD23	1:694:A:GLY:H	11	1.38
(2,43)	1:692:A:LEU:HD21	1:694:A:GLY:H	11	1.38
(2,43)	1:692:A:LEU:HD22	1:694:A:GLY:H	11	1.38
(2,43)	1:692:A:LEU:HD23	1:694:A:GLY:H	11	1.38
(1,21)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	7	1.38
(1,20)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	7	1.38
(1,19)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	7	1.38
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	8	1.35
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	8	1.35
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	8	1.35
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	8	1.35
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	8	1.35
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	8	1.35
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	8	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	8	1.35
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	8	1.35
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	8	1.35
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	8	1.35
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	8	1.35
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	8	1.35
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	8	1.35
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	8	1.35
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	8	1.35
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	8	1.35
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	8	1.35
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	8	1.35
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	8	1.35
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	8	1.35
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	8	1.35
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	8	1.35
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	8	1.35
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	8	1.35
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	8	1.35
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	8	1.35
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD21	2	1.33
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD22	2	1.33
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD23	2	1.33
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD21	2	1.33
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD22	2	1.33
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD23	2	1.33
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD21	2	1.33
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD22	2	1.33
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD23	2	1.33
(2,54)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	3	1.33
(2,54)	1:693:A:ILE:HD12	1:696:A:ARG:HH12	3	1.33
(2,53)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	3	1.33
(2,53)	1:693:A:ILE:HD12	1:696:A:ARG:HH12	3	1.33
(2,52)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	3	1.33
(2,52)	1:693:A:ILE:HD12	1:696:A:ARG:HH12	3	1.33
(2,45)	1:692:A:LEU:HD21	1:694:A:GLY:H	2	1.33
(2,45)	1:692:A:LEU:HD22	1:694:A:GLY:H	2	1.33
(2,45)	1:692:A:LEU:HD23	1:694:A:GLY:H	2	1.33
(2,44)	1:692:A:LEU:HD21	1:694:A:GLY:H	2	1.33
(2,44)	1:692:A:LEU:HD22	1:694:A:GLY:H	2	1.33
(2,44)	1:692:A:LEU:HD23	1:694:A:GLY:H	2	1.33
(2,43)	1:692:A:LEU:HD21	1:694:A:GLY:H	2	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,43)	1:692:A:LEU:HD22	1:694:A:GLY:H	2	1.33
(2,43)	1:692:A:LEU:HD23	1:694:A:GLY:H	2	1.33
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD21	8	1.32
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD22	8	1.32
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD23	8	1.32
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD21	8	1.32
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD22	8	1.32
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD23	8	1.32
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD21	8	1.32
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD22	8	1.32
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD23	8	1.32
(2,54)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	5	1.32
(2,54)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	5	1.32
(2,54)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	11	1.32
(2,54)	1:693:A:ILE:HD12	1:696:A:ARG:HH12	11	1.32
(2,53)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	5	1.32
(2,53)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	5	1.32
(2,53)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	11	1.32
(2,53)	1:693:A:ILE:HD12	1:696:A:ARG:HH12	11	1.32
(2,52)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	5	1.32
(2,52)	1:693:A:ILE:HD13	1:696:A:ARG:HH22	5	1.32
(2,52)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	11	1.32
(2,52)	1:693:A:ILE:HD12	1:696:A:ARG:HH12	11	1.32
(2,45)	1:692:A:LEU:HD21	1:694:A:GLY:H	8	1.32
(2,45)	1:692:A:LEU:HD22	1:694:A:GLY:H	8	1.32
(2,45)	1:692:A:LEU:HD23	1:694:A:GLY:H	8	1.32
(2,44)	1:692:A:LEU:HD21	1:694:A:GLY:H	8	1.32
(2,44)	1:692:A:LEU:HD22	1:694:A:GLY:H	8	1.32
(2,44)	1:692:A:LEU:HD23	1:694:A:GLY:H	8	1.32
(2,43)	1:692:A:LEU:HD21	1:694:A:GLY:H	8	1.32
(2,43)	1:692:A:LEU:HD22	1:694:A:GLY:H	8	1.32
(2,43)	1:692:A:LEU:HD23	1:694:A:GLY:H	8	1.32
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA2	4	1.31
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA3	4	1.31
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA2	4	1.31
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA3	4	1.31
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA2	4	1.31
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA3	4	1.31
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA2	13	1.3
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA3	13	1.3
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA2	13	1.3
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA3	13	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA2	13	1.3
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA3	13	1.3
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD21	5	1.3
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD22	5	1.3
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD23	5	1.3
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD21	5	1.3
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD22	5	1.3
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD23	5	1.3
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD21	5	1.3
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD22	5	1.3
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD23	5	1.3
(2,45)	1:692:A:LEU:HD21	1:694:A:GLY:H	5	1.3
(2,45)	1:692:A:LEU:HD22	1:694:A:GLY:H	5	1.3
(2,45)	1:692:A:LEU:HD23	1:694:A:GLY:H	5	1.3
(2,44)	1:692:A:LEU:HD21	1:694:A:GLY:H	5	1.3
(2,44)	1:692:A:LEU:HD22	1:694:A:GLY:H	5	1.3
(2,44)	1:692:A:LEU:HD23	1:694:A:GLY:H	5	1.3
(2,43)	1:692:A:LEU:HD21	1:694:A:GLY:H	5	1.3
(2,43)	1:692:A:LEU:HD22	1:694:A:GLY:H	5	1.3
(2,43)	1:692:A:LEU:HD23	1:694:A:GLY:H	5	1.3
(3,567)	1:706:A:ASN:H	1:703:A:SER:HA	4	1.28
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD21	9	1.27
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD22	9	1.27
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD23	9	1.27
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD21	9	1.27
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD22	9	1.27
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD23	9	1.27
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD21	9	1.27
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD22	9	1.27
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD23	9	1.27
(2,45)	1:692:A:LEU:HD21	1:694:A:GLY:H	9	1.27
(2,45)	1:692:A:LEU:HD22	1:694:A:GLY:H	9	1.27
(2,45)	1:692:A:LEU:HD23	1:694:A:GLY:H	9	1.27
(2,44)	1:692:A:LEU:HD21	1:694:A:GLY:H	9	1.27
(2,44)	1:692:A:LEU:HD22	1:694:A:GLY:H	9	1.27
(2,44)	1:692:A:LEU:HD23	1:694:A:GLY:H	9	1.27
(2,43)	1:692:A:LEU:HD21	1:694:A:GLY:H	9	1.27
(2,43)	1:692:A:LEU:HD22	1:694:A:GLY:H	9	1.27
(2,43)	1:692:A:LEU:HD23	1:694:A:GLY:H	9	1.27
(2,54)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	9	1.25
(2,54)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	9	1.25
(2,53)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	9	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,53)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	9	1.25
(2,52)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	9	1.25
(2,52)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	9	1.25
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD21	12	1.23
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD22	12	1.23
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD23	12	1.23
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD21	12	1.23
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD22	12	1.23
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD23	12	1.23
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD21	12	1.23
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD22	12	1.23
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD23	12	1.23
(2,45)	1:692:A:LEU:HD21	1:694:A:GLY:H	12	1.23
(2,45)	1:692:A:LEU:HD22	1:694:A:GLY:H	12	1.23
(2,45)	1:692:A:LEU:HD23	1:694:A:GLY:H	12	1.23
(2,44)	1:692:A:LEU:HD21	1:694:A:GLY:H	12	1.23
(2,44)	1:692:A:LEU:HD22	1:694:A:GLY:H	12	1.23
(2,44)	1:692:A:LEU:HD23	1:694:A:GLY:H	12	1.23
(2,43)	1:692:A:LEU:HD21	1:694:A:GLY:H	12	1.23
(2,43)	1:692:A:LEU:HD22	1:694:A:GLY:H	12	1.23
(2,43)	1:692:A:LEU:HD23	1:694:A:GLY:H	12	1.23
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD21	6	1.22
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD22	6	1.22
(2,57)	1:694:A:GLY:H	1:692:A:LEU:HD23	6	1.22
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD21	6	1.22
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD22	6	1.22
(2,56)	1:694:A:GLY:H	1:692:A:LEU:HD23	6	1.22
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD21	6	1.22
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD22	6	1.22
(2,55)	1:694:A:GLY:H	1:692:A:LEU:HD23	6	1.22
(2,45)	1:692:A:LEU:HD21	1:694:A:GLY:H	6	1.22
(2,45)	1:692:A:LEU:HD22	1:694:A:GLY:H	6	1.22
(2,45)	1:692:A:LEU:HD23	1:694:A:GLY:H	6	1.22
(2,44)	1:692:A:LEU:HD21	1:694:A:GLY:H	6	1.22
(2,44)	1:692:A:LEU:HD22	1:694:A:GLY:H	6	1.22
(2,44)	1:692:A:LEU:HD23	1:694:A:GLY:H	6	1.22
(2,43)	1:692:A:LEU:HD21	1:694:A:GLY:H	6	1.22
(2,43)	1:692:A:LEU:HD22	1:694:A:GLY:H	6	1.22
(2,43)	1:692:A:LEU:HD23	1:694:A:GLY:H	6	1.22
(1,21)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	8	1.22
(1,20)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	8	1.22
(1,19)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	8	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	7	1.2
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	7	1.2
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	7	1.2
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	7	1.2
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	7	1.2
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	7	1.2
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	7	1.2
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	7	1.2
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	7	1.2
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	7	1.2
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	7	1.2
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	7	1.2
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	7	1.2
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	7	1.2
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	7	1.2
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	7	1.2
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	7	1.2
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	7	1.2
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	7	1.2
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	7	1.2
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	7	1.2
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	7	1.2
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	7	1.2
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	7	1.2
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	7	1.2
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	7	1.2
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	7	1.2
(3,567)	1:706:A:ASN:H	1:703:A:SER:HA	3	1.18
(3,642)	1:701:A:VAL:HG21	1:698:A:VAL:HA	13	1.17
(3,642)	1:701:A:VAL:HG22	1:698:A:VAL:HA	13	1.17
(3,642)	1:701:A:VAL:HG23	1:698:A:VAL:HA	13	1.17
(3,351)	1:705:A:VAL:HG21	1:702:A:LEU:HG	8	1.12
(3,351)	1:705:A:VAL:HG22	1:702:A:LEU:HG	8	1.12
(3,351)	1:705:A:VAL:HG23	1:702:A:LEU:HG	8	1.12
(2,48)	1:693:A:ILE:H	1:693:A:ILE:HG12	2	1.11
(2,48)	1:693:A:ILE:H	1:693:A:ILE:HG13	2	1.11
(2,47)	1:693:A:ILE:H	1:693:A:ILE:HG12	2	1.11
(2,47)	1:693:A:ILE:H	1:693:A:ILE:HG13	2	1.11
(2,46)	1:693:A:ILE:H	1:693:A:ILE:HG12	2	1.11
(2,46)	1:693:A:ILE:H	1:693:A:ILE:HG13	2	1.11
(3,567)	1:706:A:ASN:H	1:703:A:SER:HA	1	1.09
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	13	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	13	1.08
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	13	1.08
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	13	1.08
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	13	1.08
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	13	1.08
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	13	1.08
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	13	1.08
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	13	1.08
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	13	1.08
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	13	1.08
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	13	1.08
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	13	1.08
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	13	1.08
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	13	1.08
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	13	1.08
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	13	1.08
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	13	1.08
(2,48)	1:693:A:ILE:H	1:693:A:ILE:HG12	10	1.08
(2,48)	1:693:A:ILE:H	1:693:A:ILE:HG13	10	1.08
(2,47)	1:693:A:ILE:H	1:693:A:ILE:HG12	10	1.08
(2,47)	1:693:A:ILE:H	1:693:A:ILE:HG13	10	1.08
(2,46)	1:693:A:ILE:H	1:693:A:ILE:HG12	10	1.08
(2,46)	1:693:A:ILE:H	1:693:A:ILE:HG13	10	1.08
(3,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	2	1.07
(3,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	2	1.07
(3,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	2	1.07
(3,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	2	1.07
(3,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	2	1.07
(3,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	2	1.07
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA2	3	1.07
(2,63)	1:696:A:ARG:HE	1:694:A:GLY:HA3	3	1.07
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA2	3	1.07
(2,62)	1:696:A:ARG:HE	1:694:A:GLY:HA3	3	1.07
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA2	3	1.07
(2,61)	1:696:A:ARG:HE	1:694:A:GLY:HA3	3	1.07
(3,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	3	1.06
(3,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	3	1.06
(3,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	3	1.06
(3,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	3	1.06
(3,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	3	1.06
(3,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	3	1.06
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	11	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	11	1.06
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	11	1.06
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	11	1.06
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	11	1.06
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	11	1.06
(2,48)	1:693:A:ILE:H	1:693:A:ILE:HG12	14	1.03
(2,48)	1:693:A:ILE:H	1:693:A:ILE:HG13	14	1.03
(2,47)	1:693:A:ILE:H	1:693:A:ILE:HG12	14	1.03
(2,47)	1:693:A:ILE:H	1:693:A:ILE:HG13	14	1.03
(2,46)	1:693:A:ILE:H	1:693:A:ILE:HG12	14	1.03
(2,46)	1:693:A:ILE:H	1:693:A:ILE:HG13	14	1.03
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	5	1.02
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	5	1.02
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	5	1.02
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	5	1.02
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	5	1.02
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	5	1.02
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	4	1.02
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	4	1.02
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	4	1.02
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	4	1.02
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	4	1.02
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	4	1.02
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	4	1.02
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	4	1.02
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	4	1.02
(3,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	5	1.02
(3,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	5	1.02
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	4	1.02
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	4	1.02
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	4	1.02
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	4	1.02
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	4	1.02
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	4	1.02
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	4	1.02
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	4	1.02
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	4	1.02
(3,592)	1:687:A:ILE:HG21	1:691:A:SER:HG	7	1.01
(3,592)	1:687:A:ILE:HG22	1:691:A:SER:HG	7	1.01
(3,592)	1:687:A:ILE:HG23	1:691:A:SER:HG	7	1.01
(3,592)	1:687:A:ILE:HG21	1:691:A:SER:HG	9	1.01
(3,592)	1:687:A:ILE:HG22	1:691:A:SER:HG	9	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,592)	1:687:A:ILE:HG23	1:691:A:SER:HG	9	1.01
(3,378)	1:687:A:ILE:HG21	1:691:A:SER:HG	7	1.01
(3,378)	1:687:A:ILE:HG22	1:691:A:SER:HG	7	1.01
(3,378)	1:687:A:ILE:HG23	1:691:A:SER:HG	7	1.01
(3,378)	1:687:A:ILE:HG21	1:691:A:SER:HG	9	1.01
(3,378)	1:687:A:ILE:HG22	1:691:A:SER:HG	9	1.01
(3,378)	1:687:A:ILE:HG23	1:691:A:SER:HG	9	1.01
(3,486)	1:673:A:PHE:H	1:672:A:TRP:H	3	1.0
(3,483)	1:672:A:TRP:H	1:673:A:PHE:H	3	1.0
(3,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	1	0.99
(3,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	1	0.99
(3,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	1	0.99
(3,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	1	0.99
(3,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	1	0.99
(3,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	1	0.99
(3,597)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	14	0.98
(3,597)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	14	0.98
(3,597)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	14	0.98
(3,597)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	14	0.98
(3,597)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	14	0.98
(3,597)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	14	0.98
(3,486)	1:673:A:PHE:H	1:672:A:TRP:H	5	0.97
(3,483)	1:672:A:TRP:H	1:673:A:PHE:H	5	0.97
(2,54)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	4	0.97
(2,54)	1:693:A:ILE:HD13	1:696:A:ARG:HH12	4	0.97
(2,53)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	4	0.97
(2,53)	1:693:A:ILE:HD13	1:696:A:ARG:HH12	4	0.97
(2,52)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	4	0.97
(2,52)	1:693:A:ILE:HD13	1:696:A:ARG:HH12	4	0.97
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	1	0.95
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	1	0.95
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	1	0.95
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	1	0.95
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	1	0.95
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	1	0.95
(3,592)	1:687:A:ILE:HG21	1:691:A:SER:HG	4	0.95
(3,592)	1:687:A:ILE:HG22	1:691:A:SER:HG	4	0.95
(3,592)	1:687:A:ILE:HG23	1:691:A:SER:HG	4	0.95
(3,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	6	0.95
(3,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	6	0.95
(3,378)	1:687:A:ILE:HG21	1:691:A:SER:HG	4	0.95
(3,378)	1:687:A:ILE:HG22	1:691:A:SER:HG	4	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,378)	1:687:A:ILE:HG23	1:691:A:SER:HG	4	0.95
(3,486)	1:673:A:PHE:H	1:672:A:TRP:H	7	0.94
(3,483)	1:672:A:TRP:H	1:673:A:PHE:H	7	0.94
(3,486)	1:673:A:PHE:H	1:672:A:TRP:H	1	0.93
(3,483)	1:672:A:TRP:H	1:673:A:PHE:H	1	0.93
(3,486)	1:673:A:PHE:H	1:672:A:TRP:H	12	0.92
(3,486)	1:673:A:PHE:H	1:672:A:TRP:H	13	0.92
(3,483)	1:672:A:TRP:H	1:673:A:PHE:H	12	0.92
(3,483)	1:672:A:TRP:H	1:673:A:PHE:H	13	0.92
(2,54)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	1	0.92
(2,54)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	1	0.92
(2,53)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	1	0.92
(2,53)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	1	0.92
(2,52)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	1	0.92
(2,52)	1:693:A:ILE:HD11	1:696:A:ARG:HH22	1	0.92
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	1	0.91
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	1	0.91
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	1	0.91
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	1	0.91
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	1	0.91
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	1	0.91
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	14	0.91
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	14	0.91
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	14	0.91
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	14	0.91
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	14	0.91
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	14	0.91
(3,592)	1:687:A:ILE:HG21	1:691:A:SER:HG	13	0.91
(3,592)	1:687:A:ILE:HG22	1:691:A:SER:HG	13	0.91
(3,592)	1:687:A:ILE:HG23	1:691:A:SER:HG	13	0.91
(3,378)	1:687:A:ILE:HG21	1:691:A:SER:HG	13	0.91
(3,378)	1:687:A:ILE:HG22	1:691:A:SER:HG	13	0.91
(3,378)	1:687:A:ILE:HG23	1:691:A:SER:HG	13	0.91
(3,642)	1:701:A:VAL:HG21	1:698:A:VAL:HA	6	0.9
(3,642)	1:701:A:VAL:HG22	1:698:A:VAL:HA	6	0.9
(3,642)	1:701:A:VAL:HG23	1:698:A:VAL:HA	6	0.9
(3,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	9	0.9
(3,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	9	0.9
(3,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	9	0.9
(3,599)	1:690:A:GLY:H	1:691:A:SER:H	8	0.9
(3,599)	1:690:A:GLY:H	1:691:A:SER:H	11	0.9
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	8	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	8	0.9
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	8	0.9
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	8	0.9
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	8	0.9
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	8	0.9
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	8	0.9
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	8	0.9
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	8	0.9
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	8	0.9
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	8	0.9
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	8	0.9
(3,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	9	0.9
(3,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	9	0.9
(3,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	9	0.9
(3,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	14	0.89
(3,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	14	0.89
(3,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	14	0.89
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	10	0.89
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	10	0.89
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	10	0.89
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	10	0.89
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	10	0.89
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	10	0.89
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	10	0.89
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	10	0.89
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	10	0.89
(3,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	14	0.89
(3,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	14	0.89
(3,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	14	0.89
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	10	0.89
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	10	0.89
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	10	0.89
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	10	0.89
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	10	0.89
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	10	0.89
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	10	0.89
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	10	0.89
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	10	0.89
(3,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	13	0.88
(3,504)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	13	0.88
(3,486)	1:673:A:PHE:H	1:672:A:TRP:H	8	0.88
(3,483)	1:672:A:TRP:H	1:673:A:PHE:H	8	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	9	0.88
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	9	0.88
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	9	0.88
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	9	0.88
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	9	0.88
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	9	0.88
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	9	0.88
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	9	0.88
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	9	0.88
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	9	0.88
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	9	0.88
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	9	0.88
(3,486)	1:673:A:PHE:H	1:672:A:TRP:H	4	0.87
(3,483)	1:672:A:TRP:H	1:673:A:PHE:H	4	0.87
(3,599)	1:690:A:GLY:H	1:691:A:SER:H	4	0.86
(3,592)	1:687:A:ILE:HG21	1:691:A:SER:HG	11	0.86
(3,592)	1:687:A:ILE:HG22	1:691:A:SER:HG	11	0.86
(3,592)	1:687:A:ILE:HG23	1:691:A:SER:HG	11	0.86
(3,486)	1:673:A:PHE:H	1:672:A:TRP:H	14	0.86
(3,483)	1:672:A:TRP:H	1:673:A:PHE:H	14	0.86
(3,378)	1:687:A:ILE:HG21	1:691:A:SER:HG	11	0.86
(3,378)	1:687:A:ILE:HG22	1:691:A:SER:HG	11	0.86
(3,378)	1:687:A:ILE:HG23	1:691:A:SER:HG	11	0.86
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	4	0.85
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	4	0.85
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	4	0.85
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	4	0.85
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	4	0.85
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	4	0.85
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	4	0.85
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	4	0.85
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	4	0.85
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	4	0.85
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	4	0.85
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	4	0.85
(3,561)	1:705:A:VAL:HG11	1:702:A:LEU:HA	4	0.84
(3,561)	1:705:A:VAL:HG12	1:702:A:LEU:HA	4	0.84
(3,561)	1:705:A:VAL:HG13	1:702:A:LEU:HA	4	0.84
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	13	0.84
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	13	0.84
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	13	0.84
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	13	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	13	0.84
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	13	0.84
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	13	0.84
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	13	0.84
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	13	0.84
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	13	0.84
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	13	0.84
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	13	0.84
(3,347)	1:705:A:VAL:HG11	1:702:A:LEU:HA	4	0.84
(3,347)	1:705:A:VAL:HG12	1:702:A:LEU:HA	4	0.84
(3,347)	1:705:A:VAL:HG13	1:702:A:LEU:HA	4	0.84
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	9	0.83
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	9	0.83
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	9	0.83
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	9	0.83
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	9	0.83
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	9	0.83
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	9	0.83
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	9	0.83
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	9	0.83
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	2	0.83
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	2	0.83
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	2	0.83
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	2	0.83
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	2	0.83
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	2	0.83
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	2	0.83
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	2	0.83
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	2	0.83
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	2	0.83
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	2	0.83
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	2	0.83
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	12	0.83
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	12	0.83
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	12	0.83
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	12	0.83
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	12	0.83
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	12	0.83
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	12	0.83
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	12	0.83
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	12	0.83
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	12	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	12	0.83
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	12	0.83
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	9	0.83
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	9	0.83
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	9	0.83
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	9	0.83
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	9	0.83
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	9	0.83
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	9	0.83
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	9	0.83
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	9	0.83
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	14	0.82
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	14	0.82
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	14	0.82
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	14	0.82
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	14	0.82
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	14	0.82
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	14	0.82
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	14	0.82
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	14	0.82
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	6	0.82
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	6	0.82
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	6	0.82
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	6	0.82
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	6	0.82
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	6	0.82
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	6	0.82
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	6	0.82
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	6	0.82
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	6	0.82
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	6	0.82
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	6	0.82
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	6	0.82
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	6	0.82
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	6	0.82
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	6	0.82
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	6	0.82
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	6	0.82
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	5	0.81
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	5	0.81
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	5	0.81
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	5	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	5	0.81
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	5	0.81
(3,599)	1:690:A:GLY:H	1:691:A:SER:H	12	0.8
(3,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	4	0.8
(3,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	4	0.8
(3,486)	1:673:A:PHE:H	1:672:A:TRP:H	6	0.79
(3,483)	1:672:A:TRP:H	1:673:A:PHE:H	6	0.79
(3,573)	1:707:A:ARG:H	1:704:A:LEU:HA	11	0.78
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	9	0.76
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	9	0.76
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	9	0.76
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	9	0.76
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	9	0.76
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	9	0.76
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	9	0.76
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	9	0.76
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	9	0.76
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	2	0.76
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	2	0.76
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	2	0.76
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	2	0.76
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	2	0.76
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	2	0.76
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	2	0.76
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	2	0.76
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	2	0.76
(3,592)	1:687:A:ILE:HG21	1:691:A:SER:HG	2	0.76
(3,592)	1:687:A:ILE:HG22	1:691:A:SER:HG	2	0.76
(3,592)	1:687:A:ILE:HG23	1:691:A:SER:HG	2	0.76
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	2	0.76
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	2	0.76
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	2	0.76
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	2	0.76
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	2	0.76
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	2	0.76
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	2	0.76
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	2	0.76
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	2	0.76
(3,378)	1:687:A:ILE:HG21	1:691:A:SER:HG	2	0.76
(3,378)	1:687:A:ILE:HG22	1:691:A:SER:HG	2	0.76
(3,378)	1:687:A:ILE:HG23	1:691:A:SER:HG	2	0.76
(3,348)	1:705:A:VAL:HG11	1:706:A:ASN:HA	1	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,348)	1:705:A:VAL:HG12	1:706:A:ASN:HA	1	0.76
(3,348)	1:705:A:VAL:HG13	1:706:A:ASN:HA	1	0.76
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	2	0.75
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	2	0.75
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	2	0.75
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	2	0.75
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	2	0.75
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	2	0.75
(3,605)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	12	0.75
(3,605)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	12	0.75
(3,605)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	12	0.75
(3,605)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	12	0.75
(3,605)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	12	0.75
(3,605)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	12	0.75
(3,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	8	0.75
(3,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	8	0.75
(3,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	8	0.75
(3,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	8	0.75
(3,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	8	0.75
(3,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	8	0.75
(3,391)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	12	0.75
(3,391)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	12	0.75
(3,391)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	12	0.75
(3,391)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	12	0.75
(3,391)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	12	0.75
(3,391)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	12	0.75
(3,486)	1:673:A:PHE:H	1:672:A:TRP:H	9	0.74
(3,483)	1:672:A:TRP:H	1:673:A:PHE:H	9	0.74
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	9	0.74
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	9	0.74
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	9	0.74
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	9	0.74
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	9	0.74
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	9	0.74
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	9	0.74
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	9	0.74
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	9	0.74
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	9	0.74
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	9	0.74
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	9	0.74
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	9	0.74
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	9	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	9	0.74
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	9	0.74
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	9	0.74
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	9	0.74
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	9	0.74
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	9	0.74
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	9	0.74
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	9	0.74
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	9	0.74
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	9	0.74
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	9	0.74
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	9	0.74
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	9	0.74
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	11	0.73
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	11	0.73
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	11	0.73
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	11	0.73
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	11	0.73
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	11	0.73
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	11	0.73
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	11	0.73
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	11	0.73
(2,3)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	13	0.73
(2,3)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	13	0.73
(2,3)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	13	0.73
(2,3)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	13	0.73
(2,3)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	13	0.73
(2,3)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	13	0.73
(2,2)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	13	0.73
(2,2)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	13	0.73
(2,2)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	13	0.73
(2,2)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	13	0.73
(2,2)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	13	0.73
(2,2)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	13	0.73
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	13	0.73
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	13	0.73
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	13	0.73
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	13	0.73
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	13	0.73
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	13	0.73
(3,592)	1:687:A:ILE:HG21	1:691:A:SER:HG	14	0.72
(3,592)	1:687:A:ILE:HG22	1:691:A:SER:HG	14	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,592)	1:687:A:ILE:HG23	1:691:A:SER:HG	14	0.72
(3,378)	1:687:A:ILE:HG21	1:691:A:SER:HG	14	0.72
(3,378)	1:687:A:ILE:HG22	1:691:A:SER:HG	14	0.72
(3,378)	1:687:A:ILE:HG23	1:691:A:SER:HG	14	0.72
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	9	0.72
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	9	0.72
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	9	0.72
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	9	0.72
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	9	0.72
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	9	0.72
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	7	0.71
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	7	0.71
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	7	0.71
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	7	0.71
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	7	0.71
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	7	0.71
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	7	0.71
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	7	0.71
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	7	0.71
(3,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	9	0.71
(3,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	9	0.71
(3,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	9	0.71
(3,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	9	0.71
(3,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	9	0.71
(3,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	9	0.71
(3,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	9	0.71
(3,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	9	0.71
(3,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	9	0.71
(3,567)	1:706:A:ASN:H	1:703:A:SER:HA	14	0.71
(3,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	9	0.71
(3,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	9	0.71
(3,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	9	0.71
(3,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	9	0.71
(3,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	9	0.71
(3,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	9	0.71
(3,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	9	0.71
(3,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	9	0.71
(3,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	9	0.71
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	6	0.71
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	6	0.71
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	6	0.71
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	6	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	6	0.71
(3,270)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	6	0.71
(3,605)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	6	0.7
(3,605)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	6	0.7
(3,605)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	6	0.7
(3,605)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	6	0.7
(3,605)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	6	0.7
(3,605)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	6	0.7
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	8	0.7
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	8	0.7
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	8	0.7
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	8	0.7
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	8	0.7
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	8	0.7
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	13	0.7
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	13	0.7
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	13	0.7
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	13	0.7
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	13	0.7
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	13	0.7
(3,391)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	6	0.7
(3,391)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	6	0.7
(3,391)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	6	0.7
(3,391)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	6	0.7
(3,391)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	6	0.7
(3,391)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	6	0.7
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	1	0.7
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	1	0.7
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	1	0.7
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	1	0.7
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	1	0.7
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	1	0.7
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	1	0.7
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	1	0.7
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	1	0.7
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	3	0.7
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	3	0.7
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	3	0.7
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	3	0.7
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	3	0.7
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	3	0.7
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	3	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	3	0.7
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	3	0.7
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	1	0.7
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	1	0.7
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	1	0.7
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	1	0.7
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	1	0.7
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	1	0.7
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	1	0.7
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	1	0.7
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	1	0.7
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	3	0.7
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	3	0.7
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	3	0.7
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	3	0.7
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	3	0.7
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	3	0.7
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	3	0.7
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	3	0.7
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	3	0.7
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	1	0.7
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	1	0.7
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	1	0.7
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	1	0.7
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	1	0.7
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	1	0.7
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	1	0.7
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	1	0.7
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	1	0.7
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	3	0.7
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	3	0.7
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	3	0.7
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	3	0.7
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	3	0.7
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	3	0.7
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	3	0.7
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	3	0.7
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	3	0.7
(3,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	6	0.69
(3,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	6	0.69
(3,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	6	0.69
(3,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	6	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	6	0.69
(3,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	6	0.69
(3,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	3	0.68
(3,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	3	0.68
(3,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	3	0.68
(3,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	13	0.68
(3,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	13	0.68
(3,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	13	0.68
(3,605)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	11	0.68
(3,605)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	11	0.68
(3,605)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	11	0.68
(3,605)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	11	0.68
(3,605)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	11	0.68
(3,605)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	11	0.68
(3,564)	1:705:A:VAL:HG21	1:701:A:VAL:HA	1	0.68
(3,564)	1:705:A:VAL:HG22	1:701:A:VAL:HA	1	0.68
(3,564)	1:705:A:VAL:HG23	1:701:A:VAL:HA	1	0.68
(3,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	10	0.68
(3,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	10	0.68
(3,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	10	0.68
(3,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	3	0.68
(3,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	3	0.68
(3,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	3	0.68
(3,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	13	0.68
(3,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	13	0.68
(3,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	13	0.68
(3,391)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	11	0.68
(3,391)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	11	0.68
(3,391)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	11	0.68
(3,391)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	11	0.68
(3,391)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	11	0.68
(3,391)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	11	0.68
(3,348)	1:705:A:VAL:HG11	1:706:A:ASN:HA	4	0.68
(3,348)	1:705:A:VAL:HG12	1:706:A:ASN:HA	4	0.68
(3,348)	1:705:A:VAL:HG13	1:706:A:ASN:HA	4	0.68
(3,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	10	0.68
(3,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	10	0.68
(3,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	10	0.68
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	12	0.68
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	12	0.68
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	12	0.68
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	12	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	12	0.68
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	12	0.68
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	12	0.68
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	12	0.68
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	12	0.68
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	12	0.68
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	12	0.68
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	12	0.68
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	12	0.68
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	12	0.68
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	12	0.68
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	12	0.68
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	12	0.68
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	12	0.68
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	12	0.68
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	12	0.68
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	12	0.68
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	12	0.68
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	12	0.68
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	12	0.68
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	12	0.68
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	12	0.68
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	12	0.68
(3,599)	1:690:A:GLY:H	1:691:A:SER:H	9	0.67
(3,573)	1:707:A:ARG:H	1:704:A:LEU:HA	13	0.67
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	5	0.67
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	5	0.67
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	5	0.67
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	5	0.67
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	5	0.67
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	5	0.67
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	5	0.67
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	5	0.67
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	5	0.67
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	5	0.67
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	5	0.67
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	5	0.67
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	5	0.67
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	5	0.67
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	5	0.67
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	5	0.67
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	5	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	5	0.67
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	5	0.67
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	5	0.67
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	5	0.67
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	5	0.67
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	5	0.67
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	5	0.67
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	5	0.67
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	5	0.67
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	5	0.67
(3,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	7	0.65
(3,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	7	0.65
(3,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	7	0.65
(3,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	7	0.65
(3,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	7	0.65
(3,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	7	0.65
(3,348)	1:705:A:VAL:HG11	1:706:A:ASN:HA	3	0.65
(3,348)	1:705:A:VAL:HG12	1:706:A:ASN:HA	3	0.65
(3,348)	1:705:A:VAL:HG13	1:706:A:ASN:HA	3	0.65
(3,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	8	0.65
(3,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	8	0.65
(3,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	8	0.65
(3,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	8	0.65
(3,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	8	0.65
(3,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	8	0.65
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	12	0.64
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	12	0.64
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	12	0.64
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	12	0.64
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	12	0.64
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	12	0.64
(3,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	1	0.64
(3,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	1	0.64
(3,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	1	0.64
(3,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	1	0.64
(3,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	1	0.64
(3,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	1	0.64
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	3	0.64
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	3	0.64
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	3	0.64
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	3	0.64
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	3	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	3	0.64
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	13	0.64
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	13	0.64
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	13	0.64
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	13	0.64
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	13	0.64
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	13	0.64
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	13	0.64
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	13	0.64
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	13	0.64
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	13	0.64
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	13	0.64
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	13	0.64
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	13	0.64
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	13	0.64
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	13	0.64
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	13	0.64
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	13	0.64
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	13	0.64
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	13	0.64
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	13	0.64
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	13	0.64
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	13	0.64
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	13	0.64
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	13	0.64
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	13	0.64
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	13	0.64
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	13	0.64
(3,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	4	0.63
(3,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	4	0.63
(3,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	4	0.63
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	3	0.63
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	3	0.63
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	3	0.63
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	3	0.63
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	3	0.63
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	3	0.63
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	8	0.63
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	8	0.63
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	8	0.63
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	8	0.63
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	8	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	8	0.63
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	8	0.63
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	8	0.63
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	8	0.63
(3,573)	1:707:A:ARG:H	1:704:A:LEU:HA	10	0.63
(3,573)	1:707:A:ARG:H	1:704:A:LEU:HA	12	0.63
(3,573)	1:707:A:ARG:H	1:704:A:LEU:HA	14	0.63
(3,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	9	0.63
(3,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	9	0.63
(3,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	9	0.63
(3,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	9	0.63
(3,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	9	0.63
(3,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	9	0.63
(3,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	4	0.63
(3,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	4	0.63
(3,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	4	0.63
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	8	0.63
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	8	0.63
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	8	0.63
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	8	0.63
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	8	0.63
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	8	0.63
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	8	0.63
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	8	0.63
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	8	0.63
(3,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	4	0.62
(3,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	4	0.62
(3,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	4	0.62
(3,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	4	0.62
(3,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	4	0.62
(3,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	4	0.62
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	11	0.62
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	11	0.62
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	11	0.62
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	11	0.62
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	11	0.62
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	11	0.62
(3,564)	1:705:A:VAL:HG21	1:701:A:VAL:HA	4	0.61
(3,564)	1:705:A:VAL:HG22	1:701:A:VAL:HA	4	0.61
(3,564)	1:705:A:VAL:HG23	1:701:A:VAL:HA	4	0.61
(3,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	11	0.61
(3,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	11	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	11	0.61
(3,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	14	0.61
(3,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	14	0.61
(3,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	14	0.61
(3,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	13	0.61
(3,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	13	0.61
(3,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	13	0.61
(3,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	13	0.61
(3,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	13	0.61
(3,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	13	0.61
(3,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	11	0.61
(3,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	11	0.61
(3,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	11	0.61
(3,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	14	0.61
(3,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	14	0.61
(3,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	14	0.61
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	6	0.61
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	6	0.61
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	6	0.61
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	6	0.61
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	6	0.61
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	6	0.61
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	6	0.61
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	6	0.61
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	6	0.61
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	11	0.61
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	11	0.61
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	11	0.61
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	11	0.61
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	11	0.61
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	11	0.61
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	11	0.61
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	11	0.61
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	11	0.61
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	6	0.61
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	6	0.61
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	6	0.61
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	6	0.61
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	6	0.61
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	6	0.61
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	6	0.61
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	6	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	6	0.61
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	11	0.61
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	11	0.61
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	11	0.61
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	11	0.61
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	11	0.61
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	11	0.61
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	11	0.61
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	11	0.61
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	11	0.61
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	6	0.61
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	6	0.61
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	6	0.61
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	6	0.61
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	6	0.61
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	6	0.61
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	6	0.61
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	6	0.61
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	6	0.61
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	11	0.61
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	11	0.61
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	11	0.61
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	11	0.61
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	11	0.61
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	11	0.61
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	11	0.61
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	11	0.61
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	11	0.61
(3,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	8	0.6
(3,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	8	0.6
(3,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	8	0.6
(3,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	10	0.6
(3,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	10	0.6
(3,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	10	0.6
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	5	0.6
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	5	0.6
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	5	0.6
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	5	0.6
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	5	0.6
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	5	0.6
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	5	0.6
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	5	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	5	0.6
(3,592)	1:687:A:ILE:HG21	1:691:A:SER:HG	8	0.6
(3,592)	1:687:A:ILE:HG22	1:691:A:SER:HG	8	0.6
(3,592)	1:687:A:ILE:HG23	1:691:A:SER:HG	8	0.6
(3,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	2	0.6
(3,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	2	0.6
(3,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	2	0.6
(3,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	2	0.6
(3,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	2	0.6
(3,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	2	0.6
(3,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	8	0.6
(3,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	8	0.6
(3,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	8	0.6
(3,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	10	0.6
(3,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	10	0.6
(3,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	10	0.6
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	5	0.6
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	5	0.6
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	5	0.6
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	5	0.6
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	5	0.6
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	5	0.6
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	5	0.6
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	5	0.6
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	5	0.6
(3,378)	1:687:A:ILE:HG21	1:691:A:SER:HG	8	0.6
(3,378)	1:687:A:ILE:HG22	1:691:A:SER:HG	8	0.6
(3,378)	1:687:A:ILE:HG23	1:691:A:SER:HG	8	0.6
(3,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	1	0.59
(3,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	1	0.59
(3,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	1	0.59
(3,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	2	0.59
(3,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	2	0.59
(3,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	2	0.59
(3,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	14	0.59
(3,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	14	0.59
(3,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	14	0.59
(3,599)	1:690:A:GLY:H	1:691:A:SER:H	2	0.59
(3,564)	1:705:A:VAL:HG21	1:701:A:VAL:HA	3	0.59
(3,564)	1:705:A:VAL:HG22	1:701:A:VAL:HA	3	0.59
(3,564)	1:705:A:VAL:HG23	1:701:A:VAL:HA	3	0.59
(3,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	6	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	6	0.59
(3,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	6	0.59
(3,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	6	0.59
(3,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	6	0.59
(3,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	6	0.59
(3,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	12	0.59
(3,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	12	0.59
(3,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	12	0.59
(3,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	12	0.59
(3,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	12	0.59
(3,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	12	0.59
(3,422)	1:700:A:ALA:HB1	1:697:A:ILE:HA	5	0.59
(3,422)	1:700:A:ALA:HB2	1:697:A:ILE:HA	5	0.59
(3,422)	1:700:A:ALA:HB3	1:697:A:ILE:HA	5	0.59
(3,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	1	0.59
(3,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	1	0.59
(3,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	1	0.59
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	8	0.59
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	8	0.59
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	8	0.59
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	8	0.59
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	8	0.59
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	8	0.59
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	8	0.59
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	8	0.59
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	8	0.59
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	14	0.59
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	14	0.59
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	14	0.59
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	14	0.59
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	14	0.59
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	14	0.59
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	14	0.59
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	14	0.59
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	14	0.59
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	8	0.59
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	8	0.59
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	8	0.59
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	8	0.59
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	8	0.59
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	8	0.59
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	8	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	8	0.59
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	8	0.59
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	14	0.59
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	14	0.59
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	14	0.59
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	14	0.59
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	14	0.59
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	14	0.59
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	14	0.59
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	14	0.59
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	14	0.59
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	8	0.59
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	8	0.59
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	8	0.59
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	8	0.59
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	8	0.59
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	8	0.59
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	8	0.59
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	8	0.59
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	8	0.59
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	14	0.59
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	14	0.59
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	14	0.59
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	14	0.59
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	14	0.59
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	14	0.59
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	14	0.59
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	14	0.59
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	14	0.59
(3,599)	1:690:A:GLY:H	1:691:A:SER:H	5	0.58
(3,573)	1:707:A:ARG:H	1:704:A:LEU:HA	6	0.58
(3,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	9	0.58
(3,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	9	0.58
(3,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	9	0.58
(3,486)	1:673:A:PHE:H	1:672:A:TRP:H	10	0.58
(3,483)	1:672:A:TRP:H	1:673:A:PHE:H	10	0.58
(3,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	10	0.58
(3,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	10	0.58
(3,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	10	0.58
(3,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	10	0.58
(3,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	10	0.58
(3,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	10	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	3	0.58
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	3	0.58
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	3	0.58
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	3	0.58
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	3	0.58
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	3	0.58
(3,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	9	0.58
(3,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	9	0.58
(3,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	9	0.58
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	5	0.58
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	5	0.58
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	5	0.58
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	5	0.58
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	5	0.58
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	5	0.58
(3,175)	1:692:A:LEU:HD11	1:696:A:ARG:HH21	2	0.58
(3,175)	1:692:A:LEU:HD11	1:696:A:ARG:HH22	2	0.58
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	4	0.58
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	4	0.58
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	4	0.58
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	4	0.58
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	4	0.58
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	4	0.58
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	4	0.58
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	4	0.58
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	4	0.58
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	4	0.58
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	4	0.58
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	4	0.58
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	4	0.58
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	4	0.58
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	4	0.58
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	4	0.58
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	4	0.58
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	4	0.58
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	4	0.58
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	4	0.58
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	4	0.58
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	4	0.58
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	4	0.58
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	4	0.58
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	4	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	4	0.58
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	4	0.58
(3,612)	1:695:A:LEU:H	1:694:A:GLY:H	8	0.57
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG21	2	0.57
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG22	2	0.57
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG23	2	0.57
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG21	2	0.57
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG22	2	0.57
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG23	2	0.57
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG21	2	0.57
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG22	2	0.57
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG23	2	0.57
(3,567)	1:706:A:ASN:H	1:703:A:SER:HA	5	0.57
(3,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	3	0.57
(3,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	3	0.57
(3,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	3	0.57
(3,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	12	0.57
(3,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	12	0.57
(3,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	12	0.57
(3,422)	1:700:A:ALA:HB1	1:697:A:ILE:HA	14	0.57
(3,422)	1:700:A:ALA:HB2	1:697:A:ILE:HA	14	0.57
(3,422)	1:700:A:ALA:HB3	1:697:A:ILE:HA	14	0.57
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	5	0.57
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	5	0.57
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	5	0.57
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	5	0.57
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	5	0.57
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	5	0.57
(3,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	3	0.57
(3,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	3	0.57
(3,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	3	0.57
(3,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	12	0.57
(3,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	12	0.57
(3,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	12	0.57
(3,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	11	0.56
(3,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	11	0.56
(3,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	11	0.56
(3,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	3	0.56
(3,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	3	0.56
(3,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	3	0.56
(3,486)	1:673:A:PHE:H	1:672:A:TRP:H	2	0.56
(3,483)	1:672:A:TRP:H	1:673:A:PHE:H	2	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,422)	1:700:A:ALA:HB1	1:697:A:ILE:HA	2	0.56
(3,422)	1:700:A:ALA:HB2	1:697:A:ILE:HA	2	0.56
(3,422)	1:700:A:ALA:HB3	1:697:A:ILE:HA	2	0.56
(3,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	11	0.56
(3,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	11	0.56
(3,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	11	0.56
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	10	0.56
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	10	0.56
(2,27)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	10	0.56
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	10	0.56
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	10	0.56
(2,27)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	10	0.56
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	10	0.56
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	10	0.56
(2,27)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	10	0.56
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	10	0.56
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	10	0.56
(2,26)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	10	0.56
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	10	0.56
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	10	0.56
(2,26)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	10	0.56
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	10	0.56
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	10	0.56
(2,26)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	10	0.56
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	10	0.56
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	10	0.56
(2,25)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	10	0.56
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	10	0.56
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	10	0.56
(2,25)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	10	0.56
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	10	0.56
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	10	0.56
(2,25)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	10	0.56
(3,612)	1:695:A:LEU:H	1:694:A:GLY:H	11	0.55
(3,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	4	0.55
(3,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	4	0.55
(3,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	4	0.55
(3,597)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	5	0.55
(3,597)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	5	0.55
(3,597)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	5	0.55
(3,597)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	5	0.55
(3,597)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	5	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,597)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	5	0.55
(3,422)	1:700:A:ALA:HB1	1:697:A:ILE:HA	1	0.55
(3,422)	1:700:A:ALA:HB2	1:697:A:ILE:HA	1	0.55
(3,422)	1:700:A:ALA:HB3	1:697:A:ILE:HA	1	0.55
(3,422)	1:700:A:ALA:HB1	1:697:A:ILE:HA	4	0.55
(3,422)	1:700:A:ALA:HB2	1:697:A:ILE:HA	4	0.55
(3,422)	1:700:A:ALA:HB3	1:697:A:ILE:HA	4	0.55
(3,422)	1:700:A:ALA:HB1	1:697:A:ILE:HA	12	0.55
(3,422)	1:700:A:ALA:HB2	1:697:A:ILE:HA	12	0.55
(3,422)	1:700:A:ALA:HB3	1:697:A:ILE:HA	12	0.55
(3,422)	1:700:A:ALA:HB1	1:697:A:ILE:HA	13	0.55
(3,422)	1:700:A:ALA:HB2	1:697:A:ILE:HA	13	0.55
(3,422)	1:700:A:ALA:HB3	1:697:A:ILE:HA	13	0.55
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	1	0.55
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	1	0.55
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	1	0.55
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	1	0.55
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	1	0.55
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	1	0.55
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	1	0.54
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	1	0.54
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	1	0.54
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	1	0.54
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	1	0.54
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	1	0.54
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	3	0.54
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	3	0.54
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	3	0.54
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	3	0.54
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	3	0.54
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	3	0.54
(3,554)	1:704:A:LEU:HD11	1:707:A:ARG:HE	12	0.54
(3,554)	1:704:A:LEU:HD12	1:707:A:ARG:HE	12	0.54
(3,554)	1:704:A:LEU:HD13	1:707:A:ARG:HE	12	0.54
(3,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	7	0.54
(3,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	7	0.54
(3,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	7	0.54
(3,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	7	0.54
(3,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	7	0.54
(3,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	7	0.54
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	6	0.54
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	6	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	6	0.54
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	6	0.54
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	6	0.54
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	6	0.54
(2,60)	1:696:A:ARG:H	1:693:A:ILE:HD11	7	0.54
(2,60)	1:696:A:ARG:H	1:693:A:ILE:HD12	7	0.54
(2,60)	1:696:A:ARG:H	1:693:A:ILE:HD13	7	0.54
(2,59)	1:696:A:ARG:H	1:693:A:ILE:HD11	7	0.54
(2,59)	1:696:A:ARG:H	1:693:A:ILE:HD12	7	0.54
(2,59)	1:696:A:ARG:H	1:693:A:ILE:HD13	7	0.54
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	10	0.54
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	10	0.54
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	10	0.54
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	10	0.54
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	10	0.54
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	10	0.54
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	10	0.54
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	10	0.54
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	10	0.54
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	10	0.54
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	10	0.54
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	10	0.54
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	10	0.54
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	10	0.54
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	10	0.54
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	10	0.54
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	10	0.54
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	10	0.54
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	10	0.54
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	10	0.54
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	10	0.54
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	10	0.54
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	10	0.54
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	10	0.54
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	10	0.54
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	10	0.54
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	10	0.54
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	13	0.53
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	13	0.53
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	13	0.53
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	13	0.53
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	13	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	13	0.53
(3,612)	1:695:A:LEU:H	1:694:A:GLY:H	5	0.53
(3,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	13	0.53
(3,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	13	0.53
(3,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	13	0.53
(3,599)	1:690:A:GLY:H	1:691:A:SER:H	3	0.53
(3,599)	1:690:A:GLY:H	1:691:A:SER:H	10	0.53
(3,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	5	0.53
(3,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	5	0.53
(3,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	5	0.53
(3,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	1	0.53
(3,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	1	0.53
(3,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	1	0.53
(3,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	1	0.53
(3,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	1	0.53
(3,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	1	0.53
(3,422)	1:700:A:ALA:HB1	1:697:A:ILE:HA	8	0.53
(3,422)	1:700:A:ALA:HB2	1:697:A:ILE:HA	8	0.53
(3,422)	1:700:A:ALA:HB3	1:697:A:ILE:HA	8	0.53
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	11	0.53
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	11	0.53
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	11	0.53
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	11	0.53
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	11	0.53
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	11	0.53
(3,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	5	0.53
(3,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	5	0.53
(3,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	5	0.53
(3,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	9	0.53
(3,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	9	0.53
(3,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	9	0.53
(3,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	9	0.53
(3,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	9	0.53
(3,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	9	0.53
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	3	0.52
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	3	0.52
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	3	0.52
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	3	0.52
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	3	0.52
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	3	0.52
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	4	0.52
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	4	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	4	0.52
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	4	0.52
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	4	0.52
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	4	0.52
(3,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	10	0.52
(3,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	10	0.52
(3,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	10	0.52
(3,567)	1:706:A:ASN:H	1:703:A:SER:HA	12	0.52
(3,564)	1:705:A:VAL:HG21	1:701:A:VAL:HA	8	0.52
(3,564)	1:705:A:VAL:HG22	1:701:A:VAL:HA	8	0.52
(3,564)	1:705:A:VAL:HG23	1:701:A:VAL:HA	8	0.52
(3,554)	1:704:A:LEU:HD11	1:707:A:ARG:HE	14	0.52
(3,554)	1:704:A:LEU:HD12	1:707:A:ARG:HE	14	0.52
(3,554)	1:704:A:LEU:HD13	1:707:A:ARG:HE	14	0.52
(3,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	7	0.52
(3,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	7	0.52
(3,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	7	0.52
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	4	0.52
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	4	0.52
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	4	0.52
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	4	0.52
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	4	0.52
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	4	0.52
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	7	0.52
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	7	0.52
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	7	0.52
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	7	0.52
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	7	0.52
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	7	0.52
(3,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	7	0.52
(3,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	7	0.52
(3,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	7	0.52
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	12	0.51
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	12	0.51
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	12	0.51
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	12	0.51
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	12	0.51
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	12	0.51
(3,612)	1:695:A:LEU:H	1:694:A:GLY:H	6	0.51
(3,554)	1:704:A:LEU:HD11	1:707:A:ARG:HE	6	0.51
(3,554)	1:704:A:LEU:HD12	1:707:A:ARG:HE	6	0.51
(3,554)	1:704:A:LEU:HD13	1:707:A:ARG:HE	6	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,422)	1:700:A:ALA:HB1	1:697:A:ILE:HA	3	0.51
(3,422)	1:700:A:ALA:HB2	1:697:A:ILE:HA	3	0.51
(3,422)	1:700:A:ALA:HB3	1:697:A:ILE:HA	3	0.51
(3,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	13	0.51
(3,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	13	0.51
(3,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	13	0.51
(3,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	13	0.51
(3,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	13	0.51
(3,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	13	0.51
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	10	0.5
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	10	0.5
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	10	0.5
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	10	0.5
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	10	0.5
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	10	0.5
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	3	0.5
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	3	0.5
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	3	0.5
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	3	0.5
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	3	0.5
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	3	0.5
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	3	0.5
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	3	0.5
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	3	0.5
(3,567)	1:706:A:ASN:H	1:703:A:SER:HA	10	0.5
(3,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	4	0.5
(3,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	4	0.5
(3,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	4	0.5
(3,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	4	0.5
(3,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	4	0.5
(3,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	4	0.5
(3,422)	1:700:A:ALA:HB1	1:697:A:ILE:HA	7	0.5
(3,422)	1:700:A:ALA:HB2	1:697:A:ILE:HA	7	0.5
(3,422)	1:700:A:ALA:HB3	1:697:A:ILE:HA	7	0.5
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	3	0.5
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	3	0.5
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	3	0.5
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	3	0.5
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	3	0.5
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	3	0.5
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	3	0.5
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	3	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	3	0.5
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD11	7	0.5
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD12	7	0.5
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD13	7	0.5
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD21	7	0.5
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD22	7	0.5
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD23	7	0.5
(3,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	2	0.5
(3,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	2	0.5
(3,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	2	0.5
(3,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	2	0.5
(3,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	2	0.5
(3,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	2	0.5
(3,175)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	11	0.5
(3,175)	1:692:A:LEU:HD13	1:696:A:ARG:HH12	11	0.5
(3,612)	1:695:A:LEU:H	1:694:A:GLY:H	9	0.49
(3,573)	1:707:A:ARG:H	1:704:A:LEU:HA	5	0.49
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	3	0.49
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	3	0.49
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	3	0.49
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	3	0.49
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	3	0.49
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	3	0.49
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	3	0.49
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	3	0.49
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	3	0.49
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	3	0.49
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	3	0.49
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	3	0.49
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	1	0.49
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	1	0.49
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	1	0.49
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	1	0.49
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	1	0.49
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	1	0.49
(3,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	6	0.49
(3,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	6	0.49
(3,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	6	0.49
(3,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	6	0.49
(3,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	6	0.49
(3,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	6	0.49
(3,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	12	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	12	0.49
(3,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	12	0.49
(3,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	12	0.49
(3,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	12	0.49
(3,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	12	0.49
(2,60)	1:696:A:ARG:H	1:693:A:ILE:HD11	10	0.49
(2,60)	1:696:A:ARG:H	1:693:A:ILE:HD12	10	0.49
(2,60)	1:696:A:ARG:H	1:693:A:ILE:HD13	10	0.49
(2,59)	1:696:A:ARG:H	1:693:A:ILE:HD11	10	0.49
(2,59)	1:696:A:ARG:H	1:693:A:ILE:HD12	10	0.49
(2,59)	1:696:A:ARG:H	1:693:A:ILE:HD13	10	0.49
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	2	0.49
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	2	0.49
(2,39)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	2	0.49
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	2	0.49
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	2	0.49
(2,39)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	2	0.49
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	2	0.49
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	2	0.49
(2,39)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	2	0.49
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	2	0.49
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	2	0.49
(2,38)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	2	0.49
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	2	0.49
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	2	0.49
(2,38)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	2	0.49
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	2	0.49
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	2	0.49
(2,38)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	2	0.49
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG21	2	0.49
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG22	2	0.49
(2,37)	1:687:A:ILE:HG21	1:689:A:VAL:HG23	2	0.49
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG21	2	0.49
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG22	2	0.49
(2,37)	1:687:A:ILE:HG22	1:689:A:VAL:HG23	2	0.49
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG21	2	0.49
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG22	2	0.49
(2,37)	1:687:A:ILE:HG23	1:689:A:VAL:HG23	2	0.49
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	10	0.48
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	10	0.48
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	10	0.48
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	10	0.48
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	10	0.48
(3,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	8	0.48
(3,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	8	0.48
(3,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	8	0.48
(3,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	5	0.48
(3,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	5	0.48
(3,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	5	0.48
(3,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	5	0.48
(3,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	5	0.48
(3,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	5	0.48
(3,422)	1:700:A:ALA:HB1	1:697:A:ILE:HA	9	0.48
(3,422)	1:700:A:ALA:HB2	1:697:A:ILE:HA	9	0.48
(3,422)	1:700:A:ALA:HB3	1:697:A:ILE:HA	9	0.48
(3,422)	1:700:A:ALA:HB1	1:697:A:ILE:HA	11	0.48
(3,422)	1:700:A:ALA:HB2	1:697:A:ILE:HA	11	0.48
(3,422)	1:700:A:ALA:HB3	1:697:A:ILE:HA	11	0.48
(3,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	8	0.48
(3,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	8	0.48
(3,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	8	0.48
(3,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	10	0.48
(3,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	10	0.48
(3,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	10	0.48
(3,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	10	0.48
(3,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	10	0.48
(3,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	10	0.48
(3,624)	1:698:A:VAL:HG11	1:695:A:LEU:HA	5	0.47
(3,624)	1:698:A:VAL:HG12	1:695:A:LEU:HA	5	0.47
(3,624)	1:698:A:VAL:HG13	1:695:A:LEU:HA	5	0.47
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	14	0.47
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	14	0.47
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	14	0.47
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	14	0.47
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	14	0.47
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	14	0.47
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	11	0.47
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	11	0.47
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	11	0.47
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	11	0.47
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	11	0.47
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	11	0.47
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	12	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	12	0.47
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	12	0.47
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	12	0.47
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	12	0.47
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	12	0.47
(3,592)	1:687:A:ILE:HG21	1:691:A:SER:HG	5	0.47
(3,592)	1:687:A:ILE:HG22	1:691:A:SER:HG	5	0.47
(3,592)	1:687:A:ILE:HG23	1:691:A:SER:HG	5	0.47
(3,573)	1:707:A:ARG:H	1:704:A:LEU:HA	4	0.47
(3,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	2	0.47
(3,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	2	0.47
(3,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	2	0.47
(3,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	3	0.47
(3,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	3	0.47
(3,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	3	0.47
(3,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	3	0.47
(3,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	3	0.47
(3,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	3	0.47
(3,410)	1:698:A:VAL:HG11	1:695:A:LEU:HA	5	0.47
(3,410)	1:698:A:VAL:HG12	1:695:A:LEU:HA	5	0.47
(3,410)	1:698:A:VAL:HG13	1:695:A:LEU:HA	5	0.47
(3,378)	1:687:A:ILE:HG21	1:691:A:SER:HG	5	0.47
(3,378)	1:687:A:ILE:HG22	1:691:A:SER:HG	5	0.47
(3,378)	1:687:A:ILE:HG23	1:691:A:SER:HG	5	0.47
(3,351)	1:705:A:VAL:HG21	1:702:A:LEU:HG	14	0.47
(3,351)	1:705:A:VAL:HG22	1:702:A:LEU:HG	14	0.47
(3,351)	1:705:A:VAL:HG23	1:702:A:LEU:HG	14	0.47
(3,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	2	0.47
(3,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	2	0.47
(3,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	2	0.47
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	8	0.47
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	8	0.47
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	8	0.47
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	8	0.47
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	8	0.47
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	8	0.47
(3,175)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	6	0.47
(3,175)	1:692:A:LEU:HD11	1:696:A:ARG:HH12	6	0.47
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	6	0.46
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	6	0.46
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	6	0.46
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	6	0.46
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	6	0.46
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	5	0.46
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	5	0.46
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	5	0.46
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	5	0.46
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	5	0.46
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	5	0.46
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG21	3	0.46
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG22	3	0.46
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG23	3	0.46
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG21	3	0.46
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG22	3	0.46
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG23	3	0.46
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG21	3	0.46
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG22	3	0.46
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG23	3	0.46
(3,599)	1:690:A:GLY:H	1:691:A:SER:H	13	0.46
(3,422)	1:700:A:ALA:HB1	1:697:A:ILE:HA	6	0.46
(3,422)	1:700:A:ALA:HB2	1:697:A:ILE:HA	6	0.46
(3,422)	1:700:A:ALA:HB3	1:697:A:ILE:HA	6	0.46
(2,60)	1:696:A:ARG:H	1:693:A:ILE:HD11	14	0.46
(2,60)	1:696:A:ARG:H	1:693:A:ILE:HD12	14	0.46
(2,60)	1:696:A:ARG:H	1:693:A:ILE:HD13	14	0.46
(2,59)	1:696:A:ARG:H	1:693:A:ILE:HD11	14	0.46
(2,59)	1:696:A:ARG:H	1:693:A:ILE:HD12	14	0.46
(2,59)	1:696:A:ARG:H	1:693:A:ILE:HD13	14	0.46
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	7	0.45
(3,617)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	7	0.45
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	7	0.45
(3,617)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	7	0.45
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	7	0.45
(3,617)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	7	0.45
(3,612)	1:695:A:LEU:H	1:694:A:GLY:H	3	0.45
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	6	0.45
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	6	0.45
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	6	0.45
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	6	0.45
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	6	0.45
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	6	0.45
(3,554)	1:704:A:LEU:HD11	1:707:A:ARG:HE	3	0.45
(3,554)	1:704:A:LEU:HD12	1:707:A:ARG:HE	3	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,554)	1:704:A:LEU:HD13	1:707:A:ARG:HE	3	0.45
(3,486)	1:673:A:PHE:H	1:672:A:TRP:H	11	0.45
(3,483)	1:672:A:TRP:H	1:673:A:PHE:H	11	0.45
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD11	9	0.45
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD12	9	0.45
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD13	9	0.45
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD21	9	0.45
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD22	9	0.45
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD23	9	0.45
(3,337)	1:704:A:LEU:H	1:704:A:LEU:HB2	13	0.45
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	14	0.45
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	14	0.45
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	14	0.45
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	14	0.45
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	14	0.45
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	14	0.45
(3,642)	1:701:A:VAL:HG21	1:698:A:VAL:HA	3	0.44
(3,642)	1:701:A:VAL:HG22	1:698:A:VAL:HA	3	0.44
(3,642)	1:701:A:VAL:HG23	1:698:A:VAL:HA	3	0.44
(3,573)	1:707:A:ARG:H	1:704:A:LEU:HA	9	0.44
(3,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	7	0.44
(3,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	7	0.44
(3,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	7	0.44
(3,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	7	0.44
(3,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	7	0.44
(3,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	7	0.44
(3,612)	1:695:A:LEU:H	1:694:A:GLY:H	13	0.43
(3,473)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	11	0.43
(3,473)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	11	0.43
(3,473)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	11	0.43
(3,473)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	11	0.43
(3,473)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	11	0.43
(3,473)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	11	0.43
(3,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	1	0.43
(3,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	1	0.43
(3,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	1	0.43
(3,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	1	0.43
(3,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	1	0.43
(3,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	1	0.43
(2,60)	1:696:A:ARG:H	1:693:A:ILE:HD11	2	0.43
(2,60)	1:696:A:ARG:H	1:693:A:ILE:HD12	2	0.43
(2,60)	1:696:A:ARG:H	1:693:A:ILE:HD13	2	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,59)	1:696:A:ARG:H	1:693:A:ILE:HD11	2	0.43
(2,59)	1:696:A:ARG:H	1:693:A:ILE:HD12	2	0.43
(2,59)	1:696:A:ARG:H	1:693:A:ILE:HD13	2	0.43
(3,599)	1:690:A:GLY:H	1:691:A:SER:H	14	0.42
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	12	0.42
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	12	0.42
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	12	0.42
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	12	0.42
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	12	0.42
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	12	0.42
(3,573)	1:707:A:ARG:H	1:704:A:LEU:HA	1	0.41
(3,337)	1:704:A:LEU:H	1:704:A:LEU:HB2	12	0.41
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	12	0.4
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	12	0.4
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	12	0.4
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	12	0.4
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	12	0.4
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	12	0.4
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	12	0.4
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	12	0.4
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	12	0.4
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	14	0.4
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	14	0.4
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	14	0.4
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	14	0.4
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	14	0.4
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	14	0.4
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	14	0.4
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	14	0.4
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	14	0.4
(3,592)	1:687:A:ILE:HG21	1:691:A:SER:HG	1	0.4
(3,592)	1:687:A:ILE:HG22	1:691:A:SER:HG	1	0.4
(3,592)	1:687:A:ILE:HG23	1:691:A:SER:HG	1	0.4
(3,567)	1:706:A:ASN:H	1:703:A:SER:HA	9	0.4
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	12	0.4
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	12	0.4
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	12	0.4
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	12	0.4
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	12	0.4
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	12	0.4
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	12	0.4
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	12	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	12	0.4
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	14	0.4
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	14	0.4
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	14	0.4
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	14	0.4
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	14	0.4
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	14	0.4
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	14	0.4
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	14	0.4
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	14	0.4
(3,378)	1:687:A:ILE:HG21	1:691:A:SER:HG	1	0.4
(3,378)	1:687:A:ILE:HG22	1:691:A:SER:HG	1	0.4
(3,378)	1:687:A:ILE:HG23	1:691:A:SER:HG	1	0.4
(3,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	4	0.4
(3,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	4	0.4
(3,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	4	0.4
(3,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	4	0.4
(3,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	4	0.4
(3,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	4	0.4
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG21	14	0.39
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG22	14	0.39
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG23	14	0.39
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG21	14	0.39
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG22	14	0.39
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG23	14	0.39
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG21	14	0.39
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG22	14	0.39
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG23	14	0.39
(3,567)	1:706:A:ASN:H	1:703:A:SER:HA	13	0.39
(3,642)	1:701:A:VAL:HG21	1:698:A:VAL:HA	1	0.38
(3,642)	1:701:A:VAL:HG22	1:698:A:VAL:HA	1	0.38
(3,642)	1:701:A:VAL:HG23	1:698:A:VAL:HA	1	0.38
(3,612)	1:695:A:LEU:H	1:694:A:GLY:H	1	0.38
(3,599)	1:690:A:GLY:H	1:691:A:SER:H	6	0.38
(3,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	8	0.38
(3,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	8	0.38
(3,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	5	0.38
(3,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	5	0.38
(3,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	5	0.38
(3,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	5	0.38
(3,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	5	0.38
(3,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	5	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,175)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	7	0.38
(3,175)	1:692:A:LEU:HD13	1:696:A:ARG:HH12	7	0.38
(3,175)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	13	0.38
(3,175)	1:692:A:LEU:HD13	1:696:A:ARG:HH12	13	0.38
(3,443)	1:665:A:LYS:H	1:662:A:GLU:HA	5	0.37
(3,337)	1:704:A:LEU:H	1:704:A:LEU:HB2	9	0.37
(3,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	3	0.37
(3,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	3	0.37
(3,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	3	0.37
(3,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	3	0.37
(3,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	3	0.37
(3,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	3	0.37
(3,229)	1:665:A:LYS:H	1:662:A:GLU:HA	5	0.37
(3,15)	1:665:A:LYS:H	1:662:A:GLU:HA	5	0.37
(3,622)	1:697:A:ILE:HG21	1:698:A:VAL:HA	1	0.36
(3,622)	1:697:A:ILE:HG22	1:698:A:VAL:HA	1	0.36
(3,622)	1:697:A:ILE:HG23	1:698:A:VAL:HA	1	0.36
(3,599)	1:690:A:GLY:H	1:691:A:SER:H	7	0.36
(3,511)	1:682:A:ILE:HD11	1:681:A:TYR:H	13	0.36
(3,511)	1:682:A:ILE:HD12	1:681:A:TYR:H	13	0.36
(3,511)	1:682:A:ILE:HD13	1:681:A:TYR:H	13	0.36
(3,408)	1:697:A:ILE:HG21	1:698:A:VAL:HA	1	0.36
(3,408)	1:697:A:ILE:HG22	1:698:A:VAL:HA	1	0.36
(3,408)	1:697:A:ILE:HG23	1:698:A:VAL:HA	1	0.36
(3,337)	1:704:A:LEU:H	1:704:A:LEU:HB2	5	0.36
(3,297)	1:682:A:ILE:HD11	1:681:A:TYR:H	13	0.36
(3,297)	1:682:A:ILE:HD12	1:681:A:TYR:H	13	0.36
(3,297)	1:682:A:ILE:HD13	1:681:A:TYR:H	13	0.36
(3,194)	1:697:A:ILE:HG21	1:698:A:VAL:HA	1	0.36
(3,194)	1:697:A:ILE:HG22	1:698:A:VAL:HA	1	0.36
(3,194)	1:697:A:ILE:HG23	1:698:A:VAL:HA	1	0.36
(3,612)	1:695:A:LEU:H	1:694:A:GLY:H	12	0.35
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD11	6	0.35
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD12	6	0.35
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD13	6	0.35
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD21	6	0.35
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD22	6	0.35
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD23	6	0.35
(3,573)	1:707:A:ARG:H	1:704:A:LEU:HA	2	0.35
(3,553)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	9	0.35
(3,553)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	9	0.35
(3,553)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,553)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	9	0.35
(3,553)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	9	0.35
(3,553)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	9	0.35
(3,387)	1:692:A:LEU:HD11	1:689:A:VAL:HG21	7	0.35
(3,387)	1:692:A:LEU:HD11	1:689:A:VAL:HG22	7	0.35
(3,387)	1:692:A:LEU:HD11	1:689:A:VAL:HG23	7	0.35
(3,387)	1:692:A:LEU:HD12	1:689:A:VAL:HG21	7	0.35
(3,387)	1:692:A:LEU:HD12	1:689:A:VAL:HG22	7	0.35
(3,387)	1:692:A:LEU:HD12	1:689:A:VAL:HG23	7	0.35
(3,387)	1:692:A:LEU:HD13	1:689:A:VAL:HG21	7	0.35
(3,387)	1:692:A:LEU:HD13	1:689:A:VAL:HG22	7	0.35
(3,387)	1:692:A:LEU:HD13	1:689:A:VAL:HG23	7	0.35
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	8	0.35
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	8	0.35
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	8	0.35
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	8	0.35
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	8	0.35
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	8	0.35
(3,622)	1:697:A:ILE:HG21	1:698:A:VAL:HA	5	0.34
(3,622)	1:697:A:ILE:HG22	1:698:A:VAL:HA	5	0.34
(3,622)	1:697:A:ILE:HG23	1:698:A:VAL:HA	5	0.34
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	2	0.34
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	2	0.34
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	2	0.34
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	2	0.34
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	2	0.34
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	2	0.34
(3,592)	1:687:A:ILE:HG21	1:691:A:SER:HG	3	0.34
(3,592)	1:687:A:ILE:HG22	1:691:A:SER:HG	3	0.34
(3,592)	1:687:A:ILE:HG23	1:691:A:SER:HG	3	0.34
(3,567)	1:706:A:ASN:H	1:703:A:SER:HA	7	0.34
(3,408)	1:697:A:ILE:HG21	1:698:A:VAL:HA	5	0.34
(3,408)	1:697:A:ILE:HG22	1:698:A:VAL:HA	5	0.34
(3,408)	1:697:A:ILE:HG23	1:698:A:VAL:HA	5	0.34
(3,378)	1:687:A:ILE:HG21	1:691:A:SER:HG	3	0.34
(3,378)	1:687:A:ILE:HG22	1:691:A:SER:HG	3	0.34
(3,378)	1:687:A:ILE:HG23	1:691:A:SER:HG	3	0.34
(3,348)	1:705:A:VAL:HG11	1:706:A:ASN:HA	11	0.34
(3,348)	1:705:A:VAL:HG12	1:706:A:ASN:HA	11	0.34
(3,348)	1:705:A:VAL:HG13	1:706:A:ASN:HA	11	0.34
(3,194)	1:697:A:ILE:HG21	1:698:A:VAL:HA	5	0.34
(3,194)	1:697:A:ILE:HG22	1:698:A:VAL:HA	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,194)	1:697:A:ILE:HG23	1:698:A:VAL:HA	5	0.34
(3,642)	1:701:A:VAL:HG21	1:698:A:VAL:HA	9	0.33
(3,642)	1:701:A:VAL:HG22	1:698:A:VAL:HA	9	0.33
(3,642)	1:701:A:VAL:HG23	1:698:A:VAL:HA	9	0.33
(3,622)	1:697:A:ILE:HG21	1:698:A:VAL:HA	10	0.33
(3,622)	1:697:A:ILE:HG22	1:698:A:VAL:HA	10	0.33
(3,622)	1:697:A:ILE:HG23	1:698:A:VAL:HA	10	0.33
(3,612)	1:695:A:LEU:H	1:694:A:GLY:H	4	0.33
(3,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	8	0.33
(3,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	8	0.33
(3,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	8	0.33
(3,592)	1:687:A:ILE:HG21	1:691:A:SER:HG	12	0.33
(3,592)	1:687:A:ILE:HG22	1:691:A:SER:HG	12	0.33
(3,592)	1:687:A:ILE:HG23	1:691:A:SER:HG	12	0.33
(3,482)	1:672:A:TRP:H	1:671:A:ASN:H	6	0.33
(3,408)	1:697:A:ILE:HG21	1:698:A:VAL:HA	10	0.33
(3,408)	1:697:A:ILE:HG22	1:698:A:VAL:HA	10	0.33
(3,408)	1:697:A:ILE:HG23	1:698:A:VAL:HA	10	0.33
(3,378)	1:687:A:ILE:HG21	1:691:A:SER:HG	12	0.33
(3,378)	1:687:A:ILE:HG22	1:691:A:SER:HG	12	0.33
(3,378)	1:687:A:ILE:HG23	1:691:A:SER:HG	12	0.33
(3,259)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	11	0.33
(3,259)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	11	0.33
(3,259)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	11	0.33
(3,259)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	11	0.33
(3,259)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	11	0.33
(3,259)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	11	0.33
(3,194)	1:697:A:ILE:HG21	1:698:A:VAL:HA	10	0.33
(3,194)	1:697:A:ILE:HG22	1:698:A:VAL:HA	10	0.33
(3,194)	1:697:A:ILE:HG23	1:698:A:VAL:HA	10	0.33
(3,175)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	14	0.33
(3,175)	1:692:A:LEU:HD13	1:696:A:ARG:HH12	14	0.33
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	6	0.33
(3,622)	1:697:A:ILE:HG21	1:698:A:VAL:HA	3	0.32
(3,622)	1:697:A:ILE:HG22	1:698:A:VAL:HA	3	0.32
(3,622)	1:697:A:ILE:HG23	1:698:A:VAL:HA	3	0.32
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	10	0.32
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	10	0.32
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	10	0.32
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	10	0.32
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	10	0.32
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,554)	1:704:A:LEU:HD11	1:707:A:ARG:HE	11	0.32
(3,554)	1:704:A:LEU:HD12	1:707:A:ARG:HE	11	0.32
(3,554)	1:704:A:LEU:HD13	1:707:A:ARG:HE	11	0.32
(3,408)	1:697:A:ILE:HG21	1:698:A:VAL:HA	3	0.32
(3,408)	1:697:A:ILE:HG22	1:698:A:VAL:HA	3	0.32
(3,408)	1:697:A:ILE:HG23	1:698:A:VAL:HA	3	0.32
(3,194)	1:697:A:ILE:HG21	1:698:A:VAL:HA	3	0.32
(3,194)	1:697:A:ILE:HG22	1:698:A:VAL:HA	3	0.32
(3,194)	1:697:A:ILE:HG23	1:698:A:VAL:HA	3	0.32
(3,641)	1:701:A:VAL:HG11	1:698:A:VAL:HA	12	0.31
(3,641)	1:701:A:VAL:HG12	1:698:A:VAL:HA	12	0.31
(3,641)	1:701:A:VAL:HG13	1:698:A:VAL:HA	12	0.31
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG21	13	0.31
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG22	13	0.31
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG23	13	0.31
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG21	13	0.31
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG22	13	0.31
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG23	13	0.31
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG21	13	0.31
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG22	13	0.31
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG23	13	0.31
(3,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	7	0.31
(3,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	7	0.31
(3,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	7	0.31
(3,482)	1:672:A:TRP:H	1:671:A:ASN:H	11	0.31
(3,351)	1:705:A:VAL:HG21	1:702:A:LEU:HG	12	0.31
(3,351)	1:705:A:VAL:HG22	1:702:A:LEU:HG	12	0.31
(3,351)	1:705:A:VAL:HG23	1:702:A:LEU:HG	12	0.31
(3,337)	1:704:A:LEU:H	1:704:A:LEU:HB2	14	0.31
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	14	0.31
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	11	0.31
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	4	0.3
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	4	0.3
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	4	0.3
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	4	0.3
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	4	0.3
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	4	0.3
(3,506)	1:681:A:TYR:H	1:680:A:TRP:H	10	0.3
(3,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	14	0.3
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	2	0.3
(3,339)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	2	0.3
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,339)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	2	0.3
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	2	0.3
(3,339)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	2	0.3
(3,292)	1:681:A:TYR:H	1:680:A:TRP:H	10	0.3
(3,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	8	0.3
(3,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	8	0.3
(3,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	8	0.3
(3,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	8	0.3
(3,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	8	0.3
(3,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	8	0.3
(3,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	8	0.3
(3,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	8	0.3
(3,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	8	0.3
(3,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	8	0.3
(3,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	8	0.3
(3,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	8	0.3
(3,78)	1:681:A:TYR:H	1:680:A:TRP:H	10	0.3
(3,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	14	0.3
(1,21)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	14	0.3
(1,20)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	14	0.3
(1,19)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	14	0.3
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	8	0.29
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	8	0.29
(3,623)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	8	0.29
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	8	0.29
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	8	0.29
(3,623)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	8	0.29
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	8	0.29
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	8	0.29
(3,623)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	8	0.29
(3,619)	1:696:A:ARG:H	1:695:A:LEU:H	3	0.29
(3,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	13	0.29
(3,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	13	0.29
(3,567)	1:706:A:ASN:H	1:703:A:SER:HA	2	0.29
(3,405)	1:696:A:ARG:H	1:695:A:LEU:H	3	0.29
(3,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	13	0.29
(3,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	13	0.29
(3,337)	1:704:A:LEU:H	1:704:A:LEU:HB2	1	0.29
(3,337)	1:704:A:LEU:H	1:704:A:LEU:HB2	4	0.29
(3,191)	1:696:A:ARG:H	1:695:A:LEU:H	3	0.29
(3,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	13	0.29
(3,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,612)	1:695:A:LEU:H	1:694:A:GLY:H	14	0.28
(3,598)	1:690:A:GLY:H	1:689:A:VAL:H	6	0.28
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	11	0.28
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	11	0.28
(3,593)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	11	0.28
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	11	0.28
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	11	0.28
(3,593)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	11	0.28
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	11	0.28
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	11	0.28
(3,593)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	11	0.28
(3,531)	1:689:A:VAL:H	1:690:A:GLY:H	6	0.28
(3,506)	1:681:A:TYR:H	1:680:A:TRP:H	6	0.28
(3,384)	1:690:A:GLY:H	1:689:A:VAL:H	6	0.28
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	11	0.28
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	11	0.28
(3,379)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	11	0.28
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	11	0.28
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	11	0.28
(3,379)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	11	0.28
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	11	0.28
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	11	0.28
(3,379)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	11	0.28
(3,348)	1:705:A:VAL:HG11	1:706:A:ASN:HA	13	0.28
(3,348)	1:705:A:VAL:HG12	1:706:A:ASN:HA	13	0.28
(3,348)	1:705:A:VAL:HG13	1:706:A:ASN:HA	13	0.28
(3,337)	1:704:A:LEU:H	1:704:A:LEU:HB2	6	0.28
(3,337)	1:704:A:LEU:H	1:704:A:LEU:HB2	8	0.28
(3,292)	1:681:A:TYR:H	1:680:A:TRP:H	6	0.28
(3,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	9	0.28
(3,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	9	0.28
(3,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	9	0.28
(3,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	9	0.28
(3,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	9	0.28
(3,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	9	0.28
(3,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	9	0.28
(3,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	9	0.28
(3,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	9	0.28
(3,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	9	0.28
(3,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	9	0.28
(3,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	9	0.28
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,78)	1:681:A:TYR:H	1:680:A:TRP:H	6	0.28
(3,619)	1:696:A:ARG:H	1:695:A:LEU:H	4	0.27
(3,612)	1:695:A:LEU:H	1:694:A:GLY:H	2	0.27
(3,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	4	0.27
(3,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	4	0.27
(3,573)	1:707:A:ARG:H	1:704:A:LEU:HA	3	0.27
(3,573)	1:707:A:ARG:H	1:704:A:LEU:HA	7	0.27
(3,444)	1:665:A:LYS:H	1:664:A:ASP:HA	5	0.27
(3,405)	1:696:A:ARG:H	1:695:A:LEU:H	4	0.27
(3,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	4	0.27
(3,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	4	0.27
(3,351)	1:705:A:VAL:HG21	1:702:A:LEU:HG	5	0.27
(3,351)	1:705:A:VAL:HG22	1:702:A:LEU:HG	5	0.27
(3,351)	1:705:A:VAL:HG23	1:702:A:LEU:HG	5	0.27
(3,337)	1:704:A:LEU:H	1:704:A:LEU:HB2	10	0.27
(3,230)	1:665:A:LYS:H	1:664:A:ASP:HA	5	0.27
(3,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	14	0.27
(3,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	14	0.27
(3,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	14	0.27
(3,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	14	0.27
(3,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	14	0.27
(3,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	14	0.27
(3,191)	1:696:A:ARG:H	1:695:A:LEU:H	4	0.27
(3,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	4	0.27
(3,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	4	0.27
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	9	0.27
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	5	0.27
(3,619)	1:696:A:ARG:H	1:695:A:LEU:H	7	0.26
(3,612)	1:695:A:LEU:H	1:694:A:GLY:H	10	0.26
(3,568)	1:706:A:ASN:H	1:704:A:LEU:H	4	0.26
(3,545)	1:704:A:LEU:H	1:701:A:VAL:HA	10	0.26
(3,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	8	0.26
(3,468)	1:669:A:LEU:H	1:666:A:TRP:HA	6	0.26
(3,405)	1:696:A:ARG:H	1:695:A:LEU:H	7	0.26
(3,351)	1:705:A:VAL:HG21	1:702:A:LEU:HG	13	0.26
(3,351)	1:705:A:VAL:HG22	1:702:A:LEU:HG	13	0.26
(3,351)	1:705:A:VAL:HG23	1:702:A:LEU:HG	13	0.26
(3,348)	1:705:A:VAL:HG11	1:706:A:ASN:HA	9	0.26
(3,348)	1:705:A:VAL:HG12	1:706:A:ASN:HA	9	0.26
(3,348)	1:705:A:VAL:HG13	1:706:A:ASN:HA	9	0.26
(3,348)	1:705:A:VAL:HG11	1:706:A:ASN:HA	10	0.26
(3,348)	1:705:A:VAL:HG12	1:706:A:ASN:HA	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,348)	1:705:A:VAL:HG13	1:706:A:ASN:HA	10	0.26
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	10	0.26
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	10	0.26
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	10	0.26
(3,254)	1:669:A:LEU:H	1:666:A:TRP:HA	6	0.26
(3,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	9	0.26
(3,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	9	0.26
(3,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	9	0.26
(3,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	9	0.26
(3,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	9	0.26
(3,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	9	0.26
(3,191)	1:696:A:ARG:H	1:695:A:LEU:H	7	0.26
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	4	0.26
(3,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	8	0.26
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	10	0.26
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	10	0.26
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	10	0.26
(3,40)	1:669:A:LEU:H	1:666:A:TRP:HA	6	0.26
(3,598)	1:690:A:GLY:H	1:689:A:VAL:H	1	0.25
(3,598)	1:690:A:GLY:H	1:689:A:VAL:H	3	0.25
(3,597)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	11	0.25
(3,597)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	11	0.25
(3,597)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	11	0.25
(3,597)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	11	0.25
(3,597)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	11	0.25
(3,597)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	11	0.25
(3,545)	1:704:A:LEU:H	1:701:A:VAL:HA	5	0.25
(3,531)	1:689:A:VAL:H	1:690:A:GLY:H	1	0.25
(3,531)	1:689:A:VAL:H	1:690:A:GLY:H	3	0.25
(3,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	12	0.25
(3,384)	1:690:A:GLY:H	1:689:A:VAL:H	1	0.25
(3,384)	1:690:A:GLY:H	1:689:A:VAL:H	3	0.25
(3,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	4	0.25
(3,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	4	0.25
(3,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	4	0.25
(3,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	4	0.25
(3,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	4	0.25
(3,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	4	0.25
(3,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	4	0.25
(3,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	4	0.25
(3,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	4	0.25
(3,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	4	0.25
(3,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	4	0.25
(3,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	4	0.25
(3,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	4	0.25
(3,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	4	0.25
(3,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	4	0.25
(3,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	4	0.25
(3,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	4	0.25
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	1	0.25
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	3	0.25
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	3	0.25
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	11	0.25
(3,80)	1:682:A:ILE:HG21	1:679:A:LEU:H	8	0.25
(3,80)	1:682:A:ILE:HG22	1:679:A:LEU:H	8	0.25
(3,80)	1:682:A:ILE:HG23	1:679:A:LEU:H	8	0.25
(3,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	12	0.25
(3,619)	1:696:A:ARG:H	1:695:A:LEU:H	8	0.24
(3,619)	1:696:A:ARG:H	1:695:A:LEU:H	9	0.24
(3,619)	1:696:A:ARG:H	1:695:A:LEU:H	10	0.24
(3,619)	1:696:A:ARG:H	1:695:A:LEU:H	12	0.24
(3,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	6	0.24
(3,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	6	0.24
(3,591)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	6	0.24
(3,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	6	0.24
(3,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	6	0.24
(3,591)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	6	0.24
(3,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	6	0.24
(3,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	6	0.24
(3,591)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	6	0.24
(3,567)	1:706:A:ASN:H	1:703:A:SER:HA	6	0.24
(3,444)	1:665:A:LYS:H	1:664:A:ASP:HA	13	0.24
(3,405)	1:696:A:ARG:H	1:695:A:LEU:H	8	0.24
(3,405)	1:696:A:ARG:H	1:695:A:LEU:H	9	0.24
(3,405)	1:696:A:ARG:H	1:695:A:LEU:H	10	0.24
(3,405)	1:696:A:ARG:H	1:695:A:LEU:H	12	0.24
(3,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	6	0.24
(3,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	6	0.24
(3,377)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	6	0.24
(3,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	6	0.24
(3,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	6	0.24
(3,377)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	6	0.24
(3,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	6	0.24
(3,377)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	6	0.24
(3,230)	1:665:A:LYS:H	1:664:A:ASP:HA	13	0.24
(3,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	13	0.24
(3,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	13	0.24
(3,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	13	0.24
(3,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	13	0.24
(3,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	13	0.24
(3,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	13	0.24
(3,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	13	0.24
(3,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	13	0.24
(3,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	13	0.24
(3,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	13	0.24
(3,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	13	0.24
(3,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	13	0.24
(3,191)	1:696:A:ARG:H	1:695:A:LEU:H	8	0.24
(3,191)	1:696:A:ARG:H	1:695:A:LEU:H	9	0.24
(3,191)	1:696:A:ARG:H	1:695:A:LEU:H	10	0.24
(3,191)	1:696:A:ARG:H	1:695:A:LEU:H	12	0.24
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	13	0.24
(3,632)	1:700:A:ALA:H	1:699:A:PHE:HA	2	0.23
(3,602)	1:692:A:LEU:HD11	1:691:A:SER:HB2	11	0.23
(3,602)	1:692:A:LEU:HD11	1:691:A:SER:HB3	11	0.23
(3,602)	1:692:A:LEU:HD12	1:691:A:SER:HB2	11	0.23
(3,602)	1:692:A:LEU:HD12	1:691:A:SER:HB3	11	0.23
(3,602)	1:692:A:LEU:HD13	1:691:A:SER:HB2	11	0.23
(3,602)	1:692:A:LEU:HD13	1:691:A:SER:HB3	11	0.23
(3,597)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	8	0.23
(3,597)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	8	0.23
(3,597)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	8	0.23
(3,597)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	8	0.23
(3,597)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	8	0.23
(3,597)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	8	0.23
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD11	11	0.23
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD12	11	0.23
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD13	11	0.23
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD21	11	0.23
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD22	11	0.23
(3,581)	1:707:A:ARG:HE	1:704:A:LEU:HD23	11	0.23
(3,565)	1:705:A:VAL:HG21	1:702:A:LEU:HG	3	0.23
(3,565)	1:705:A:VAL:HG22	1:702:A:LEU:HG	3	0.23
(3,565)	1:705:A:VAL:HG23	1:702:A:LEU:HG	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,444)	1:665:A:LYS:H	1:664:A:ASP:HA	3	0.23
(3,418)	1:700:A:ALA:H	1:699:A:PHE:HA	2	0.23
(3,388)	1:692:A:LEU:HD11	1:691:A:SER:HB2	11	0.23
(3,388)	1:692:A:LEU:HD11	1:691:A:SER:HB3	11	0.23
(3,388)	1:692:A:LEU:HD12	1:691:A:SER:HB2	11	0.23
(3,388)	1:692:A:LEU:HD12	1:691:A:SER:HB3	11	0.23
(3,388)	1:692:A:LEU:HD13	1:691:A:SER:HB2	11	0.23
(3,388)	1:692:A:LEU:HD13	1:691:A:SER:HB3	11	0.23
(3,348)	1:705:A:VAL:HG11	1:706:A:ASN:HA	6	0.23
(3,348)	1:705:A:VAL:HG12	1:706:A:ASN:HA	6	0.23
(3,348)	1:705:A:VAL:HG13	1:706:A:ASN:HA	6	0.23
(3,337)	1:704:A:LEU:H	1:704:A:LEU:HB2	2	0.23
(3,337)	1:704:A:LEU:H	1:704:A:LEU:HB2	11	0.23
(3,289)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	14	0.23
(3,289)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	14	0.23
(3,289)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	14	0.23
(3,289)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	14	0.23
(3,289)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	14	0.23
(3,289)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	14	0.23
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	9	0.23
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	9	0.23
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	9	0.23
(3,230)	1:665:A:LYS:H	1:664:A:ASP:HA	3	0.23
(3,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	2	0.23
(3,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	2	0.23
(3,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	2	0.23
(3,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	2	0.23
(3,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	2	0.23
(3,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	2	0.23
(3,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	2	0.23
(3,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	2	0.23
(3,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	2	0.23
(3,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	2	0.23
(3,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	2	0.23
(3,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	2	0.23
(3,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	12	0.23
(3,215)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	12	0.23
(3,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	12	0.23
(3,215)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	12	0.23
(3,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	12	0.23
(3,215)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	12	0.23
(3,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,215)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	12	0.23
(3,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	12	0.23
(3,215)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	12	0.23
(3,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	12	0.23
(3,215)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	12	0.23
(3,204)	1:700:A:ALA:H	1:699:A:PHE:HA	2	0.23
(3,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	3	0.23
(3,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	3	0.23
(3,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	3	0.23
(3,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	3	0.23
(3,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	3	0.23
(3,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	3	0.23
(3,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	1	0.23
(3,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	1	0.23
(3,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	1	0.23
(3,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	1	0.23
(3,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	1	0.23
(3,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	1	0.23
(3,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	2	0.23
(3,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	2	0.23
(3,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	2	0.23
(3,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	2	0.23
(3,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	2	0.23
(3,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	2	0.23
(3,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	13	0.23
(3,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	13	0.23
(3,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	13	0.23
(3,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	13	0.23
(3,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	13	0.23
(3,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	13	0.23
(3,174)	1:692:A:LEU:HD11	1:691:A:SER:HB2	11	0.23
(3,174)	1:692:A:LEU:HD11	1:691:A:SER:HB3	11	0.23
(3,174)	1:692:A:LEU:HD12	1:691:A:SER:HB2	11	0.23
(3,174)	1:692:A:LEU:HD12	1:691:A:SER:HB3	11	0.23
(3,174)	1:692:A:LEU:HD13	1:691:A:SER:HB2	11	0.23
(3,174)	1:692:A:LEU:HD13	1:691:A:SER:HB3	11	0.23
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	6	0.23
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	1	0.23
(3,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	14	0.23
(3,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	14	0.23
(3,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	14	0.23
(3,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	14	0.23
(3,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	14	0.23
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	9	0.23
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	9	0.23
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	9	0.23
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	9	0.23
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	9	0.23
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	9	0.23
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	9	0.23
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	9	0.23
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	9	0.23
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	3	0.23
(3,632)	1:700:A:ALA:H	1:699:A:PHE:HA	4	0.22
(3,632)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.22
(3,619)	1:696:A:ARG:H	1:695:A:LEU:H	1	0.22
(3,619)	1:696:A:ARG:H	1:695:A:LEU:H	11	0.22
(3,619)	1:696:A:ARG:H	1:695:A:LEU:H	13	0.22
(3,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	11	0.22
(3,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	11	0.22
(3,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	11	0.22
(3,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	1	0.22
(3,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	1	0.22
(3,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	1	0.22
(3,600)	1:692:A:LEU:HD11	1:689:A:VAL:HA	9	0.22
(3,600)	1:692:A:LEU:HD12	1:689:A:VAL:HA	9	0.22
(3,600)	1:692:A:LEU:HD13	1:689:A:VAL:HA	9	0.22
(3,598)	1:690:A:GLY:H	1:689:A:VAL:H	12	0.22
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	9	0.22
(3,596)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	9	0.22
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	9	0.22
(3,596)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	9	0.22
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	9	0.22
(3,596)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	9	0.22
(3,579)	1:707:A:ARG:H	1:707:A:ARG:HG2	8	0.22
(3,579)	1:707:A:ARG:H	1:707:A:ARG:HG3	8	0.22
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	1	0.22
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	1	0.22
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	1	0.22
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	1	0.22
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	1	0.22
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	1	0.22
(3,531)	1:689:A:VAL:H	1:690:A:GLY:H	12	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	5	0.22
(3,512)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	5	0.22
(3,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	5	0.22
(3,512)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	5	0.22
(3,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	5	0.22
(3,512)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	5	0.22
(3,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	5	0.22
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	9	0.22
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	9	0.22
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	9	0.22
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	9	0.22
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	9	0.22
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	9	0.22
(3,444)	1:665:A:LYS:H	1:664:A:ASP:HA	12	0.22
(3,418)	1:700:A:ALA:H	1:699:A:PHE:HA	4	0.22
(3,418)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.22
(3,405)	1:696:A:ARG:H	1:695:A:LEU:H	1	0.22
(3,405)	1:696:A:ARG:H	1:695:A:LEU:H	11	0.22
(3,405)	1:696:A:ARG:H	1:695:A:LEU:H	13	0.22
(3,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	11	0.22
(3,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	11	0.22
(3,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	11	0.22
(3,384)	1:690:A:GLY:H	1:689:A:VAL:H	12	0.22
(3,365)	1:707:A:ARG:H	1:707:A:ARG:HG2	8	0.22
(3,365)	1:707:A:ARG:H	1:707:A:ARG:HG3	8	0.22
(3,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	5	0.22
(3,298)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	5	0.22
(3,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	5	0.22
(3,298)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	5	0.22
(3,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	5	0.22
(3,298)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	5	0.22
(3,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	1	0.22
(3,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	1	0.22
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	6	0.22
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	6	0.22
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	6	0.22
(3,230)	1:665:A:LYS:H	1:664:A:ASP:HA	12	0.22
(3,204)	1:700:A:ALA:H	1:699:A:PHE:HA	4	0.22
(3,204)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.22
(3,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	9	0.22
(3,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	9	0.22
(3,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	9	0.22
(3,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	9	0.22
(3,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	9	0.22
(3,191)	1:696:A:ARG:H	1:695:A:LEU:H	1	0.22
(3,191)	1:696:A:ARG:H	1:695:A:LEU:H	11	0.22
(3,191)	1:696:A:ARG:H	1:695:A:LEU:H	13	0.22
(3,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	11	0.22
(3,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	11	0.22
(3,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	11	0.22
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HG2	8	0.22
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HG3	8	0.22
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	1	0.22
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	1	0.22
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	1	0.22
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	1	0.22
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	1	0.22
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	1	0.22
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	12	0.22
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	3	0.22
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	5	0.22
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	10	0.22
(3,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	5	0.22
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	6	0.22
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	6	0.22
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	6	0.22
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	12	0.22
(3,632)	1:700:A:ALA:H	1:699:A:PHE:HA	1	0.21
(3,632)	1:700:A:ALA:H	1:699:A:PHE:HA	3	0.21
(3,632)	1:700:A:ALA:H	1:699:A:PHE:HA	6	0.21
(3,632)	1:700:A:ALA:H	1:699:A:PHE:HA	9	0.21
(3,632)	1:700:A:ALA:H	1:699:A:PHE:HA	10	0.21
(3,632)	1:700:A:ALA:H	1:699:A:PHE:HA	13	0.21
(3,619)	1:696:A:ARG:H	1:695:A:LEU:H	6	0.21
(3,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	5	0.21
(3,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	5	0.21
(3,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	5	0.21
(3,598)	1:690:A:GLY:H	1:689:A:VAL:H	13	0.21
(3,567)	1:706:A:ASN:H	1:703:A:SER:HA	8	0.21
(3,554)	1:704:A:LEU:HD11	1:707:A:ARG:HE	4	0.21
(3,554)	1:704:A:LEU:HD12	1:707:A:ARG:HE	4	0.21
(3,554)	1:704:A:LEU:HD13	1:707:A:ARG:HE	4	0.21
(3,545)	1:704:A:LEU:H	1:701:A:VAL:HA	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,531)	1:689:A:VAL:H	1:690:A:GLY:H	13	0.21
(3,482)	1:672:A:TRP:H	1:671:A:ASN:H	2	0.21
(3,444)	1:665:A:LYS:H	1:664:A:ASP:HA	9	0.21
(3,439)	1:664:A:ASP:H	1:663:A:LEU:HA	2	0.21
(3,439)	1:664:A:ASP:H	1:663:A:LEU:HA	8	0.21
(3,439)	1:664:A:ASP:H	1:663:A:LEU:HA	9	0.21
(3,439)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.21
(3,418)	1:700:A:ALA:H	1:699:A:PHE:HA	1	0.21
(3,418)	1:700:A:ALA:H	1:699:A:PHE:HA	3	0.21
(3,418)	1:700:A:ALA:H	1:699:A:PHE:HA	6	0.21
(3,418)	1:700:A:ALA:H	1:699:A:PHE:HA	9	0.21
(3,418)	1:700:A:ALA:H	1:699:A:PHE:HA	10	0.21
(3,418)	1:700:A:ALA:H	1:699:A:PHE:HA	13	0.21
(3,405)	1:696:A:ARG:H	1:695:A:LEU:H	6	0.21
(3,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	5	0.21
(3,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	5	0.21
(3,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	5	0.21
(3,384)	1:690:A:GLY:H	1:689:A:VAL:H	13	0.21
(3,271)	1:672:A:TRP:HE1	1:671:A:ASN:H	8	0.21
(3,267)	1:671:A:ASN:H	1:672:A:TRP:HE1	8	0.21
(3,230)	1:665:A:LYS:H	1:664:A:ASP:HA	9	0.21
(3,225)	1:664:A:ASP:H	1:663:A:LEU:HA	2	0.21
(3,225)	1:664:A:ASP:H	1:663:A:LEU:HA	8	0.21
(3,225)	1:664:A:ASP:H	1:663:A:LEU:HA	9	0.21
(3,225)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.21
(3,204)	1:700:A:ALA:H	1:699:A:PHE:HA	1	0.21
(3,204)	1:700:A:ALA:H	1:699:A:PHE:HA	3	0.21
(3,204)	1:700:A:ALA:H	1:699:A:PHE:HA	6	0.21
(3,204)	1:700:A:ALA:H	1:699:A:PHE:HA	9	0.21
(3,204)	1:700:A:ALA:H	1:699:A:PHE:HA	10	0.21
(3,204)	1:700:A:ALA:H	1:699:A:PHE:HA	13	0.21
(3,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	1	0.21
(3,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	1	0.21
(3,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	1	0.21
(3,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	1	0.21
(3,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	1	0.21
(3,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	1	0.21
(3,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	3	0.21
(3,198)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	3	0.21
(3,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	3	0.21
(3,198)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	3	0.21
(3,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,198)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	3	0.21
(3,191)	1:696:A:ARG:H	1:695:A:LEU:H	6	0.21
(3,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	5	0.21
(3,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	5	0.21
(3,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	5	0.21
(3,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	9	0.21
(3,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	9	0.21
(3,163)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	9	0.21
(3,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	9	0.21
(3,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	9	0.21
(3,163)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	9	0.21
(3,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	9	0.21
(3,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	9	0.21
(3,163)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	9	0.21
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	13	0.21
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	9	0.21
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	10	0.21
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	13	0.21
(3,57)	1:672:A:TRP:HE1	1:671:A:ASN:H	8	0.21
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	14	0.21
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	14	0.21
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	14	0.21
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	14	0.21
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	14	0.21
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	14	0.21
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	2	0.21
(3,53)	1:671:A:ASN:H	1:672:A:TRP:HE1	8	0.21
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	13	0.21
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	13	0.21
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	13	0.21
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	13	0.21
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	13	0.21
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	13	0.21
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	9	0.21
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	2	0.21
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	8	0.21
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	9	0.21
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.21
(3,632)	1:700:A:ALA:H	1:699:A:PHE:HA	5	0.2
(3,632)	1:700:A:ALA:H	1:699:A:PHE:HA	7	0.2
(3,632)	1:700:A:ALA:H	1:699:A:PHE:HA	8	0.2
(3,632)	1:700:A:ALA:H	1:699:A:PHE:HA	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	4	0.2
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	4	0.2
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	4	0.2
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	4	0.2
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	4	0.2
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	4	0.2
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	13	0.2
(3,621)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	13	0.2
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	13	0.2
(3,621)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	13	0.2
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	13	0.2
(3,621)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	13	0.2
(3,619)	1:696:A:ARG:H	1:695:A:LEU:H	14	0.2
(3,579)	1:707:A:ARG:H	1:707:A:ARG:HG2	6	0.2
(3,579)	1:707:A:ARG:H	1:707:A:ARG:HG3	6	0.2
(3,545)	1:704:A:LEU:H	1:701:A:VAL:HA	13	0.2
(3,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	6	0.2
(3,482)	1:672:A:TRP:H	1:671:A:ASN:H	10	0.2
(3,482)	1:672:A:TRP:H	1:671:A:ASN:H	13	0.2
(3,482)	1:672:A:TRP:H	1:671:A:ASN:H	14	0.2
(3,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	5	0.2
(3,444)	1:665:A:LYS:H	1:664:A:ASP:HA	1	0.2
(3,443)	1:665:A:LYS:H	1:662:A:GLU:HA	12	0.2
(3,439)	1:664:A:ASP:H	1:663:A:LEU:HA	4	0.2
(3,439)	1:664:A:ASP:H	1:663:A:LEU:HA	7	0.2
(3,439)	1:664:A:ASP:H	1:663:A:LEU:HA	11	0.2
(3,422)	1:700:A:ALA:HB1	1:697:A:ILE:HA	10	0.2
(3,422)	1:700:A:ALA:HB2	1:697:A:ILE:HA	10	0.2
(3,422)	1:700:A:ALA:HB3	1:697:A:ILE:HA	10	0.2
(3,418)	1:700:A:ALA:H	1:699:A:PHE:HA	5	0.2
(3,418)	1:700:A:ALA:H	1:699:A:PHE:HA	7	0.2
(3,418)	1:700:A:ALA:H	1:699:A:PHE:HA	8	0.2
(3,418)	1:700:A:ALA:H	1:699:A:PHE:HA	11	0.2
(3,405)	1:696:A:ARG:H	1:695:A:LEU:H	14	0.2
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	14	0.2
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	14	0.2
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	14	0.2
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	14	0.2
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	14	0.2
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	14	0.2
(3,365)	1:707:A:ARG:H	1:707:A:ARG:HG2	6	0.2
(3,365)	1:707:A:ARG:H	1:707:A:ARG:HG3	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	1	0.2
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	1	0.2
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	1	0.2
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	11	0.2
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	11	0.2
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	11	0.2
(3,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	5	0.2
(3,230)	1:665:A:LYS:H	1:664:A:ASP:HA	1	0.2
(3,229)	1:665:A:LYS:H	1:662:A:GLU:HA	12	0.2
(3,225)	1:664:A:ASP:H	1:663:A:LEU:HA	4	0.2
(3,225)	1:664:A:ASP:H	1:663:A:LEU:HA	7	0.2
(3,225)	1:664:A:ASP:H	1:663:A:LEU:HA	11	0.2
(3,204)	1:700:A:ALA:H	1:699:A:PHE:HA	5	0.2
(3,204)	1:700:A:ALA:H	1:699:A:PHE:HA	7	0.2
(3,204)	1:700:A:ALA:H	1:699:A:PHE:HA	8	0.2
(3,204)	1:700:A:ALA:H	1:699:A:PHE:HA	11	0.2
(3,191)	1:696:A:ARG:H	1:695:A:LEU:H	14	0.2
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	14	0.2
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	14	0.2
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	14	0.2
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	14	0.2
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	14	0.2
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	14	0.2
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HG2	6	0.2
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HG3	6	0.2
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	12	0.2
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	14	0.2
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	7	0.2
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	12	0.2
(3,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	6	0.2
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	1	0.2
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	1	0.2
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	1	0.2
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	11	0.2
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	11	0.2
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	11	0.2
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	10	0.2
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	13	0.2
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	14	0.2
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	2	0.2
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	2	0.2
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	2	0.2
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	2	0.2
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	2	0.2
(3,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	5	0.2
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	1	0.2
(3,15)	1:665:A:LYS:H	1:662:A:GLU:HA	12	0.2
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	4	0.2
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	7	0.2
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	11	0.2
(3,632)	1:700:A:ALA:H	1:699:A:PHE:HA	12	0.19
(3,620)	1:696:A:ARG:H	1:696:A:ARG:HE	14	0.19
(3,619)	1:696:A:ARG:H	1:695:A:LEU:H	2	0.19
(3,602)	1:692:A:LEU:HD11	1:691:A:SER:HB2	8	0.19
(3,602)	1:692:A:LEU:HD11	1:691:A:SER:HB3	8	0.19
(3,602)	1:692:A:LEU:HD12	1:691:A:SER:HB2	8	0.19
(3,602)	1:692:A:LEU:HD12	1:691:A:SER:HB3	8	0.19
(3,602)	1:692:A:LEU:HD13	1:691:A:SER:HB2	8	0.19
(3,602)	1:692:A:LEU:HD13	1:691:A:SER:HB3	8	0.19
(3,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	13	0.19
(3,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	13	0.19
(3,505)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	13	0.19
(3,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	9	0.19
(3,482)	1:672:A:TRP:H	1:671:A:ASN:H	3	0.19
(3,482)	1:672:A:TRP:H	1:671:A:ASN:H	7	0.19
(3,448)	1:665:A:LYS:H	1:666:A:TRP:HD1	14	0.19
(3,443)	1:665:A:LYS:H	1:662:A:GLU:HA	3	0.19
(3,439)	1:664:A:ASP:H	1:663:A:LEU:HA	5	0.19
(3,439)	1:664:A:ASP:H	1:663:A:LEU:HA	6	0.19
(3,439)	1:664:A:ASP:H	1:663:A:LEU:HA	10	0.19
(3,418)	1:700:A:ALA:H	1:699:A:PHE:HA	12	0.19
(3,406)	1:696:A:ARG:H	1:696:A:ARG:HE	14	0.19
(3,405)	1:696:A:ARG:H	1:695:A:LEU:H	2	0.19
(3,388)	1:692:A:LEU:HD11	1:691:A:SER:HB2	8	0.19
(3,388)	1:692:A:LEU:HD11	1:691:A:SER:HB3	8	0.19
(3,388)	1:692:A:LEU:HD12	1:691:A:SER:HB2	8	0.19
(3,388)	1:692:A:LEU:HD12	1:691:A:SER:HB3	8	0.19
(3,388)	1:692:A:LEU:HD13	1:691:A:SER:HB2	8	0.19
(3,388)	1:692:A:LEU:HD13	1:691:A:SER:HB3	8	0.19
(3,351)	1:705:A:VAL:HG21	1:702:A:LEU:HG	9	0.19
(3,351)	1:705:A:VAL:HG22	1:702:A:LEU:HG	9	0.19
(3,351)	1:705:A:VAL:HG23	1:702:A:LEU:HG	9	0.19
(3,348)	1:705:A:VAL:HG11	1:706:A:ASN:HA	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,348)	1:705:A:VAL:HG12	1:706:A:ASN:HA	12	0.19
(3,348)	1:705:A:VAL:HG13	1:706:A:ASN:HA	12	0.19
(3,348)	1:705:A:VAL:HG11	1:706:A:ASN:HA	14	0.19
(3,348)	1:705:A:VAL:HG12	1:706:A:ASN:HA	14	0.19
(3,348)	1:705:A:VAL:HG13	1:706:A:ASN:HA	14	0.19
(3,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	13	0.19
(3,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	13	0.19
(3,291)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	13	0.19
(3,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	10	0.19
(3,290)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	10	0.19
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	2	0.19
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	2	0.19
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	2	0.19
(3,234)	1:665:A:LYS:H	1:666:A:TRP:HD1	14	0.19
(3,229)	1:665:A:LYS:H	1:662:A:GLU:HA	3	0.19
(3,225)	1:664:A:ASP:H	1:663:A:LEU:HA	5	0.19
(3,225)	1:664:A:ASP:H	1:663:A:LEU:HA	6	0.19
(3,225)	1:664:A:ASP:H	1:663:A:LEU:HA	10	0.19
(3,204)	1:700:A:ALA:H	1:699:A:PHE:HA	12	0.19
(3,191)	1:696:A:ARG:H	1:695:A:LEU:H	2	0.19
(3,174)	1:692:A:LEU:HD11	1:691:A:SER:HB2	8	0.19
(3,174)	1:692:A:LEU:HD11	1:691:A:SER:HB3	8	0.19
(3,174)	1:692:A:LEU:HD12	1:691:A:SER:HB2	8	0.19
(3,174)	1:692:A:LEU:HD12	1:691:A:SER:HB3	8	0.19
(3,174)	1:692:A:LEU:HD13	1:691:A:SER:HB2	8	0.19
(3,174)	1:692:A:LEU:HD13	1:691:A:SER:HB3	8	0.19
(3,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	13	0.19
(3,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	13	0.19
(3,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	13	0.19
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	6	0.19
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	12	0.19
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	2	0.19
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	6	0.19
(3,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	13	0.19
(3,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	13	0.19
(3,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	13	0.19
(3,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	9	0.19
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	2	0.19
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	2	0.19
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	2	0.19
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	3	0.19
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	6	0.19
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	6	0.19
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	6	0.19
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	6	0.19
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	6	0.19
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	6	0.19
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	12	0.19
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	12	0.19
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	12	0.19
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	12	0.19
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	12	0.19
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	12	0.19
(3,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	14	0.19
(3,15)	1:665:A:LYS:H	1:662:A:GLU:HA	3	0.19
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	5	0.19
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	6	0.19
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	10	0.19
(1,21)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	3	0.19
(1,20)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	3	0.19
(1,19)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	3	0.19
(3,641)	1:701:A:VAL:HG11	1:698:A:VAL:HA	10	0.18
(3,641)	1:701:A:VAL:HG12	1:698:A:VAL:HA	10	0.18
(3,641)	1:701:A:VAL:HG13	1:698:A:VAL:HA	10	0.18
(3,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	3	0.18
(3,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	3	0.18
(3,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	3	0.18
(3,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	8	0.18
(3,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	8	0.18
(3,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	8	0.18
(3,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	13	0.18
(3,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	13	0.18
(3,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	13	0.18
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG21	9	0.18
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG22	9	0.18
(3,601)	1:692:A:LEU:HD11	1:689:A:VAL:HG23	9	0.18
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG21	9	0.18
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG22	9	0.18
(3,601)	1:692:A:LEU:HD12	1:689:A:VAL:HG23	9	0.18
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG21	9	0.18
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG22	9	0.18
(3,601)	1:692:A:LEU:HD13	1:689:A:VAL:HG23	9	0.18
(3,598)	1:690:A:GLY:H	1:689:A:VAL:H	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	5	0.18
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	5	0.18
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	5	0.18
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	5	0.18
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	5	0.18
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	5	0.18
(3,545)	1:704:A:LEU:H	1:701:A:VAL:HA	11	0.18
(3,531)	1:689:A:VAL:H	1:690:A:GLY:H	10	0.18
(3,444)	1:665:A:LYS:H	1:664:A:ASP:HA	11	0.18
(3,444)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.18
(3,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	3	0.18
(3,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	3	0.18
(3,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	3	0.18
(3,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	8	0.18
(3,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	8	0.18
(3,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	8	0.18
(3,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	13	0.18
(3,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	13	0.18
(3,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	13	0.18
(3,384)	1:690:A:GLY:H	1:689:A:VAL:H	10	0.18
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD11	10	0.18
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD12	10	0.18
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD13	10	0.18
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD21	10	0.18
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD22	10	0.18
(3,367)	1:707:A:ARG:HE	1:704:A:LEU:HD23	10	0.18
(3,350)	1:705:A:VAL:HG21	1:701:A:VAL:HA	1	0.18
(3,350)	1:705:A:VAL:HG22	1:701:A:VAL:HA	1	0.18
(3,350)	1:705:A:VAL:HG23	1:701:A:VAL:HA	1	0.18
(3,348)	1:705:A:VAL:HG11	1:706:A:ASN:HA	7	0.18
(3,348)	1:705:A:VAL:HG12	1:706:A:ASN:HA	7	0.18
(3,348)	1:705:A:VAL:HG13	1:706:A:ASN:HA	7	0.18
(3,337)	1:704:A:LEU:H	1:704:A:LEU:HB2	3	0.18
(3,337)	1:704:A:LEU:H	1:704:A:LEU:HB2	7	0.18
(3,289)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	12	0.18
(3,289)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	12	0.18
(3,289)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	12	0.18
(3,289)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	12	0.18
(3,289)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	12	0.18
(3,289)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	12	0.18
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	5	0.18
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	5	0.18
(3,260)	1:670:A:TRP:H	1:667:A:ALA:HA	2	0.18
(3,230)	1:665:A:LYS:H	1:664:A:ASP:HA	11	0.18
(3,230)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.18
(3,196)	1:698:A:VAL:HG11	1:695:A:LEU:HA	12	0.18
(3,196)	1:698:A:VAL:HG12	1:695:A:LEU:HA	12	0.18
(3,196)	1:698:A:VAL:HG13	1:695:A:LEU:HA	12	0.18
(3,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	3	0.18
(3,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	3	0.18
(3,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	3	0.18
(3,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	3	0.18
(3,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	3	0.18
(3,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	3	0.18
(3,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	3	0.18
(3,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	3	0.18
(3,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	3	0.18
(3,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	8	0.18
(3,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	8	0.18
(3,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	8	0.18
(3,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	13	0.18
(3,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	13	0.18
(3,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	13	0.18
(3,178)	1:693:A:ILE:HD11	1:697:A:ILE:H	10	0.18
(3,178)	1:693:A:ILE:HD12	1:697:A:ILE:H	10	0.18
(3,178)	1:693:A:ILE:HD13	1:697:A:ILE:H	10	0.18
(3,175)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	5	0.18
(3,175)	1:692:A:LEU:HD11	1:696:A:ARG:HH12	5	0.18
(3,175)	1:692:A:LEU:HD12	1:696:A:ARG:HH21	8	0.18
(3,175)	1:692:A:LEU:HD12	1:696:A:ARG:HH22	8	0.18
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	5	0.18
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	5	0.18
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	5	0.18
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	5	0.18
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	5	0.18
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	5	0.18
(3,136)	1:705:A:VAL:HG21	1:701:A:VAL:HA	1	0.18
(3,136)	1:705:A:VAL:HG22	1:701:A:VAL:HA	1	0.18
(3,136)	1:705:A:VAL:HG23	1:701:A:VAL:HA	1	0.18
(3,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	9	0.18
(3,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	9	0.18
(3,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	9	0.18
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	2	0.18
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	4	0.18
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	5	0.18
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	8	0.18
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	2	0.18
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	9	0.18
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	10	0.18
(3,83)	1:682:A:ILE:HD11	1:681:A:TYR:H	10	0.18
(3,83)	1:682:A:ILE:HD12	1:681:A:TYR:H	10	0.18
(3,83)	1:682:A:ILE:HD13	1:681:A:TYR:H	10	0.18
(3,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	12	0.18
(3,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	12	0.18
(3,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	12	0.18
(3,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	12	0.18
(3,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	12	0.18
(3,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	12	0.18
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	5	0.18
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	5	0.18
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	5	0.18
(3,46)	1:670:A:TRP:H	1:667:A:ALA:HA	2	0.18
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	10	0.18
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	10	0.18
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	10	0.18
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	10	0.18
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	10	0.18
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	10	0.18
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	11	0.18
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.18
(2,66)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	5	0.18
(2,66)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	5	0.18
(2,66)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	5	0.18
(2,66)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	5	0.18
(2,66)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	5	0.18
(2,66)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	5	0.18
(2,65)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	5	0.18
(2,65)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	5	0.18
(2,65)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	5	0.18
(2,65)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	5	0.18
(2,65)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	5	0.18
(2,65)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	5	0.18
(2,64)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	5	0.18
(2,64)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,64)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	5	0.18
(2,64)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	5	0.18
(2,64)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	5	0.18
(2,64)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	5	0.18
(3,620)	1:696:A:ARG:H	1:696:A:ARG:HE	5	0.17
(3,619)	1:696:A:ARG:H	1:695:A:LEU:H	5	0.17
(3,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	4	0.17
(3,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	4	0.17
(3,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	4	0.17
(3,602)	1:692:A:LEU:HD11	1:691:A:SER:HB2	5	0.17
(3,602)	1:692:A:LEU:HD11	1:691:A:SER:HB3	5	0.17
(3,602)	1:692:A:LEU:HD12	1:691:A:SER:HB2	5	0.17
(3,602)	1:692:A:LEU:HD12	1:691:A:SER:HB3	5	0.17
(3,602)	1:692:A:LEU:HD13	1:691:A:SER:HB2	5	0.17
(3,602)	1:692:A:LEU:HD13	1:691:A:SER:HB3	5	0.17
(3,598)	1:690:A:GLY:H	1:689:A:VAL:H	2	0.17
(3,598)	1:690:A:GLY:H	1:689:A:VAL:H	4	0.17
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	3	0.17
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	3	0.17
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	3	0.17
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	3	0.17
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	3	0.17
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	3	0.17
(3,545)	1:704:A:LEU:H	1:701:A:VAL:HA	12	0.17
(3,531)	1:689:A:VAL:H	1:690:A:GLY:H	2	0.17
(3,531)	1:689:A:VAL:H	1:690:A:GLY:H	4	0.17
(3,522)	1:684:A:ILE:HG21	1:688:A:ILE:H	5	0.17
(3,522)	1:684:A:ILE:HG22	1:688:A:ILE:H	5	0.17
(3,522)	1:684:A:ILE:HG23	1:688:A:ILE:H	5	0.17
(3,516)	1:684:A:ILE:HD11	1:681:A:TYR:HA	12	0.17
(3,516)	1:684:A:ILE:HD12	1:681:A:TYR:HA	12	0.17
(3,516)	1:684:A:ILE:HD13	1:681:A:TYR:HA	12	0.17
(3,516)	1:684:A:ILE:HD11	1:681:A:TYR:HA	14	0.17
(3,516)	1:684:A:ILE:HD12	1:681:A:TYR:HA	14	0.17
(3,516)	1:684:A:ILE:HD13	1:681:A:TYR:HA	14	0.17
(3,482)	1:672:A:TRP:H	1:671:A:ASN:H	9	0.17
(3,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	3	0.17
(3,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	13	0.17
(3,448)	1:665:A:LYS:H	1:666:A:TRP:HD1	6	0.17
(3,444)	1:665:A:LYS:H	1:664:A:ASP:HA	4	0.17
(3,444)	1:665:A:LYS:H	1:664:A:ASP:HA	10	0.17
(3,406)	1:696:A:ARG:H	1:696:A:ARG:HE	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,405)	1:696:A:ARG:H	1:695:A:LEU:H	5	0.17
(3,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	3	0.17
(3,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	3	0.17
(3,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	3	0.17
(3,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	3	0.17
(3,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	3	0.17
(3,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	3	0.17
(3,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	7	0.17
(3,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	7	0.17
(3,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	7	0.17
(3,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	7	0.17
(3,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	7	0.17
(3,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	7	0.17
(3,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	4	0.17
(3,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	4	0.17
(3,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	4	0.17
(3,388)	1:692:A:LEU:HD11	1:691:A:SER:HB2	5	0.17
(3,388)	1:692:A:LEU:HD11	1:691:A:SER:HB3	5	0.17
(3,388)	1:692:A:LEU:HD12	1:691:A:SER:HB2	5	0.17
(3,388)	1:692:A:LEU:HD12	1:691:A:SER:HB3	5	0.17
(3,388)	1:692:A:LEU:HD13	1:691:A:SER:HB2	5	0.17
(3,388)	1:692:A:LEU:HD13	1:691:A:SER:HB3	5	0.17
(3,384)	1:690:A:GLY:H	1:689:A:VAL:H	2	0.17
(3,384)	1:690:A:GLY:H	1:689:A:VAL:H	4	0.17
(3,348)	1:705:A:VAL:HG11	1:706:A:ASN:HA	5	0.17
(3,348)	1:705:A:VAL:HG12	1:706:A:ASN:HA	5	0.17
(3,348)	1:705:A:VAL:HG13	1:706:A:ASN:HA	5	0.17
(3,303)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	2	0.17
(3,303)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	2	0.17
(3,303)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	2	0.17
(3,303)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	2	0.17
(3,303)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	2	0.17
(3,303)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	2	0.17
(3,302)	1:684:A:ILE:HD11	1:681:A:TYR:HA	12	0.17
(3,302)	1:684:A:ILE:HD12	1:681:A:TYR:HA	12	0.17
(3,302)	1:684:A:ILE:HD13	1:681:A:TYR:HA	12	0.17
(3,302)	1:684:A:ILE:HD11	1:681:A:TYR:HA	14	0.17
(3,302)	1:684:A:ILE:HD12	1:681:A:TYR:HA	14	0.17
(3,302)	1:684:A:ILE:HD13	1:681:A:TYR:HA	14	0.17
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	4	0.17
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	4	0.17
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,260)	1:670:A:TRP:H	1:667:A:ALA:HA	11	0.17
(3,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	3	0.17
(3,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	13	0.17
(3,234)	1:665:A:LYS:H	1:666:A:TRP:HD1	6	0.17
(3,230)	1:665:A:LYS:H	1:664:A:ASP:HA	4	0.17
(3,230)	1:665:A:LYS:H	1:664:A:ASP:HA	10	0.17
(3,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	2	0.17
(3,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	2	0.17
(3,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	2	0.17
(3,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	2	0.17
(3,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	2	0.17
(3,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	2	0.17
(3,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	13	0.17
(3,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	13	0.17
(3,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	13	0.17
(3,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	13	0.17
(3,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	13	0.17
(3,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	13	0.17
(3,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	14	0.17
(3,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	14	0.17
(3,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	14	0.17
(3,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	14	0.17
(3,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	14	0.17
(3,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	14	0.17
(3,191)	1:696:A:ARG:H	1:695:A:LEU:H	5	0.17
(3,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	3	0.17
(3,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	3	0.17
(3,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	3	0.17
(3,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	3	0.17
(3,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	3	0.17
(3,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	3	0.17
(3,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	7	0.17
(3,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	7	0.17
(3,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	7	0.17
(3,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	7	0.17
(3,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	7	0.17
(3,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	7	0.17
(3,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	4	0.17
(3,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	4	0.17
(3,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	4	0.17
(3,174)	1:692:A:LEU:HD11	1:691:A:SER:HB2	5	0.17
(3,174)	1:692:A:LEU:HD11	1:691:A:SER:HB3	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,174)	1:692:A:LEU:HD12	1:691:A:SER:HB2	5	0.17
(3,174)	1:692:A:LEU:HD12	1:691:A:SER:HB3	5	0.17
(3,174)	1:692:A:LEU:HD13	1:691:A:SER:HB2	5	0.17
(3,174)	1:692:A:LEU:HD13	1:691:A:SER:HB3	5	0.17
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	3	0.17
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	3	0.17
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	3	0.17
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	3	0.17
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	3	0.17
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	3	0.17
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	2	0.17
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	4	0.17
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	1	0.17
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	11	0.17
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	5	0.17
(3,88)	1:684:A:ILE:HD11	1:681:A:TYR:HA	12	0.17
(3,88)	1:684:A:ILE:HD12	1:681:A:TYR:HA	12	0.17
(3,88)	1:684:A:ILE:HD13	1:681:A:TYR:HA	12	0.17
(3,88)	1:684:A:ILE:HD11	1:681:A:TYR:HA	14	0.17
(3,88)	1:684:A:ILE:HD12	1:681:A:TYR:HA	14	0.17
(3,88)	1:684:A:ILE:HD13	1:681:A:TYR:HA	14	0.17
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	4	0.17
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	4	0.17
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	4	0.17
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	9	0.17
(3,46)	1:670:A:TRP:H	1:667:A:ALA:HA	11	0.17
(3,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	3	0.17
(3,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	13	0.17
(3,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	6	0.17
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	4	0.17
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	10	0.17
(3,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	6	0.16
(3,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	6	0.16
(3,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	6	0.16
(3,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	7	0.16
(3,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	7	0.16
(3,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	7	0.16
(3,594)	1:688:A:ILE:HG21	1:692:A:LEU:HG	14	0.16
(3,594)	1:688:A:ILE:HG22	1:692:A:LEU:HG	14	0.16
(3,594)	1:688:A:ILE:HG23	1:692:A:LEU:HG	14	0.16
(3,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	6	0.16
(3,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	7	0.16
(3,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	7	0.16
(3,567)	1:706:A:ASN:H	1:703:A:SER:HA	11	0.16
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	12	0.16
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	12	0.16
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	12	0.16
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	12	0.16
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	12	0.16
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	12	0.16
(3,482)	1:672:A:TRP:H	1:671:A:ASN:H	1	0.16
(3,482)	1:672:A:TRP:H	1:671:A:ASN:H	4	0.16
(3,462)	1:667:A:ALA:HB1	1:664:A:ASP:HA	13	0.16
(3,462)	1:667:A:ALA:HB2	1:664:A:ASP:HA	13	0.16
(3,462)	1:667:A:ALA:HB3	1:664:A:ASP:HA	13	0.16
(3,444)	1:665:A:LYS:H	1:664:A:ASP:HA	2	0.16
(3,444)	1:665:A:LYS:H	1:664:A:ASP:HA	6	0.16
(3,444)	1:665:A:LYS:H	1:664:A:ASP:HA	7	0.16
(3,444)	1:665:A:LYS:H	1:664:A:ASP:HA	8	0.16
(3,439)	1:664:A:ASP:H	1:663:A:LEU:HA	3	0.16
(3,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	6	0.16
(3,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	6	0.16
(3,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	6	0.16
(3,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	7	0.16
(3,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	7	0.16
(3,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	7	0.16
(3,380)	1:688:A:ILE:HG21	1:692:A:LEU:HG	14	0.16
(3,380)	1:688:A:ILE:HG22	1:692:A:LEU:HG	14	0.16
(3,380)	1:688:A:ILE:HG23	1:692:A:LEU:HG	14	0.16
(3,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	6	0.16
(3,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	6	0.16
(3,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	7	0.16
(3,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	7	0.16
(3,260)	1:670:A:TRP:H	1:667:A:ALA:HA	7	0.16
(3,248)	1:667:A:ALA:HB1	1:664:A:ASP:HA	13	0.16
(3,248)	1:667:A:ALA:HB2	1:664:A:ASP:HA	13	0.16
(3,248)	1:667:A:ALA:HB3	1:664:A:ASP:HA	13	0.16
(3,230)	1:665:A:LYS:H	1:664:A:ASP:HA	2	0.16
(3,230)	1:665:A:LYS:H	1:664:A:ASP:HA	6	0.16
(3,230)	1:665:A:LYS:H	1:664:A:ASP:HA	7	0.16
(3,230)	1:665:A:LYS:H	1:664:A:ASP:HA	8	0.16
(3,225)	1:664:A:ASP:H	1:663:A:LEU:HA	3	0.16
(3,193)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,193)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	9	0.16
(3,193)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	9	0.16
(3,193)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	9	0.16
(3,193)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	9	0.16
(3,193)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	9	0.16
(3,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	1	0.16
(3,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	1	0.16
(3,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	1	0.16
(3,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	1	0.16
(3,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	1	0.16
(3,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	1	0.16
(3,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	6	0.16
(3,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	6	0.16
(3,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	6	0.16
(3,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	7	0.16
(3,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	7	0.16
(3,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	7	0.16
(3,166)	1:688:A:ILE:HG21	1:692:A:LEU:HG	14	0.16
(3,166)	1:688:A:ILE:HG22	1:692:A:LEU:HG	14	0.16
(3,166)	1:688:A:ILE:HG23	1:692:A:LEU:HG	14	0.16
(3,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	6	0.16
(3,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	6	0.16
(3,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	7	0.16
(3,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	7	0.16
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	12	0.16
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	12	0.16
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	12	0.16
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	12	0.16
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	12	0.16
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	12	0.16
(3,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	11	0.16
(3,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	11	0.16
(3,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	11	0.16
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	7	0.16
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	9	0.16
(3,80)	1:682:A:ILE:HG21	1:679:A:LEU:H	7	0.16
(3,80)	1:682:A:ILE:HG22	1:679:A:LEU:H	7	0.16
(3,80)	1:682:A:ILE:HG23	1:679:A:LEU:H	7	0.16
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	1	0.16
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	4	0.16
(3,46)	1:670:A:TRP:H	1:667:A:ALA:HA	7	0.16
(3,34)	1:667:A:ALA:HB1	1:664:A:ASP:HA	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,34)	1:667:A:ALA:HB2	1:664:A:ASP:HA	13	0.16
(3,34)	1:667:A:ALA:HB3	1:664:A:ASP:HA	13	0.16
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	2	0.16
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	6	0.16
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	7	0.16
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	8	0.16
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	3	0.16
(3,598)	1:690:A:GLY:H	1:689:A:VAL:H	9	0.15
(3,598)	1:690:A:GLY:H	1:689:A:VAL:H	14	0.15
(3,536)	1:702:A:LEU:H	1:704:A:LEU:H	10	0.15
(3,531)	1:689:A:VAL:H	1:690:A:GLY:H	9	0.15
(3,531)	1:689:A:VAL:H	1:690:A:GLY:H	14	0.15
(3,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	9	0.15
(3,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	9	0.15
(3,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	9	0.15
(3,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	9	0.15
(3,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	9	0.15
(3,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	9	0.15
(3,482)	1:672:A:TRP:H	1:671:A:ASN:H	5	0.15
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	1	0.15
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	1	0.15
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	1	0.15
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	1	0.15
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	1	0.15
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	1	0.15
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	1	0.15
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	1	0.15
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	1	0.15
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	1	0.15
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	1	0.15
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	1	0.15
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	2	0.15
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	2	0.15
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	2	0.15
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	2	0.15
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	2	0.15
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	2	0.15
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	9	0.15
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	9	0.15
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	9	0.15
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	9	0.15
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	9	0.15
(3,384)	1:690:A:GLY:H	1:689:A:VAL:H	9	0.15
(3,384)	1:690:A:GLY:H	1:689:A:VAL:H	14	0.15
(3,342)	1:705:A:VAL:H	1:702:A:LEU:HA	10	0.15
(3,336)	1:704:A:LEU:H	1:704:A:LEU:HB3	7	0.15
(3,322)	1:702:A:LEU:H	1:704:A:LEU:H	10	0.15
(3,260)	1:670:A:TRP:H	1:667:A:ALA:HA	6	0.15
(3,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	4	0.15
(3,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	4	0.15
(3,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	4	0.15
(3,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	4	0.15
(3,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	4	0.15
(3,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	4	0.15
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	2	0.15
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	2	0.15
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	2	0.15
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	2	0.15
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	2	0.15
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	2	0.15
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	9	0.15
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	9	0.15
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	9	0.15
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	9	0.15
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	9	0.15
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	9	0.15
(3,177)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	12	0.15
(3,177)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	12	0.15
(3,177)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	12	0.15
(3,177)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	12	0.15
(3,177)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	12	0.15
(3,177)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	12	0.15
(3,128)	1:705:A:VAL:H	1:702:A:LEU:HA	10	0.15
(3,108)	1:702:A:LEU:H	1:704:A:LEU:H	10	0.15
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	9	0.15
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	14	0.15
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	4	0.15
(3,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	9	0.15
(3,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	9	0.15
(3,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	9	0.15
(3,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	9	0.15
(3,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	9	0.15
(3,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	5	0.15
(3,46)	1:670:A:TRP:H	1:667:A:ALA:HA	6	0.15
(2,66)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	8	0.15
(2,66)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	8	0.15
(2,66)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	8	0.15
(2,66)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	8	0.15
(2,66)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	8	0.15
(2,66)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	8	0.15
(2,65)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	8	0.15
(2,65)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	8	0.15
(2,65)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	8	0.15
(2,65)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	8	0.15
(2,65)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	8	0.15
(2,65)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	8	0.15
(2,64)	1:700:A:ALA:HB1	1:699:A:PHE:HD1	8	0.15
(2,64)	1:700:A:ALA:HB1	1:699:A:PHE:HD2	8	0.15
(2,64)	1:700:A:ALA:HB2	1:699:A:PHE:HD1	8	0.15
(2,64)	1:700:A:ALA:HB2	1:699:A:PHE:HD2	8	0.15
(2,64)	1:700:A:ALA:HB3	1:699:A:PHE:HD1	8	0.15
(2,64)	1:700:A:ALA:HB3	1:699:A:PHE:HD2	8	0.15
(3,607)	1:693:A:ILE:HG21	1:690:A:GLY:HA2	7	0.14
(3,607)	1:693:A:ILE:HG21	1:690:A:GLY:HA3	7	0.14
(3,607)	1:693:A:ILE:HG22	1:690:A:GLY:HA2	7	0.14
(3,607)	1:693:A:ILE:HG22	1:690:A:GLY:HA3	7	0.14
(3,607)	1:693:A:ILE:HG23	1:690:A:GLY:HA2	7	0.14
(3,607)	1:693:A:ILE:HG23	1:690:A:GLY:HA3	7	0.14
(3,594)	1:688:A:ILE:HG21	1:692:A:LEU:HG	2	0.14
(3,594)	1:688:A:ILE:HG22	1:692:A:LEU:HG	2	0.14
(3,594)	1:688:A:ILE:HG23	1:692:A:LEU:HG	2	0.14
(3,588)	1:686:A:ILE:HD11	1:685:A:PHE:H	14	0.14
(3,588)	1:686:A:ILE:HD12	1:685:A:PHE:H	14	0.14
(3,588)	1:686:A:ILE:HD13	1:685:A:PHE:H	14	0.14
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	14	0.14
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	14	0.14
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	14	0.14
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	14	0.14
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	14	0.14
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	14	0.14
(3,545)	1:704:A:LEU:H	1:701:A:VAL:HA	6	0.14
(3,545)	1:704:A:LEU:H	1:701:A:VAL:HA	9	0.14
(3,517)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	14	0.14
(3,517)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,517)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	14	0.14
(3,517)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	14	0.14
(3,517)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	14	0.14
(3,517)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	14	0.14
(3,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	4	0.14
(3,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	4	0.14
(3,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	4	0.14
(3,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	4	0.14
(3,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	4	0.14
(3,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	4	0.14
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	3	0.14
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	3	0.14
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	3	0.14
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	3	0.14
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	3	0.14
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	3	0.14
(3,482)	1:672:A:TRP:H	1:671:A:ASN:H	12	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	5	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	5	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	5	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	5	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	5	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	5	0.14
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	5	0.14
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	5	0.14
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	5	0.14
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	5	0.14
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	5	0.14
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	5	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	5	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	5	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	5	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	5	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	5	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	5	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	13	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	13	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	13	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	13	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	13	0.14
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	13	0.14
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	13	0.14
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	13	0.14
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	13	0.14
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	13	0.14
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	13	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	13	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	13	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	13	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	13	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	13	0.14
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	13	0.14
(3,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	9	0.14
(3,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	14	0.14
(3,443)	1:665:A:LYS:H	1:662:A:GLU:HA	13	0.14
(3,403)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	1	0.14
(3,403)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	1	0.14
(3,403)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	1	0.14
(3,403)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	1	0.14
(3,403)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	1	0.14
(3,403)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	1	0.14
(3,403)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	3	0.14
(3,403)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	3	0.14
(3,403)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	3	0.14
(3,403)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	3	0.14
(3,403)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	3	0.14
(3,403)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	3	0.14
(3,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	8	0.14
(3,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	8	0.14
(3,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	8	0.14
(3,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	8	0.14
(3,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	8	0.14
(3,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	8	0.14
(3,393)	1:693:A:ILE:HG21	1:690:A:GLY:HA2	7	0.14
(3,393)	1:693:A:ILE:HG21	1:690:A:GLY:HA3	7	0.14
(3,393)	1:693:A:ILE:HG22	1:690:A:GLY:HA2	7	0.14
(3,393)	1:693:A:ILE:HG22	1:690:A:GLY:HA3	7	0.14
(3,393)	1:693:A:ILE:HG23	1:690:A:GLY:HA2	7	0.14
(3,393)	1:693:A:ILE:HG23	1:690:A:GLY:HA3	7	0.14
(3,380)	1:688:A:ILE:HG21	1:692:A:LEU:HG	2	0.14
(3,380)	1:688:A:ILE:HG22	1:692:A:LEU:HG	2	0.14
(3,380)	1:688:A:ILE:HG23	1:692:A:LEU:HG	2	0.14
(3,374)	1:686:A:ILE:HD11	1:685:A:PHE:H	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,374)	1:686:A:ILE:HD12	1:685:A:PHE:H	14	0.14
(3,374)	1:686:A:ILE:HD13	1:685:A:PHE:H	14	0.14
(3,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	4	0.14
(3,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	4	0.14
(3,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	4	0.14
(3,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	4	0.14
(3,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	4	0.14
(3,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	4	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	5	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	5	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	5	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	5	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	5	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	5	0.14
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	5	0.14
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	5	0.14
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	5	0.14
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	5	0.14
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	5	0.14
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	5	0.14
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	5	0.14
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	5	0.14
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	5	0.14
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	5	0.14
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	5	0.14
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	5	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	13	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	13	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	13	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	13	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	13	0.14
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	13	0.14
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	13	0.14
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	13	0.14
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	13	0.14
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	13	0.14
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	13	0.14
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	13	0.14
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	13	0.14
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	13	0.14
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	13	0.14
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	13	0.14
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	13	0.14
(3,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	9	0.14
(3,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	14	0.14
(3,229)	1:665:A:LYS:H	1:662:A:GLU:HA	13	0.14
(3,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	6	0.14
(3,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	6	0.14
(3,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	6	0.14
(3,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	6	0.14
(3,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	6	0.14
(3,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	6	0.14
(3,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	6	0.14
(3,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	6	0.14
(3,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	6	0.14
(3,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	8	0.14
(3,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	8	0.14
(3,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	8	0.14
(3,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	8	0.14
(3,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	8	0.14
(3,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	8	0.14
(3,179)	1:693:A:ILE:HG21	1:690:A:GLY:HA2	7	0.14
(3,179)	1:693:A:ILE:HG21	1:690:A:GLY:HA3	7	0.14
(3,179)	1:693:A:ILE:HG22	1:690:A:GLY:HA2	7	0.14
(3,179)	1:693:A:ILE:HG22	1:690:A:GLY:HA3	7	0.14
(3,179)	1:693:A:ILE:HG23	1:690:A:GLY:HA2	7	0.14
(3,179)	1:693:A:ILE:HG23	1:690:A:GLY:HA3	7	0.14
(3,178)	1:693:A:ILE:HD11	1:697:A:ILE:H	2	0.14
(3,178)	1:693:A:ILE:HD12	1:697:A:ILE:H	2	0.14
(3,178)	1:693:A:ILE:HD13	1:697:A:ILE:H	2	0.14
(3,166)	1:688:A:ILE:HG21	1:692:A:LEU:HG	2	0.14
(3,166)	1:688:A:ILE:HG22	1:692:A:LEU:HG	2	0.14
(3,166)	1:688:A:ILE:HG23	1:692:A:LEU:HG	2	0.14
(3,160)	1:686:A:ILE:HD11	1:685:A:PHE:H	14	0.14
(3,160)	1:686:A:ILE:HD12	1:685:A:PHE:H	14	0.14
(3,160)	1:686:A:ILE:HD13	1:685:A:PHE:H	14	0.14
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	14	0.14
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	14	0.14
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	14	0.14
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	14	0.14
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	14	0.14
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	14	0.14
(3,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	14	0.14
(3,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	14	0.14
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	11	0.14
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	13	0.14
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	8	0.14
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	13	0.14
(3,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	14	0.14
(3,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	14	0.14
(3,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	14	0.14
(3,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	14	0.14
(3,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	14	0.14
(3,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	14	0.14
(3,83)	1:682:A:ILE:HD11	1:681:A:TYR:H	1	0.14
(3,83)	1:682:A:ILE:HD12	1:681:A:TYR:H	1	0.14
(3,83)	1:682:A:ILE:HD13	1:681:A:TYR:H	1	0.14
(3,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	4	0.14
(3,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	4	0.14
(3,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	4	0.14
(3,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	4	0.14
(3,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	4	0.14
(3,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	4	0.14
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	12	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	5	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	5	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	5	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	5	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	5	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	5	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	10	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	10	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	10	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	10	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	10	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	10	0.14
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	7	0.14
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	7	0.14
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	7	0.14
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	7	0.14
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	7	0.14
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	7	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	5	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	5	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	5	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	5	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	5	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	5	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	5	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	5	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	5	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	5	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	5	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	5	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	5	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	5	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	5	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	5	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	5	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	13	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	13	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	13	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	13	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	13	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	13	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	13	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	13	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	13	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	13	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	13	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	13	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	13	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	13	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	13	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	13	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	13	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	13	0.14
(3,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	9	0.14
(3,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	14	0.14
(3,15)	1:665:A:LYS:H	1:662:A:GLU:HA	13	0.14
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	6	0.14
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	6	0.14
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	6	0.14
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	6	0.14
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	6	0.14
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	6	0.14
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	6	0.14
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	6	0.14
(3,620)	1:696:A:ARG:H	1:696:A:ARG:HE	2	0.13
(3,620)	1:696:A:ARG:H	1:696:A:ARG:HE	12	0.13
(3,598)	1:690:A:GLY:H	1:689:A:VAL:H	5	0.13
(3,598)	1:690:A:GLY:H	1:689:A:VAL:H	7	0.13
(3,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	8	0.13
(3,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	8	0.13
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	7	0.13
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	7	0.13
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	7	0.13
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	7	0.13
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	7	0.13
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	7	0.13
(3,565)	1:705:A:VAL:HG21	1:702:A:LEU:HG	4	0.13
(3,565)	1:705:A:VAL:HG22	1:702:A:LEU:HG	4	0.13
(3,565)	1:705:A:VAL:HG23	1:702:A:LEU:HG	4	0.13
(3,555)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	3	0.13
(3,555)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	3	0.13
(3,555)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	3	0.13
(3,555)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	3	0.13
(3,555)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	3	0.13
(3,555)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	3	0.13
(3,555)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	3	0.13
(3,555)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	3	0.13
(3,555)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	3	0.13
(3,531)	1:689:A:VAL:H	1:690:A:GLY:H	5	0.13
(3,531)	1:689:A:VAL:H	1:690:A:GLY:H	7	0.13
(3,517)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	8	0.13
(3,517)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	8	0.13
(3,517)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	8	0.13
(3,517)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	8	0.13
(3,517)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	8	0.13
(3,517)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	8	0.13
(3,406)	1:696:A:ARG:H	1:696:A:ARG:HE	2	0.13
(3,406)	1:696:A:ARG:H	1:696:A:ARG:HE	12	0.13
(3,403)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	13	0.13
(3,403)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	13	0.13
(3,403)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	13	0.13
(3,403)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,403)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	13	0.13
(3,403)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	13	0.13
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	3	0.13
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	3	0.13
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	3	0.13
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	3	0.13
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	3	0.13
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	3	0.13
(3,384)	1:690:A:GLY:H	1:689:A:VAL:H	5	0.13
(3,384)	1:690:A:GLY:H	1:689:A:VAL:H	7	0.13
(3,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	8	0.13
(3,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	8	0.13
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	13	0.13
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	13	0.13
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	13	0.13
(3,271)	1:672:A:TRP:HE1	1:671:A:ASN:H	6	0.13
(3,267)	1:671:A:ASN:H	1:672:A:TRP:HE1	6	0.13
(3,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	4	0.13
(3,199)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	4	0.13
(3,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	4	0.13
(3,199)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	4	0.13
(3,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	4	0.13
(3,199)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	4	0.13
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	3	0.13
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	3	0.13
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	3	0.13
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	3	0.13
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	3	0.13
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	3	0.13
(3,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	8	0.13
(3,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	8	0.13
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	7	0.13
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	7	0.13
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	7	0.13
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	7	0.13
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	7	0.13
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	7	0.13
(3,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	12	0.13
(3,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	12	0.13
(3,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	12	0.13
(3,127)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	3	0.13
(3,127)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,127)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	3	0.13
(3,127)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	3	0.13
(3,127)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	3	0.13
(3,127)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	3	0.13
(3,127)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	3	0.13
(3,127)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	3	0.13
(3,127)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	3	0.13
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	5	0.13
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	7	0.13
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	3	0.13
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	4	0.13
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	12	0.13
(3,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	8	0.13
(3,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	8	0.13
(3,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	8	0.13
(3,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	8	0.13
(3,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	8	0.13
(3,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	8	0.13
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	13	0.13
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	13	0.13
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	13	0.13
(3,57)	1:672:A:TRP:HE1	1:671:A:ASN:H	6	0.13
(3,53)	1:671:A:ASN:H	1:672:A:TRP:HE1	6	0.13
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	9	0.13
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	9	0.13
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	9	0.13
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	9	0.13
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	9	0.13
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	9	0.13
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	1	0.13
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	1	0.13
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	1	0.13
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	1	0.13
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	1	0.13
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	1	0.13
(3,625)	1:698:A:VAL:HG11	1:695:A:LEU:HG	6	0.12
(3,625)	1:698:A:VAL:HG12	1:695:A:LEU:HG	6	0.12
(3,625)	1:698:A:VAL:HG13	1:695:A:LEU:HG	6	0.12
(3,625)	1:698:A:VAL:HG11	1:695:A:LEU:HG	9	0.12
(3,625)	1:698:A:VAL:HG12	1:695:A:LEU:HG	9	0.12
(3,625)	1:698:A:VAL:HG13	1:695:A:LEU:HG	9	0.12
(3,615)	1:695:A:LEU:HD21	1:698:A:VAL:HB	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,615)	1:695:A:LEU:HD22	1:698:A:VAL:HB	12	0.12
(3,615)	1:695:A:LEU:HD23	1:698:A:VAL:HB	12	0.12
(3,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	14	0.12
(3,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	14	0.12
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	6	0.12
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	6	0.12
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	6	0.12
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	6	0.12
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	6	0.12
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	6	0.12
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	8	0.12
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	8	0.12
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	8	0.12
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	8	0.12
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	8	0.12
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	8	0.12
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	9	0.12
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	9	0.12
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	9	0.12
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	9	0.12
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	9	0.12
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	9	0.12
(3,565)	1:705:A:VAL:HG21	1:702:A:LEU:HG	8	0.12
(3,565)	1:705:A:VAL:HG22	1:702:A:LEU:HG	8	0.12
(3,565)	1:705:A:VAL:HG23	1:702:A:LEU:HG	8	0.12
(3,545)	1:704:A:LEU:H	1:701:A:VAL:HA	1	0.12
(3,501)	1:678:A:TRP:HE1	1:682:A:ILE:H	10	0.12
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	11	0.12
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	11	0.12
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	11	0.12
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	11	0.12
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	11	0.12
(3,500)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	11	0.12
(3,494)	1:676:A:THR:HG21	1:679:A:LEU:H	8	0.12
(3,494)	1:676:A:THR:HG22	1:679:A:LEU:H	8	0.12
(3,494)	1:676:A:THR:HG23	1:679:A:LEU:H	8	0.12
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	14	0.12
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	14	0.12
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	14	0.12
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	14	0.12
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	14	0.12
(3,463)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	14	0.12
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	14	0.12
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	14	0.12
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	14	0.12
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	14	0.12
(3,463)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	14	0.12
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	14	0.12
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	14	0.12
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	14	0.12
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	14	0.12
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	14	0.12
(3,463)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	14	0.12
(3,460)	1:667:A:ALA:H	1:666:A:TRP:HD1	11	0.12
(3,457)	1:667:A:ALA:H	1:664:A:ASP:HA	5	0.12
(3,439)	1:664:A:ASP:H	1:663:A:LEU:HA	13	0.12
(3,411)	1:698:A:VAL:HG11	1:695:A:LEU:HG	6	0.12
(3,411)	1:698:A:VAL:HG12	1:695:A:LEU:HG	6	0.12
(3,411)	1:698:A:VAL:HG13	1:695:A:LEU:HG	6	0.12
(3,411)	1:698:A:VAL:HG11	1:695:A:LEU:HG	9	0.12
(3,411)	1:698:A:VAL:HG12	1:695:A:LEU:HG	9	0.12
(3,411)	1:698:A:VAL:HG13	1:695:A:LEU:HG	9	0.12
(3,403)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	4	0.12
(3,403)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	4	0.12
(3,403)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	4	0.12
(3,403)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	4	0.12
(3,403)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	4	0.12
(3,403)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	4	0.12
(3,401)	1:695:A:LEU:HD21	1:698:A:VAL:HB	12	0.12
(3,401)	1:695:A:LEU:HD22	1:698:A:VAL:HB	12	0.12
(3,401)	1:695:A:LEU:HD23	1:698:A:VAL:HB	12	0.12
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	4	0.12
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	4	0.12
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	4	0.12
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	4	0.12
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	4	0.12
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	4	0.12
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	5	0.12
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	5	0.12
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	5	0.12
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	5	0.12
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	5	0.12
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	9	0.12
(3,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	9	0.12
(3,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	9	0.12
(3,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	9	0.12
(3,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	9	0.12
(3,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	9	0.12
(3,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	14	0.12
(3,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	14	0.12
(3,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	8	0.12
(3,352)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	8	0.12
(3,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	8	0.12
(3,352)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	8	0.12
(3,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	8	0.12
(3,352)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	8	0.12
(3,348)	1:705:A:VAL:HG11	1:706:A:ASN:HA	2	0.12
(3,348)	1:705:A:VAL:HG12	1:706:A:ASN:HA	2	0.12
(3,348)	1:705:A:VAL:HG13	1:706:A:ASN:HA	2	0.12
(3,348)	1:705:A:VAL:HG11	1:706:A:ASN:HA	8	0.12
(3,348)	1:705:A:VAL:HG12	1:706:A:ASN:HA	8	0.12
(3,348)	1:705:A:VAL:HG13	1:706:A:ASN:HA	8	0.12
(3,342)	1:705:A:VAL:H	1:702:A:LEU:HA	7	0.12
(3,342)	1:705:A:VAL:H	1:702:A:LEU:HA	14	0.12
(3,336)	1:704:A:LEU:H	1:704:A:LEU:HB3	3	0.12
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	7	0.12
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	7	0.12
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	7	0.12
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	7	0.12
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	7	0.12
(3,286)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	7	0.12
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	14	0.12
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	14	0.12
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	14	0.12
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	14	0.12
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	14	0.12
(3,249)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	14	0.12
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	14	0.12
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	14	0.12
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	14	0.12
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	14	0.12
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	14	0.12
(3,249)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	14	0.12
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	14	0.12
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	14	0.12
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	14	0.12
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	14	0.12
(3,249)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	14	0.12
(3,246)	1:667:A:ALA:H	1:666:A:TRP:HD1	11	0.12
(3,243)	1:667:A:ALA:H	1:664:A:ASP:HA	5	0.12
(3,225)	1:664:A:ASP:H	1:663:A:LEU:HA	13	0.12
(3,213)	1:701:A:VAL:HG11	1:698:A:VAL:HA	6	0.12
(3,213)	1:701:A:VAL:HG12	1:698:A:VAL:HA	6	0.12
(3,213)	1:701:A:VAL:HG13	1:698:A:VAL:HA	6	0.12
(3,197)	1:698:A:VAL:HG11	1:695:A:LEU:HG	6	0.12
(3,197)	1:698:A:VAL:HG12	1:695:A:LEU:HG	6	0.12
(3,197)	1:698:A:VAL:HG13	1:695:A:LEU:HG	6	0.12
(3,197)	1:698:A:VAL:HG11	1:695:A:LEU:HG	9	0.12
(3,197)	1:698:A:VAL:HG12	1:695:A:LEU:HG	9	0.12
(3,197)	1:698:A:VAL:HG13	1:695:A:LEU:HG	9	0.12
(3,187)	1:695:A:LEU:HD21	1:698:A:VAL:HB	12	0.12
(3,187)	1:695:A:LEU:HD22	1:698:A:VAL:HB	12	0.12
(3,187)	1:695:A:LEU:HD23	1:698:A:VAL:HB	12	0.12
(3,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	13	0.12
(3,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	13	0.12
(3,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	13	0.12
(3,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	13	0.12
(3,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	13	0.12
(3,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	13	0.12
(3,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	14	0.12
(3,186)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	14	0.12
(3,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	14	0.12
(3,186)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	14	0.12
(3,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	14	0.12
(3,186)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	14	0.12
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	4	0.12
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	4	0.12
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	4	0.12
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	4	0.12
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	4	0.12
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	4	0.12
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	5	0.12
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	5	0.12
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	5	0.12
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	5	0.12
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	5	0.12
(3,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	9	0.12
(3,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	9	0.12
(3,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	9	0.12
(3,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	9	0.12
(3,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	9	0.12
(3,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	9	0.12
(3,178)	1:693:A:ILE:HD11	1:697:A:ILE:H	6	0.12
(3,178)	1:693:A:ILE:HD12	1:697:A:ILE:H	6	0.12
(3,178)	1:693:A:ILE:HD13	1:697:A:ILE:H	6	0.12
(3,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	14	0.12
(3,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	14	0.12
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	6	0.12
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	6	0.12
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	6	0.12
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	6	0.12
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	6	0.12
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	6	0.12
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	9	0.12
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	9	0.12
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	9	0.12
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	9	0.12
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	9	0.12
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	9	0.12
(3,137)	1:705:A:VAL:HG21	1:702:A:LEU:HG	8	0.12
(3,137)	1:705:A:VAL:HG22	1:702:A:LEU:HG	8	0.12
(3,137)	1:705:A:VAL:HG23	1:702:A:LEU:HG	8	0.12
(3,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	5	0.12
(3,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	5	0.12
(3,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	5	0.12
(3,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	6	0.12
(3,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	6	0.12
(3,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	6	0.12
(3,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	7	0.12
(3,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	7	0.12
(3,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	7	0.12
(3,128)	1:705:A:VAL:H	1:702:A:LEU:HA	7	0.12
(3,128)	1:705:A:VAL:H	1:702:A:LEU:HA	14	0.12
(3,105)	1:702:A:LEU:H	1:700:A:ALA:H	2	0.12
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	1	0.12
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	2	0.12
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	13	0.12
(3,83)	1:682:A:ILE:HD11	1:681:A:TYR:H	4	0.12
(3,83)	1:682:A:ILE:HD12	1:681:A:TYR:H	4	0.12
(3,83)	1:682:A:ILE:HD13	1:681:A:TYR:H	4	0.12
(3,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	10	0.12
(3,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	9	0.12
(3,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	9	0.12
(3,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	9	0.12
(3,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	9	0.12
(3,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	9	0.12
(3,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	9	0.12
(3,66)	1:676:A:THR:HG21	1:679:A:LEU:H	8	0.12
(3,66)	1:676:A:THR:HG22	1:679:A:LEU:H	8	0.12
(3,66)	1:676:A:THR:HG23	1:679:A:LEU:H	8	0.12
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	14	0.12
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	14	0.12
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	14	0.12
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	14	0.12
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	14	0.12
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	14	0.12
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	14	0.12
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	14	0.12
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	14	0.12
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	14	0.12
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	14	0.12
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	14	0.12
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	14	0.12
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	14	0.12
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	14	0.12
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	14	0.12
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	14	0.12
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	14	0.12
(3,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	11	0.12
(3,29)	1:667:A:ALA:H	1:664:A:ASP:HA	5	0.12
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	13	0.12
(3,625)	1:698:A:VAL:HG11	1:695:A:LEU:HG	8	0.11
(3,625)	1:698:A:VAL:HG12	1:695:A:LEU:HG	8	0.11
(3,625)	1:698:A:VAL:HG13	1:695:A:LEU:HG	8	0.11
(3,609)	1:693:A:ILE:HG21	1:694:A:GLY:H	1	0.11
(3,609)	1:693:A:ILE:HG22	1:694:A:GLY:H	1	0.11
(3,609)	1:693:A:ILE:HG23	1:694:A:GLY:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,602)	1:692:A:LEU:HD11	1:691:A:SER:HB2	10	0.11
(3,602)	1:692:A:LEU:HD11	1:691:A:SER:HB3	10	0.11
(3,602)	1:692:A:LEU:HD12	1:691:A:SER:HB2	10	0.11
(3,602)	1:692:A:LEU:HD12	1:691:A:SER:HB3	10	0.11
(3,602)	1:692:A:LEU:HD13	1:691:A:SER:HB2	10	0.11
(3,602)	1:692:A:LEU:HD13	1:691:A:SER:HB3	10	0.11
(3,598)	1:690:A:GLY:H	1:689:A:VAL:H	11	0.11
(3,597)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	9	0.11
(3,597)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	9	0.11
(3,597)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	9	0.11
(3,597)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	9	0.11
(3,597)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	9	0.11
(3,597)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	9	0.11
(3,580)	1:707:A:ARG:H	1:707:A:ARG:HD2	2	0.11
(3,580)	1:707:A:ARG:H	1:707:A:ARG:HD3	2	0.11
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	2	0.11
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	2	0.11
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	2	0.11
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	2	0.11
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	2	0.11
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	2	0.11
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	13	0.11
(3,566)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	13	0.11
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	13	0.11
(3,566)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	13	0.11
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	13	0.11
(3,566)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	13	0.11
(3,531)	1:689:A:VAL:H	1:690:A:GLY:H	11	0.11
(3,516)	1:684:A:ILE:HD11	1:681:A:TYR:HA	13	0.11
(3,516)	1:684:A:ILE:HD12	1:681:A:TYR:HA	13	0.11
(3,516)	1:684:A:ILE:HD13	1:681:A:TYR:HA	13	0.11
(3,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	11	0.11
(3,510)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	11	0.11
(3,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	11	0.11
(3,510)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	11	0.11
(3,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	11	0.11
(3,510)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	11	0.11
(3,507)	1:681:A:TYR:H	1:682:A:ILE:H	3	0.11
(3,507)	1:681:A:TYR:H	1:682:A:ILE:H	14	0.11
(3,492)	1:676:A:THR:HG21	1:669:A:LEU:HA	13	0.11
(3,492)	1:676:A:THR:HG22	1:669:A:LEU:HA	13	0.11
(3,492)	1:676:A:THR:HG23	1:669:A:LEU:HA	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,487)	1:674:A:ASP:H	1:677:A:ASN:H	8	0.11
(3,482)	1:672:A:TRP:H	1:671:A:ASN:H	8	0.11
(3,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	1	0.11
(3,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	1	0.11
(3,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	1	0.11
(3,439)	1:664:A:ASP:H	1:663:A:LEU:HA	1	0.11
(3,439)	1:664:A:ASP:H	1:663:A:LEU:HA	12	0.11
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	11	0.11
(3,429)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	11	0.11
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	11	0.11
(3,429)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	11	0.11
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	11	0.11
(3,429)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	11	0.11
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	11	0.11
(3,429)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	11	0.11
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	11	0.11
(3,429)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	11	0.11
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	11	0.11
(3,429)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	11	0.11
(3,411)	1:698:A:VAL:HG11	1:695:A:LEU:HG	8	0.11
(3,411)	1:698:A:VAL:HG12	1:695:A:LEU:HG	8	0.11
(3,411)	1:698:A:VAL:HG13	1:695:A:LEU:HG	8	0.11
(3,403)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	12	0.11
(3,403)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	12	0.11
(3,403)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	12	0.11
(3,403)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	12	0.11
(3,403)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	12	0.11
(3,403)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	12	0.11
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	8	0.11
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	8	0.11
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	8	0.11
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	8	0.11
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	8	0.11
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	8	0.11
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	13	0.11
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	13	0.11
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	13	0.11
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	13	0.11
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	13	0.11
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	13	0.11
(3,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	4	0.11
(3,396)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	4	0.11
(3,396)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	4	0.11
(3,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	4	0.11
(3,396)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	4	0.11
(3,395)	1:693:A:ILE:HG21	1:694:A:GLY:H	1	0.11
(3,395)	1:693:A:ILE:HG22	1:694:A:GLY:H	1	0.11
(3,395)	1:693:A:ILE:HG23	1:694:A:GLY:H	1	0.11
(3,388)	1:692:A:LEU:HD11	1:691:A:SER:HB2	10	0.11
(3,388)	1:692:A:LEU:HD11	1:691:A:SER:HB3	10	0.11
(3,388)	1:692:A:LEU:HD12	1:691:A:SER:HB2	10	0.11
(3,388)	1:692:A:LEU:HD12	1:691:A:SER:HB3	10	0.11
(3,388)	1:692:A:LEU:HD13	1:691:A:SER:HB2	10	0.11
(3,388)	1:692:A:LEU:HD13	1:691:A:SER:HB3	10	0.11
(3,384)	1:690:A:GLY:H	1:689:A:VAL:H	11	0.11
(3,366)	1:707:A:ARG:H	1:707:A:ARG:HD2	2	0.11
(3,366)	1:707:A:ARG:H	1:707:A:ARG:HD3	2	0.11
(3,350)	1:705:A:VAL:HG21	1:701:A:VAL:HA	4	0.11
(3,350)	1:705:A:VAL:HG22	1:701:A:VAL:HA	4	0.11
(3,350)	1:705:A:VAL:HG23	1:701:A:VAL:HA	4	0.11
(3,336)	1:704:A:LEU:H	1:704:A:LEU:HB3	8	0.11
(3,302)	1:684:A:ILE:HD11	1:681:A:TYR:HA	13	0.11
(3,302)	1:684:A:ILE:HD12	1:681:A:TYR:HA	13	0.11
(3,302)	1:684:A:ILE:HD13	1:681:A:TYR:HA	13	0.11
(3,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	11	0.11
(3,296)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	11	0.11
(3,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	11	0.11
(3,296)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	11	0.11
(3,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	11	0.11
(3,296)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	11	0.11
(3,293)	1:681:A:TYR:H	1:682:A:ILE:H	3	0.11
(3,293)	1:681:A:TYR:H	1:682:A:ILE:H	14	0.11
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	7	0.11
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	7	0.11
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	7	0.11
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	8	0.11
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	8	0.11
(3,285)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	8	0.11
(3,278)	1:676:A:THR:HG21	1:669:A:LEU:HA	13	0.11
(3,278)	1:676:A:THR:HG22	1:669:A:LEU:HA	13	0.11
(3,278)	1:676:A:THR:HG23	1:669:A:LEU:HA	13	0.11
(3,273)	1:674:A:ASP:H	1:677:A:ASN:H	8	0.11
(3,271)	1:672:A:TRP:HE1	1:671:A:ASN:H	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,267)	1:671:A:ASN:H	1:672:A:TRP:HE1	13	0.11
(3,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	1	0.11
(3,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	1	0.11
(3,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	1	0.11
(3,225)	1:664:A:ASP:H	1:663:A:LEU:HA	1	0.11
(3,225)	1:664:A:ASP:H	1:663:A:LEU:HA	12	0.11
(3,197)	1:698:A:VAL:HG11	1:695:A:LEU:HG	8	0.11
(3,197)	1:698:A:VAL:HG12	1:695:A:LEU:HG	8	0.11
(3,197)	1:698:A:VAL:HG13	1:695:A:LEU:HG	8	0.11
(3,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	13	0.11
(3,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	13	0.11
(3,195)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	13	0.11
(3,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	13	0.11
(3,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	13	0.11
(3,195)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	13	0.11
(3,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	13	0.11
(3,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	13	0.11
(3,195)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	13	0.11
(3,193)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	8	0.11
(3,193)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	8	0.11
(3,193)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	8	0.11
(3,193)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	8	0.11
(3,193)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	8	0.11
(3,193)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	8	0.11
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	8	0.11
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	8	0.11
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	8	0.11
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	8	0.11
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	8	0.11
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	8	0.11
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	13	0.11
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	13	0.11
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	13	0.11
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	13	0.11
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	13	0.11
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	13	0.11
(3,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	4	0.11
(3,182)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	4	0.11
(3,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	4	0.11
(3,182)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	4	0.11
(3,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	4	0.11
(3,182)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,181)	1:693:A:ILE:HG21	1:694:A:GLY:H	1	0.11
(3,181)	1:693:A:ILE:HG22	1:694:A:GLY:H	1	0.11
(3,181)	1:693:A:ILE:HG23	1:694:A:GLY:H	1	0.11
(3,174)	1:692:A:LEU:HD11	1:691:A:SER:HB2	10	0.11
(3,174)	1:692:A:LEU:HD11	1:691:A:SER:HB3	10	0.11
(3,174)	1:692:A:LEU:HD12	1:691:A:SER:HB2	10	0.11
(3,174)	1:692:A:LEU:HD12	1:691:A:SER:HB3	10	0.11
(3,174)	1:692:A:LEU:HD13	1:691:A:SER:HB2	10	0.11
(3,174)	1:692:A:LEU:HD13	1:691:A:SER:HB3	10	0.11
(3,152)	1:707:A:ARG:H	1:707:A:ARG:HD2	2	0.11
(3,152)	1:707:A:ARG:H	1:707:A:ARG:HD3	2	0.11
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	2	0.11
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	2	0.11
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	2	0.11
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	2	0.11
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	2	0.11
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	2	0.11
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	13	0.11
(3,138)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	13	0.11
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	13	0.11
(3,138)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	13	0.11
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	13	0.11
(3,138)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	13	0.11
(3,136)	1:705:A:VAL:HG21	1:701:A:VAL:HA	4	0.11
(3,136)	1:705:A:VAL:HG22	1:701:A:VAL:HA	4	0.11
(3,136)	1:705:A:VAL:HG23	1:701:A:VAL:HA	4	0.11
(3,133)	1:705:A:VAL:HG11	1:702:A:LEU:HA	2	0.11
(3,133)	1:705:A:VAL:HG12	1:702:A:LEU:HA	2	0.11
(3,133)	1:705:A:VAL:HG13	1:702:A:LEU:HA	2	0.11
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	11	0.11
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	11	0.11
(3,88)	1:684:A:ILE:HD11	1:681:A:TYR:HA	13	0.11
(3,88)	1:684:A:ILE:HD12	1:681:A:TYR:HA	13	0.11
(3,88)	1:684:A:ILE:HD13	1:681:A:TYR:HA	13	0.11
(3,83)	1:682:A:ILE:HD11	1:681:A:TYR:H	11	0.11
(3,83)	1:682:A:ILE:HD12	1:681:A:TYR:H	11	0.11
(3,83)	1:682:A:ILE:HD13	1:681:A:TYR:H	11	0.11
(3,83)	1:682:A:ILE:HD11	1:681:A:TYR:H	14	0.11
(3,83)	1:682:A:ILE:HD12	1:681:A:TYR:H	14	0.11
(3,83)	1:682:A:ILE:HD13	1:681:A:TYR:H	14	0.11
(3,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	11	0.11
(3,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	11	0.11
(3,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	11	0.11
(3,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	11	0.11
(3,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	11	0.11
(3,79)	1:681:A:TYR:H	1:682:A:ILE:H	3	0.11
(3,79)	1:681:A:TYR:H	1:682:A:ILE:H	14	0.11
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	7	0.11
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	7	0.11
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	7	0.11
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	8	0.11
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	8	0.11
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	8	0.11
(3,64)	1:676:A:THR:HG21	1:669:A:LEU:HA	13	0.11
(3,64)	1:676:A:THR:HG22	1:669:A:LEU:HA	13	0.11
(3,64)	1:676:A:THR:HG23	1:669:A:LEU:HA	13	0.11
(3,59)	1:674:A:ASP:H	1:677:A:ASN:H	8	0.11
(3,57)	1:672:A:TRP:HE1	1:671:A:ASN:H	13	0.11
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	8	0.11
(3,53)	1:671:A:ASN:H	1:672:A:TRP:HE1	13	0.11
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	1	0.11
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	1	0.11
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	1	0.11
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	1	0.11
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	12	0.11
(3,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	7	0.1
(3,520)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	7	0.1
(3,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	7	0.1
(3,520)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	7	0.1
(3,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	7	0.1
(3,520)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	7	0.1
(3,516)	1:684:A:ILE:HD11	1:681:A:TYR:HA	11	0.1
(3,516)	1:684:A:ILE:HD12	1:681:A:TYR:HA	11	0.1
(3,516)	1:684:A:ILE:HD13	1:681:A:TYR:HA	11	0.1
(3,507)	1:681:A:TYR:H	1:682:A:ILE:H	11	0.1
(3,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	7	0.1
(3,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	7	0.1
(3,478)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	7	0.1
(3,468)	1:669:A:LEU:H	1:666:A:TRP:HA	4	0.1
(3,404)	1:696:A:ARG:H	1:693:A:ILE:HA	12	0.1
(3,401)	1:695:A:LEU:HD21	1:698:A:VAL:HB	2	0.1
(3,401)	1:695:A:LEU:HD22	1:698:A:VAL:HB	2	0.1
(3,401)	1:695:A:LEU:HD23	1:698:A:VAL:HB	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,401)	1:695:A:LEU:HD21	1:698:A:VAL:HB	14	0.1
(3,401)	1:695:A:LEU:HD22	1:698:A:VAL:HB	14	0.1
(3,401)	1:695:A:LEU:HD23	1:698:A:VAL:HB	14	0.1
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB2	1	0.1
(3,399)	1:695:A:LEU:HD11	1:691:A:SER:HB3	1	0.1
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB2	1	0.1
(3,399)	1:695:A:LEU:HD12	1:691:A:SER:HB3	1	0.1
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB2	1	0.1
(3,399)	1:695:A:LEU:HD13	1:691:A:SER:HB3	1	0.1
(3,336)	1:704:A:LEU:H	1:704:A:LEU:HB3	11	0.1
(3,302)	1:684:A:ILE:HD11	1:681:A:TYR:HA	11	0.1
(3,302)	1:684:A:ILE:HD12	1:681:A:TYR:HA	11	0.1
(3,302)	1:684:A:ILE:HD13	1:681:A:TYR:HA	11	0.1
(3,293)	1:681:A:TYR:H	1:682:A:ILE:H	11	0.1
(3,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	7	0.1
(3,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	7	0.1
(3,264)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	7	0.1
(3,254)	1:669:A:LEU:H	1:666:A:TRP:HA	4	0.1
(3,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	10	0.1
(3,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	10	0.1
(3,223)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	10	0.1
(3,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	10	0.1
(3,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	10	0.1
(3,223)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	10	0.1
(3,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	10	0.1
(3,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	10	0.1
(3,223)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	10	0.1
(3,214)	1:701:A:VAL:HG21	1:698:A:VAL:HA	8	0.1
(3,214)	1:701:A:VAL:HG22	1:698:A:VAL:HA	8	0.1
(3,214)	1:701:A:VAL:HG23	1:698:A:VAL:HA	8	0.1
(3,190)	1:696:A:ARG:H	1:693:A:ILE:HA	12	0.1
(3,187)	1:695:A:LEU:HD21	1:698:A:VAL:HB	2	0.1
(3,187)	1:695:A:LEU:HD22	1:698:A:VAL:HB	2	0.1
(3,187)	1:695:A:LEU:HD23	1:698:A:VAL:HB	2	0.1
(3,187)	1:695:A:LEU:HD21	1:698:A:VAL:HB	14	0.1
(3,187)	1:695:A:LEU:HD22	1:698:A:VAL:HB	14	0.1
(3,187)	1:695:A:LEU:HD23	1:698:A:VAL:HB	14	0.1
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB2	1	0.1
(3,185)	1:695:A:LEU:HD11	1:691:A:SER:HB3	1	0.1
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB2	1	0.1
(3,185)	1:695:A:LEU:HD12	1:691:A:SER:HB3	1	0.1
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB2	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,185)	1:695:A:LEU:HD13	1:691:A:SER:HB3	1	0.1
(3,177)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	6	0.1
(3,177)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	6	0.1
(3,177)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	6	0.1
(3,177)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	6	0.1
(3,177)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	6	0.1
(3,177)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	6	0.1
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	1	0.1
(3,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	7	0.1
(3,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	7	0.1
(3,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	7	0.1
(3,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	7	0.1
(3,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	7	0.1
(3,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	7	0.1
(3,88)	1:684:A:ILE:HD11	1:681:A:TYR:HA	11	0.1
(3,88)	1:684:A:ILE:HD12	1:681:A:TYR:HA	11	0.1
(3,88)	1:684:A:ILE:HD13	1:681:A:TYR:HA	11	0.1
(3,79)	1:681:A:TYR:H	1:682:A:ILE:H	11	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	1	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	1	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	1	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	1	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	1	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	1	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	7	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	7	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	7	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	7	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	7	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	7	0.1
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	8	0.1
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	8	0.1
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	8	0.1
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	8	0.1
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	8	0.1
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	8	0.1
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	7	0.1
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	7	0.1
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	7	0.1
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	4	0.1
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	4	0.1
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	4	0.1
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	4	0.1
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	4	0.1
(3,40)	1:669:A:LEU:H	1:666:A:TRP:HA	4	0.1
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	10	0.1
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	10	0.1
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	10	0.1
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	10	0.1
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	10	0.1
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	10	0.1
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	10	0.1
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	10	0.1
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	10	0.1
(3,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	8	0.1
(3,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	8	0.1
(3,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	8	0.1
(3,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	8	0.1
(3,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	8	0.1
(3,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	8	0.1
(3,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	8	0.1
(3,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	8	0.1
(3,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	8	0.1
(3,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	8	0.1
(3,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	8	0.1
(3,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	8	0.1

10 Dihedral-angle violation analysis

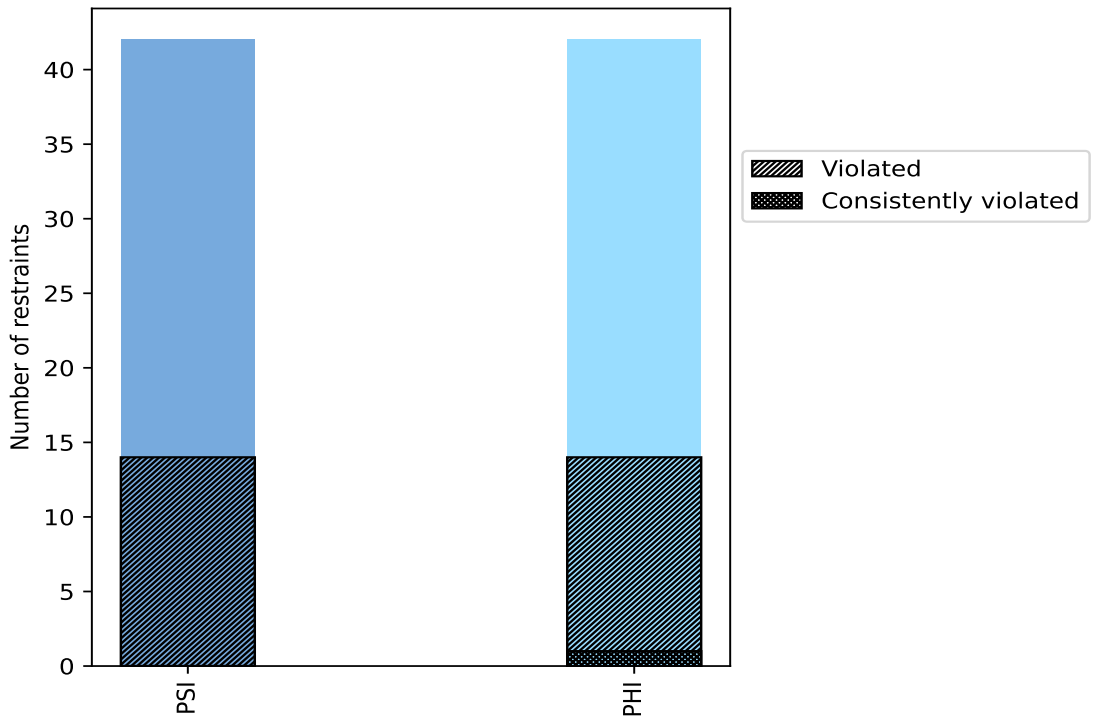
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	42	50.0	14	33.3	16.7	0	0.0	0.0
PHI	42	50.0	14	33.3	16.7	1	2.4	1.2
Total	84	100.0	28	33.3	33.3	1	1.2	1.2

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



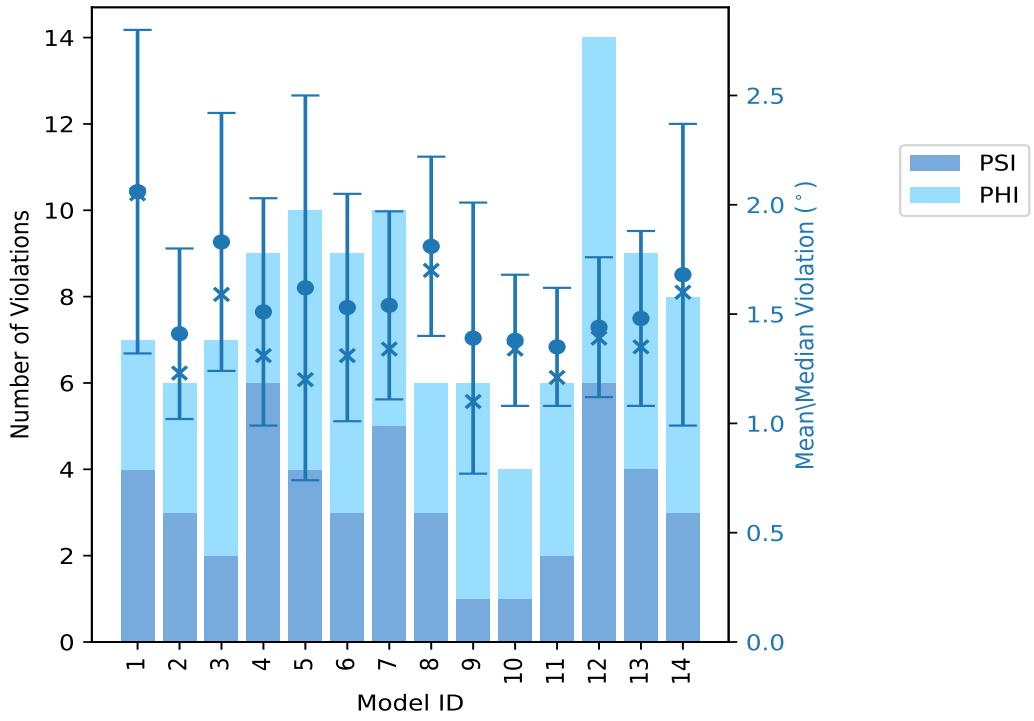
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	4	3	7	2.06	3.36	0.74	2.05
2	3	3	6	1.41	2.19	0.39	1.23
3	2	5	7	1.83	3.11	0.59	1.59
4	6	3	9	1.51	2.73	0.52	1.31
5	4	6	10	1.62	4.01	0.88	1.2
6	3	6	9	1.53	2.83	0.52	1.31
7	5	5	10	1.54	2.42	0.43	1.34
8	3	3	6	1.81	2.53	0.41	1.7
9	1	5	6	1.39	2.76	0.62	1.1
10	1	3	4	1.38	1.77	0.3	1.34
11	2	4	6	1.35	1.82	0.27	1.21
12	6	8	14	1.44	2.12	0.32	1.39
13	4	5	9	1.48	2.15	0.4	1.35
14	3	5	8	1.68	3.34	0.69	1.6

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



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

on the right

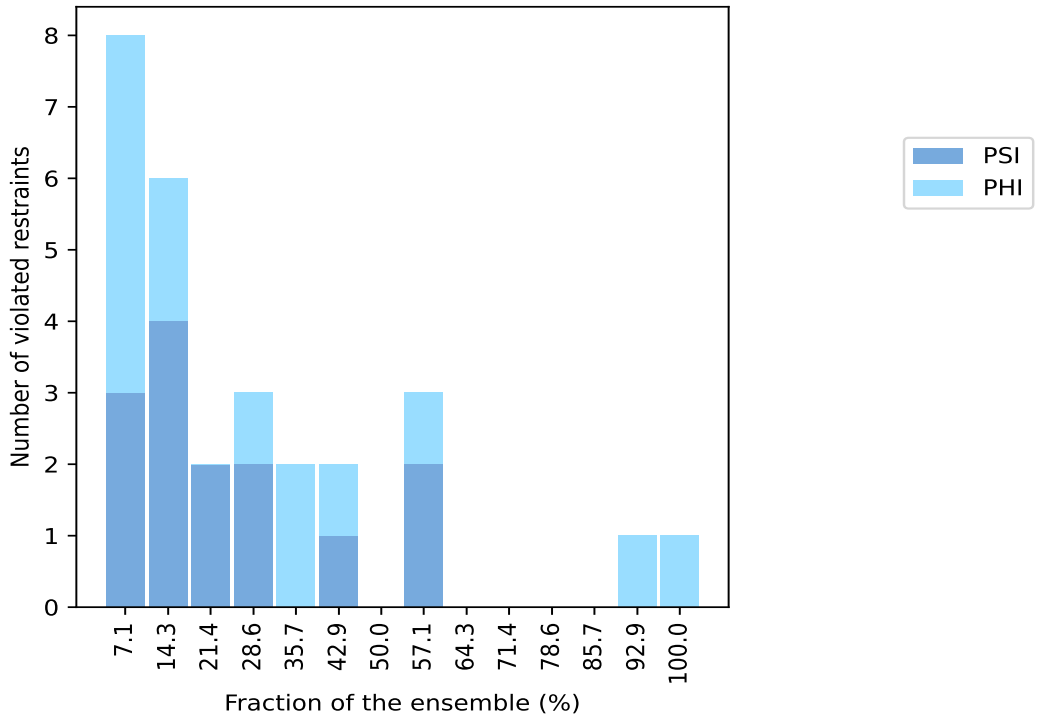
10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
3	5	8	1	7.1
4	2	6	2	14.3
2	0	2	3	21.4
2	1	3	4	28.6
0	2	2	5	35.7
1	1	2	6	42.9
0	0	0	7	50.0
2	1	3	8	57.1
0	0	0	9	64.3
0	0	0	10	71.4
0	0	0	11	78.6
0	0	0	12	85.7
0	1	1	13	92.9
0	1	1	14	100.0

[1] Number of models with violations

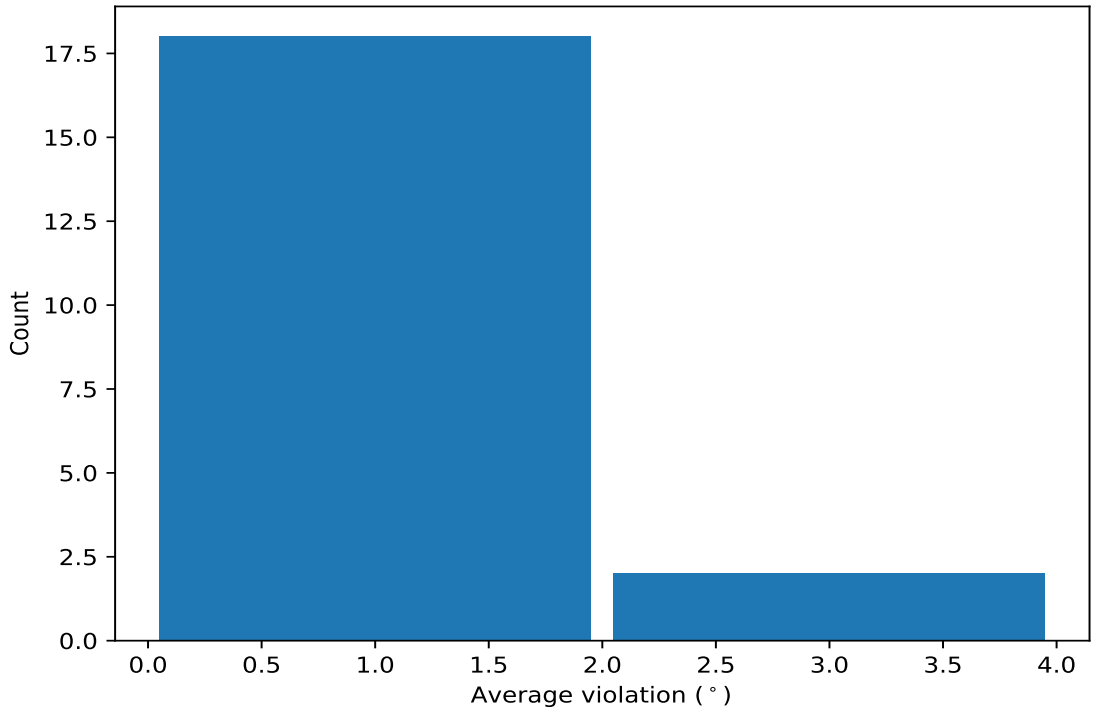
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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



10.4.2 Table: Most violated dihedral-angle restraints

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

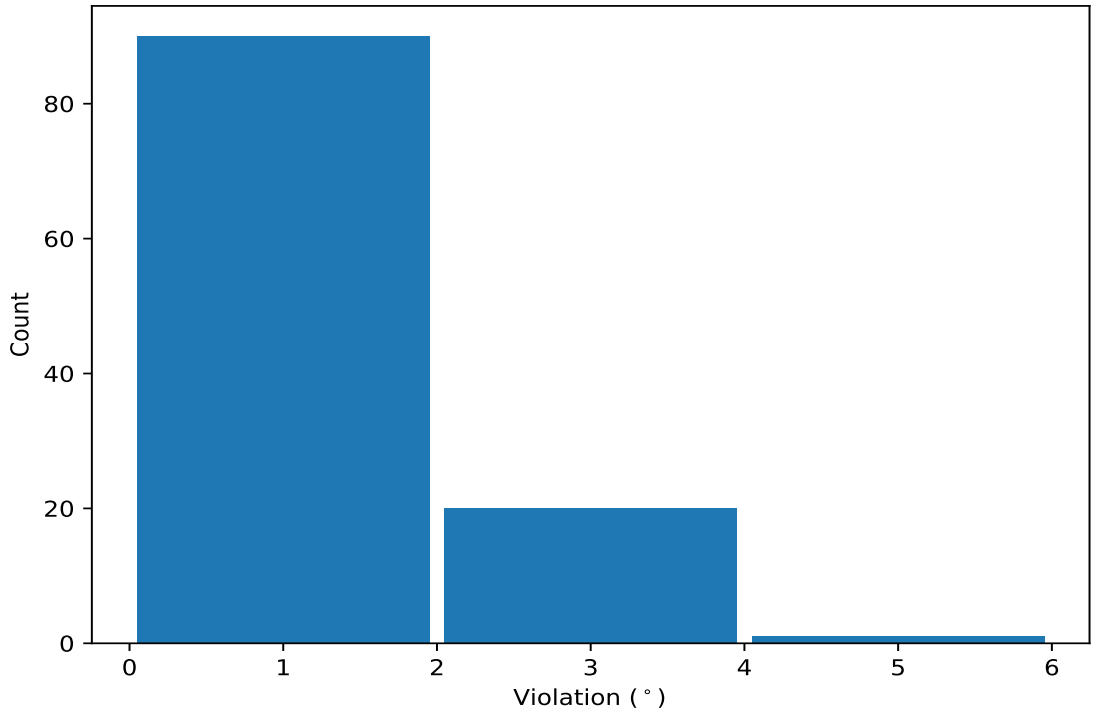
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	14	2.21	0.78	2.07
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	13	1.51	0.35	1.44
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	8	2.25	0.72	2.0
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	8	1.84	0.54	1.89
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	8	1.76	0.32	1.76
(1,62)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	6	1.45	0.3	1.44
(1,59)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	6	1.27	0.17	1.23
(1,21)	1:673:C:PHE:C	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	5	1.23	0.02	1.24
(1,19)	1:671:C:ASN:C	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	5	1.18	0.13	1.16
(1,20)	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	1:673:C:PHE:N	4	1.5	0.17	1.44
(1,63)	1:697:C:ILE:C	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	4	1.39	0.42	1.18
(1,52)	1:692:C:LEU:N	1:692:C:LEU:CA	1:692:C:LEU:C	1:693:C:ILE:N	4	1.2	0.1	1.19
(1,58)	1:695:C:LEU:N	1:695:C:LEU:CA	1:695:C:LEU:C	1:696:C:ARG:N	3	1.33	0.16	1.31
(1,68)	1:700:C:ALA:N	1:700:C:ALA:CA	1:700:C:ALA:C	1:701:C:VAL:N	3	1.08	0.07	1.07
(1,38)	1:684:C:ILE:N	1:684:C:ILE:CA	1:684:C:ILE:C	1:685:C:PHE:N	2	1.36	0.17	1.36
(1,65)	1:698:C:VAL:C	1:699:C:PHE:N	1:699:C:PHE:CA	1:699:C:PHE:C	2	1.18	0.02	1.18
(1,64)	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	1:699:C:PHE:N	2	1.14	0.08	1.14
(1,41)	1:685:C:PHE:C	1:686:C:ILE:N	1:686:C:ILE:CA	1:686:C:ILE:C	2	1.14	0.03	1.14
(1,40)	1:685:C:PHE:N	1:685:C:PHE:CA	1:685:C:PHE:C	1:686:C:ILE:N	2	1.14	0.09	1.14
(1,46)	1:688:C:ILE:N	1:688:C:ILE:CA	1:688:C:ILE:C	1:689:C:VAL:N	2	1.11	0.0	1.11

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints (i)

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	5	4.01
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1	3.36
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	14	3.34
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	3	3.11
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	6	2.83
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	9	2.76
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	4	2.73
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	1	2.6
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	8	2.53
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	7	2.42
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	1	2.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	5	2.32
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	2	2.19
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	13	2.15
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	8	2.14
(1,34)	1:682:C:ILE:N	1:682:C:ILE:CA	1:682:C:ILE:C	1:683:C:ARG:N	12	2.12
(1,63)	1:697:C:ILE:C	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	3	2.1
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	1	2.05
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	12	2.01
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	13	2.0
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	4	2.0
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	7	1.97
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	13	1.89
(1,62)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	3	1.88
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	6	1.88
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	7	1.88
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	7	1.82
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	11	1.82
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	14	1.81
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	10	1.77
(1,20)	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	1:673:C:PHE:N	8	1.77
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	5	1.76
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	14	1.76
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	1	1.75
(1,62)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	6	1.73
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	8	1.64
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	14	1.64
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	12	1.63
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	12	1.63
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	11	1.6
(1,39)	1:684:C:ILE:C	1:685:C:PHE:N	1:685:C:PHE:CA	1:685:C:PHE:C	3	1.59
(1,59)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	2	1.58
(1,62)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	14	1.57
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	10	1.55
(1,58)	1:695:C:LEU:N	1:695:C:LEU:CA	1:695:C:LEU:C	1:696:C:ARG:N	12	1.54
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	12	1.54
(1,38)	1:684:C:ILE:N	1:684:C:ILE:CA	1:684:C:ILE:C	1:685:C:PHE:N	3	1.53
(1,35)	1:682:C:ILE:C	1:683:C:ARG:N	1:683:C:ARG:CA	1:683:C:ARG:C	12	1.53
(1,20)	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	1:673:C:PHE:N	4	1.53
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	4	1.52
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	8	1.44
(1,29)	1:677:C:ASN:C	1:678:C:TRP:N	1:678:C:TRP:CA	1:678:C:TRP:C	13	1.43
(1,19)	1:671:C:ASN:C	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	3	1.42
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	9	1.37
(1,59)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	6	1.35
(1,20)	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	1:673:C:PHE:N	7	1.35
(1,20)	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	1:673:C:PHE:N	13	1.35
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	8	1.33
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	7	1.33
(1,52)	1:692:C:LEU:N	1:692:C:LEU:CA	1:692:C:LEU:C	1:693:C:ILE:N	2	1.32
(1,62)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	4	1.31
(1,58)	1:695:C:LEU:N	1:695:C:LEU:CA	1:695:C:LEU:C	1:696:C:ARG:N	6	1.31

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,63)	1:697:C:ILE:C	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	6	1.28
(1,21)	1:673:C:PHE:C	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	5	1.26
(1,59)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	12	1.25
(1,52)	1:692:C:LEU:N	1:692:C:LEU:CA	1:692:C:LEU:C	1:693:C:ILE:N	4	1.25
(1,21)	1:673:C:PHE:C	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	12	1.24
(1,21)	1:673:C:PHE:C	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	14	1.24
(1,64)	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	1:699:C:PHE:N	11	1.23
(1,40)	1:685:C:PHE:N	1:685:C:PHE:CA	1:685:C:PHE:C	1:686:C:ILE:N	7	1.23
(1,59)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	5	1.22
(1,21)	1:673:C:PHE:C	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	7	1.22
(1,44)	1:687:C:ILE:N	1:687:C:ILE:CA	1:687:C:ILE:C	1:688:C:ILE:N	6	1.21
(1,65)	1:698:C:VAL:C	1:699:C:PHE:N	1:699:C:PHE:CA	1:699:C:PHE:C	12	1.2
(1,19)	1:671:C:ASN:C	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	11	1.2
(1,59)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	3	1.19
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	5	1.19
(1,38)	1:684:C:ILE:N	1:684:C:ILE:CA	1:684:C:ILE:C	1:685:C:PHE:N	5	1.19
(1,21)	1:673:C:PHE:C	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	13	1.19
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	13	1.18
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	12	1.18
(1,68)	1:700:C:ALA:N	1:700:C:ALA:CA	1:700:C:ALA:C	1:701:C:VAL:N	1	1.17
(1,41)	1:685:C:PHE:C	1:686:C:ILE:N	1:686:C:ILE:CA	1:686:C:ILE:C	12	1.17
(1,65)	1:698:C:VAL:C	1:699:C:PHE:N	1:699:C:PHE:CA	1:699:C:PHE:C	11	1.16
(1,19)	1:671:C:ASN:C	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	6	1.16
(1,58)	1:695:C:LEU:N	1:695:C:LEU:CA	1:695:C:LEU:C	1:696:C:ARG:N	2	1.15
(1,52)	1:692:C:LEU:N	1:692:C:LEU:CA	1:692:C:LEU:C	1:693:C:ILE:N	10	1.14
(1,62)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	9	1.12
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	13	1.12
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	2	1.11
(1,46)	1:688:C:ILE:N	1:688:C:ILE:CA	1:688:C:ILE:C	1:689:C:VAL:N	1	1.11
(1,46)	1:688:C:ILE:N	1:688:C:ILE:CA	1:688:C:ILE:C	1:689:C:VAL:N	2	1.11
(1,41)	1:685:C:PHE:C	1:686:C:ILE:N	1:686:C:ILE:CA	1:686:C:ILE:C	7	1.11
(1,63)	1:697:C:ILE:C	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	5	1.09
(1,63)	1:697:C:ILE:C	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	14	1.08
(1,62)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	5	1.08
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	4	1.08
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	5	1.08
(1,12)	1:668:C:SER:N	1:668:C:SER:CA	1:668:C:SER:C	1:669:C:LEU:N	4	1.08
(1,68)	1:700:C:ALA:N	1:700:C:ALA:CA	1:700:C:ALA:C	1:701:C:VAL:N	7	1.07
(1,52)	1:692:C:LEU:N	1:692:C:LEU:CA	1:692:C:LEU:C	1:693:C:ILE:N	11	1.07
(1,19)	1:671:C:ASN:C	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	9	1.07
(1,64)	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	1:699:C:PHE:N	12	1.06
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	4	1.06
(1,45)	1:687:C:ILE:C	1:688:C:ILE:N	1:688:C:ILE:CA	1:688:C:ILE:C	6	1.05
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	14	1.04
(1,40)	1:685:C:PHE:N	1:685:C:PHE:CA	1:685:C:PHE:C	1:686:C:ILE:N	12	1.04
(1,19)	1:671:C:ASN:C	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	10	1.04
(1,59)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	9	1.02
(1,57)	1:694:C:GLY:C	1:695:C:LEU:N	1:695:C:LEU:CA	1:695:C:LEU:C	9	1.01
(1,68)	1:700:C:ALA:N	1:700:C:ALA:CA	1:700:C:ALA:C	1:701:C:VAL:N	13	1.0