



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 10:33 PM UTC

PDB ID : 2LYL / pdb_00002lyl
BMRB ID : 17894
Title : NOE-based 3D structure of the predissociated homodimer of CylR2 in equilibrium with monomer at 266K (-7 Celsius degrees)
Authors : Jaremko, M.; Jaremko, L.; Kim, H.; Cho, M.; Schwieters, C.D.; Giller, K.; Becker, S.; Zweckstetter, M.
Deposited on : 2012-09-19

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

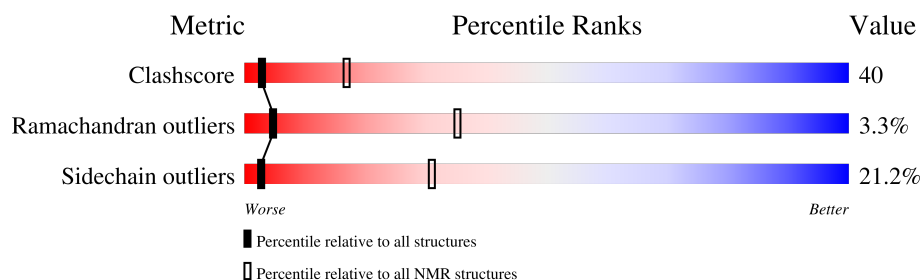
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

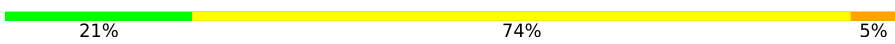
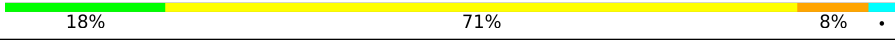
The overall completeness of chemical shifts assignment is 37%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	66	
1	B	66	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:66, B:67-B:130 (130)	1.43	17

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2234 atoms, of which 1146 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CylR2.

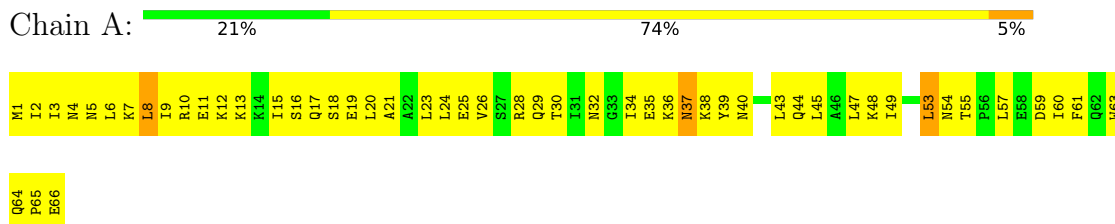
Mol	Chain	Residues	Atoms						Trace
1	A	66	Total	C	H	N	O	S	0
			1117	351	573	91	101	1	
1	B	66	Total	C	H	N	O	S	0
			1117	351	573	91	101	1	

4 Residue-property plots

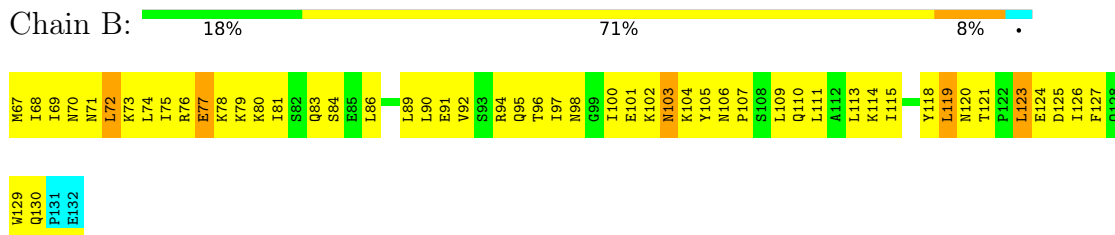
4.1 Average score per residue in the NMR ensemble

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: CylR2



• Molecule 1: CylR2

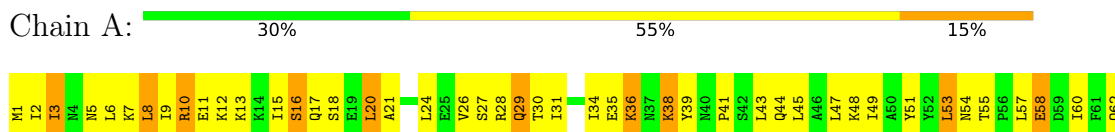


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

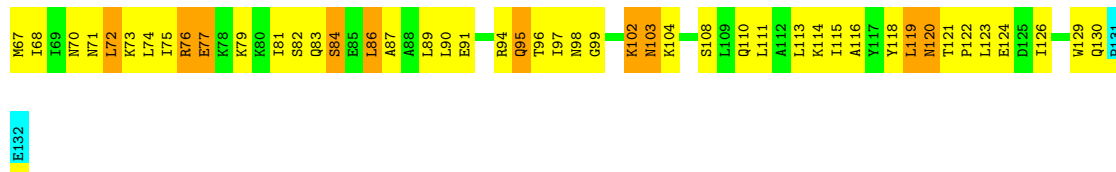
• Molecule 1: CylR2





- Molecule 1: CylR2

Chain B: 27% 55% 15% .



4.2.2 Score per residue for model 2

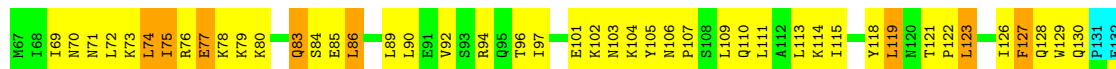
- Molecule 1: CylR2

Chain A: 39% 52% 9%



- Molecule 1: CylR2

Chain B: 29% 56% 12% .



4.2.3 Score per residue for model 3

- Molecule 1: CylR2

Chain A: 33% 50% 17%



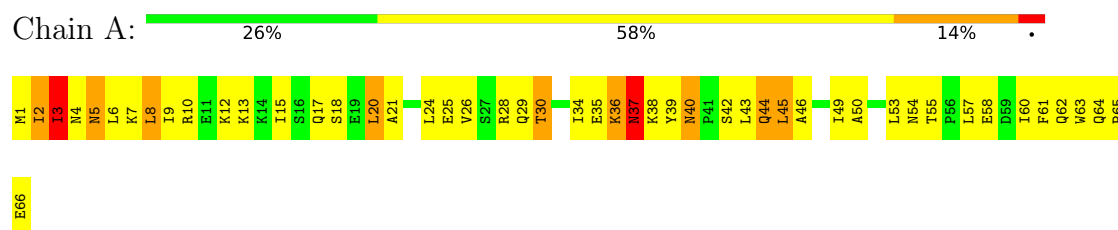
- Molecule 1: CylR2

Chain B: 32% 52% 14% .

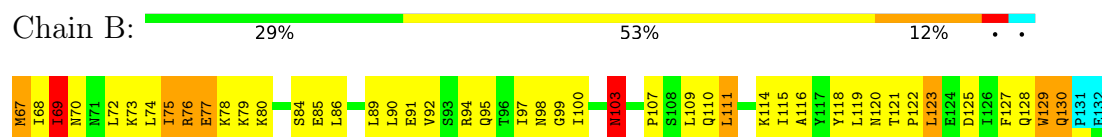


4.2.4 Score per residue for model 4

- Molecule 1: CylR2

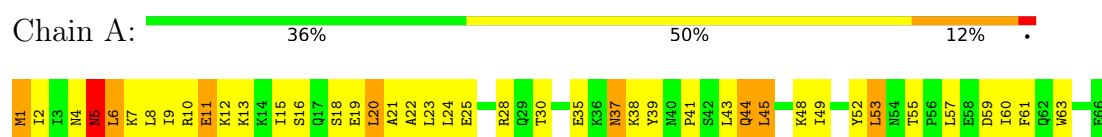


- Molecule 1: CylR2

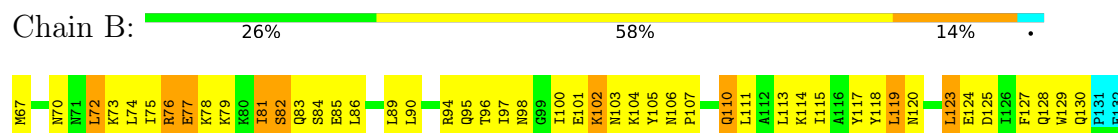


4.2.5 Score per residue for model 5

- Molecule 1: CylR2

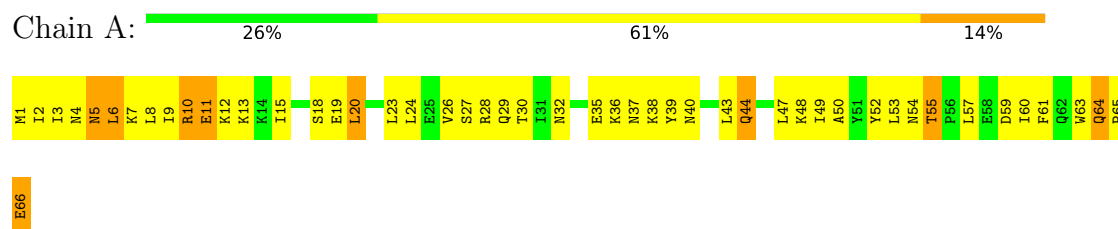


- Molecule 1: CylR2

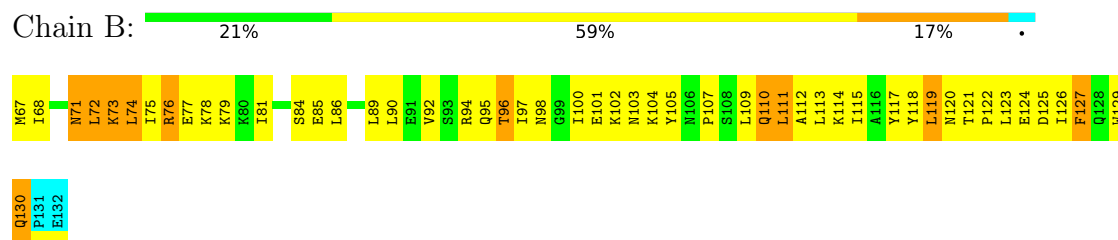


4.2.6 Score per residue for model 6

- Molecule 1: CylR2



- Molecule 1: CylR2

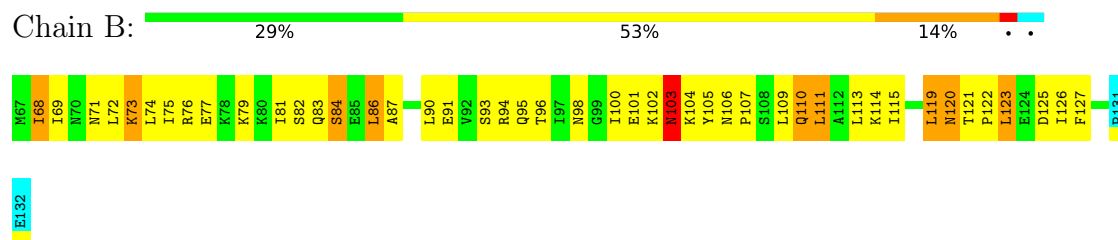


4.2.7 Score per residue for model 7

- Molecule 1: CylR2



- Molecule 1: CylR2



4.2.8 Score per residue for model 8

- Molecule 1: CylR2

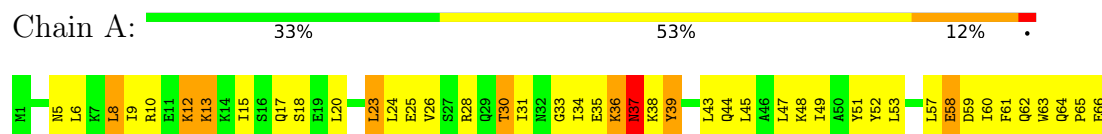


- Molecule 1: CylR2

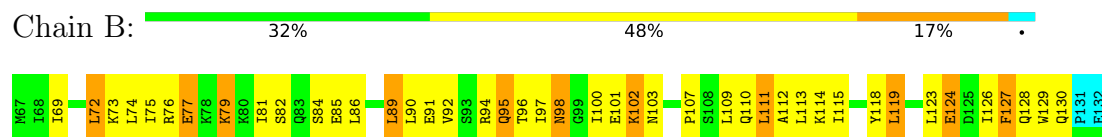


4.2.9 Score per residue for model 9

- Molecule 1: CylR2

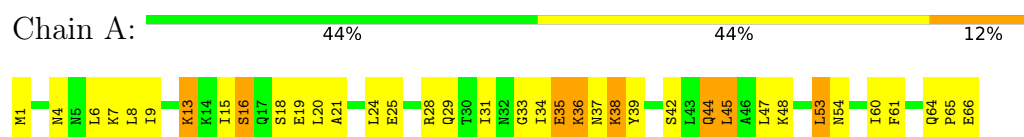


- Molecule 1: CylR2

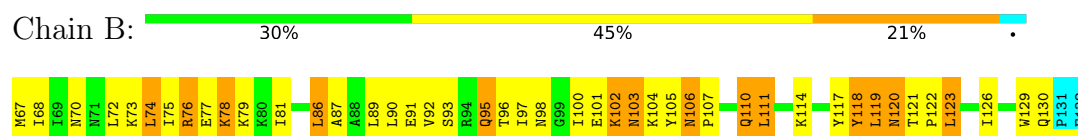


4.2.10 Score per residue for model 10

- Molecule 1: CylR2

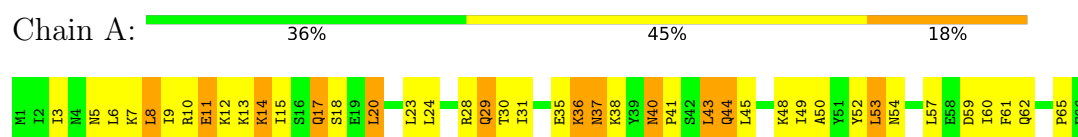


- Molecule 1: CylR2

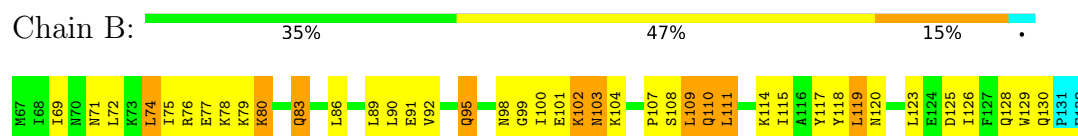


4.2.11 Score per residue for model 11

- Molecule 1: CylR2



- Molecule 1: CylR2



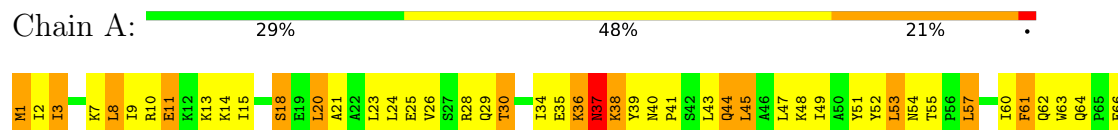
4.2.12 Score per residue for model 12

- Molecule 1: CylR2

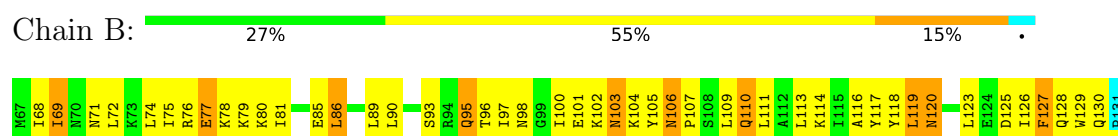
P131
E132

4.2.15 Score per residue for model 15

- Molecule 1: CylR2



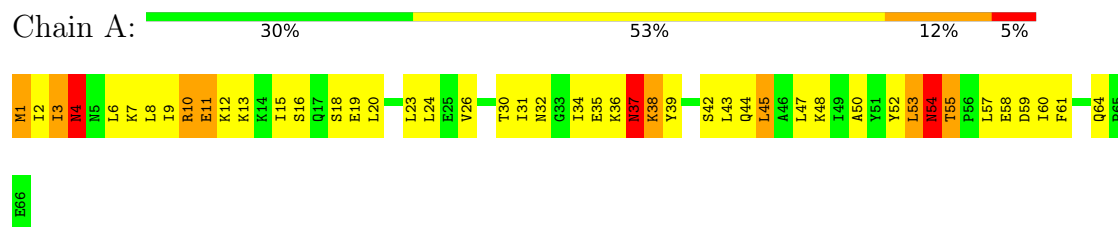
- Molecule 1: CylR2



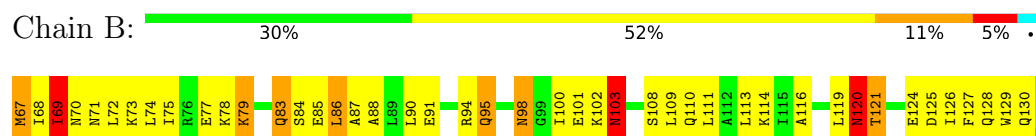
E132

4.2.16 Score per residue for model 16

- Molecule 1: CylR2



- Molecule 1: CylR2



4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: CylR2





• Molecule 1: CylR2

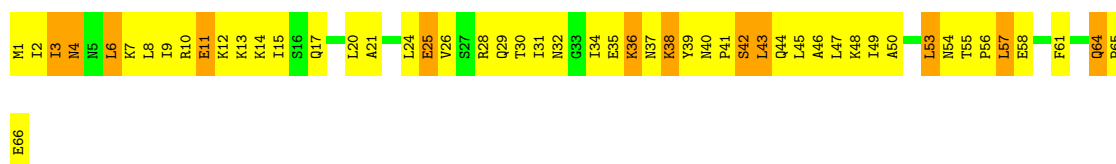
Chain B: 32% 45% 18%



4.2.18 Score per residue for model 18

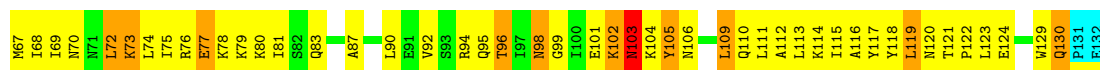
• Molecule 1: CylR2

Chain A: 21% 61% 18%



• Molecule 1: CylR2

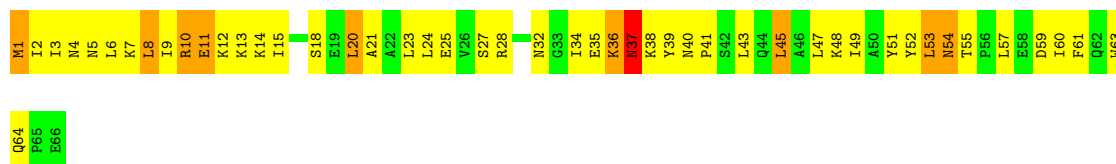
Chain B: 26% 55% 15%



4.2.19 Score per residue for model 19

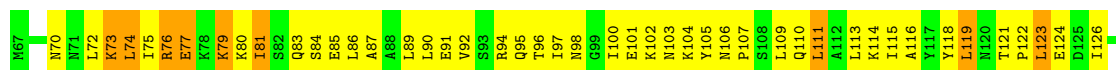
• Molecule 1: CylR2

Chain A: 27% 58% 14%



• Molecule 1: CylR2

Chain B: 24% 58% 15%



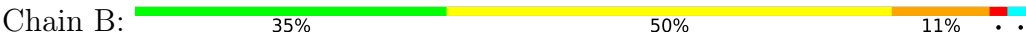


4.2.20 Score per residue for model 20

• Molecule 1: CylR2



• Molecule 1: CylR2



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	3.0
X-PLOR NIH	refinement	2.28

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	717
Number of shifts mapped to atoms	717
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	37%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.80±0.02	0±0/552 (0.0± 0.0%)	1.05±0.02	0±0/743 (0.0± 0.1%)
1	B	0.79±0.02	0±0/535 (0.0± 0.0%)	1.05±0.02	0±0/723 (0.0± 0.1%)
All	All	0.80	0/21740 (0.0%)	1.05	12/29320 (0.0%)

There are no bond-length outliers.

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(°)	Ideal(°)	Models	
								Worst	Total
1	B	127	PHE	CA-CB-CG	-6.93	106.87	113.80	2	7
1	A	61	PHE	CA-CB-CG	-5.73	108.07	113.80	9	5

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	544	573	575	49±7
1	B	527	560	559	47±8
All	All	21420	22660	22680	1750

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 40.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:LEU:HD12	1:B:113:LEU:HD11	0.97	1.34	16	1
1:A:23:LEU:HD12	1:A:52:TYR:CD2	0.93	1.98	9	1
1:A:20:LEU:HD22	1:A:21:ALA:N	0.90	1.80	1	4
1:B:86:LEU:HD22	1:B:87:ALA:N	0.90	1.81	1	4
1:B:89:LEU:HD12	1:B:118:TYR:CD2	0.88	2.04	9	1
1:A:57:LEU:HD11	1:B:109:LEU:HD23	0.86	1.46	8	1
1:B:74:LEU:H	1:B:74:LEU:HD12	0.85	1.29	11	1
1:B:69:ILE:HD11	1:B:130:GLN:CG	0.83	2.03	15	2
1:B:69:ILE:HD11	1:B:130:GLN:HG2	0.79	1.53	4	2
1:A:1:MET:SD	1:A:1:MET:N	0.79	2.52	5	3
1:A:2:ILE:O	1:A:3:ILE:HD12	0.77	1.79	4	1
1:A:9:ILE:HD13	1:A:60:ILE:HG22	0.77	1.55	15	6
1:A:3:ILE:HD11	1:A:64:GLN:CG	0.76	2.09	15	2
1:A:43:LEU:HD22	1:A:43:LEU:C	0.76	2.04	18	1
1:B:86:LEU:H	1:B:86:LEU:HD13	0.76	1.40	7	3
1:A:43:LEU:HD13	1:A:44:GLN:H	0.75	1.40	18	1
1:A:3:ILE:HD11	1:A:64:GLN:HG2	0.75	1.57	4	2
1:A:57:LEU:HD13	1:A:60:ILE:HD11	0.75	1.59	1	4
1:B:89:LEU:HD13	1:B:118:TYR:CD1	0.74	2.17	15	5
1:B:75:ILE:HG22	1:B:119:LEU:HD21	0.74	1.58	4	1
1:A:20:LEU:HD21	1:A:31:ILE:HG21	0.74	1.59	1	4
1:B:72:LEU:HD23	1:B:126:ILE:HG22	0.74	1.59	13	1
1:B:96:THR:HG23	1:B:104:LYS:HZ2	0.74	1.41	15	1
1:B:75:ILE:HD13	1:B:126:ILE:HG22	0.72	1.61	16	5
1:A:2:ILE:HD11	1:B:108:SER:HB2	0.72	1.59	14	1
1:B:69:ILE:HD12	1:B:69:ILE:N	0.71	1.99	15	1
1:A:3:ILE:HD12	1:A:3:ILE:N	0.71	1.99	15	1
1:A:43:LEU:HD22	1:A:44:GLN:N	0.71	2.00	18	1
1:A:64:GLN:CB	1:A:65:PRO:HD3	0.71	2.16	20	2
1:A:64:GLN:HB2	1:A:65:PRO:CD	0.70	2.16	6	2
1:A:24:LEU:HB2	1:A:26:VAL:HG22	0.70	1.62	14	12
1:B:90:LEU:HB2	1:B:92:VAL:HG22	0.70	1.61	14	11
1:A:53:LEU:HD13	1:A:53:LEU:O	0.70	1.86	7	7
1:A:9:ILE:CG2	1:A:53:LEU:HD11	0.70	2.16	6	3
1:B:67:MET:N	1:B:67:MET:SD	0.70	2.64	20	3
1:B:123:LEU:HD13	1:B:126:ILE:HD11	0.69	1.64	1	3
1:B:69:ILE:HG21	1:B:128:GLN:HE21	0.69	1.46	15	3
1:A:53:LEU:O	1:A:54:ASN:ND2	0.69	2.25	14	2
1:A:4:ASN:OD1	1:A:34:ILE:HG22	0.69	1.87	16	1
1:A:6:LEU:O	1:A:6:LEU:HD22	0.69	1.87	17	9
1:A:2:ILE:C	1:A:3:ILE:HD12	0.69	2.11	4	1
1:B:87:ALA:HB1	1:B:92:VAL:O	0.69	1.87	20	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:ILE:HD11	1:B:108:SER:CB	0.69	2.18	14	1
1:A:9:ILE:HG22	1:A:53:LEU:HD11	0.69	1.63	19	6
1:A:47:LEU:HD11	1:B:123:LEU:HD12	0.69	1.64	14	3
1:B:100:ILE:HG23	1:B:105:TYR:O	0.69	1.87	13	1
1:B:86:LEU:CD2	1:B:97:ILE:HG21	0.68	2.18	10	5
1:A:57:LEU:C	1:A:57:LEU:HD13	0.68	2.14	16	3
1:A:57:LEU:HB2	1:B:113:LEU:HD21	0.68	1.66	9	1
1:A:3:ILE:HD12	1:A:3:ILE:H	0.67	1.48	15	1
1:B:68:ILE:HG21	1:B:106:ASN:CG	0.67	2.14	15	1
1:B:100:ILE:HG21	1:B:107:PRO:HD3	0.67	1.66	15	7
1:A:1:MET:SD	1:A:2:ILE:N	0.67	2.68	16	2
1:A:8:LEU:HD12	1:A:8:LEU:H	0.67	1.49	11	1
1:A:53:LEU:HD22	1:A:53:LEU:O	0.67	1.90	16	1
1:B:69:ILE:HD13	1:B:128:GLN:CG	0.66	2.20	4	1
1:A:3:ILE:HD11	1:A:64:GLN:HG3	0.66	1.65	15	1
1:A:20:LEU:HD23	1:A:31:ILE:HG21	0.66	1.66	8	4
1:A:8:LEU:HD12	1:A:8:LEU:N	0.66	2.04	11	1
1:B:86:LEU:HD23	1:B:97:ILE:HG21	0.66	1.68	10	5
1:A:18:SER:OG	1:A:28:ARG:NH1	0.65	2.29	6	13
1:B:86:LEU:HD21	1:B:97:ILE:HG21	0.65	1.65	12	2
1:B:67:MET:SD	1:B:68:ILE:N	0.65	2.68	14	1
1:B:68:ILE:C	1:B:69:ILE:HD12	0.65	2.14	4	1
1:B:68:ILE:O	1:B:69:ILE:HD12	0.65	1.91	4	1
1:A:30:THR:HG23	1:A:38:LYS:HG2	0.65	1.68	18	1
1:B:69:ILE:HD13	1:B:128:GLN:HG2	0.65	1.69	4	1
1:A:20:LEU:HD13	1:A:20:LEU:H	0.65	1.52	7	4
1:B:116:ALA:HB1	1:B:121:THR:O	0.65	1.91	16	6
1:A:47:LEU:HD22	1:B:124:GLU:HG3	0.65	1.67	3	1
1:A:2:ILE:HG21	1:A:40:ASN:CB	0.64	2.22	14	4
1:B:119:LEU:HD13	1:B:119:LEU:O	0.64	1.93	3	1
1:A:58:GLU:H	1:A:58:GLU:CD	0.64	2.00	9	6
1:A:8:LEU:H	1:A:8:LEU:CD1	0.64	2.03	11	1
1:B:69:ILE:HD12	1:B:69:ILE:H	0.64	1.49	15	1
1:A:20:LEU:C	1:A:20:LEU:HD23	0.64	2.18	13	3
1:A:63:TRP:N	1:A:63:TRP:CD1	0.64	2.66	3	1
1:A:31:ILE:HD13	1:A:34:ILE:HD12	0.64	1.69	9	3
1:B:119:LEU:O	1:B:119:LEU:HD22	0.64	1.93	14	1
1:B:73:LYS:O	1:B:77:GLU:HG3	0.63	1.94	16	7
1:B:75:ILE:HG22	1:B:119:LEU:HD12	0.63	1.71	8	1
1:B:89:LEU:N	1:B:89:LEU:HD23	0.63	2.08	9	1
1:A:48:LYS:HG3	1:B:129:TRP:CZ3	0.63	2.28	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:LEU:HD21	1:B:123:LEU:HG	0.63	1.71	14	1
1:A:34:ILE:HG23	1:A:39:TYR:O	0.63	1.94	16	2
1:A:53:LEU:HD13	1:A:54:ASN:HD22	0.63	1.53	16	1
1:A:2:ILE:HG21	1:A:40:ASN:ND2	0.63	2.09	19	1
1:B:72:LEU:HD22	1:B:72:LEU:O	0.63	1.94	20	11
1:B:67:MET:SD	1:B:67:MET:N	0.62	2.72	14	1
1:A:9:ILE:HD13	1:A:60:ILE:CG2	0.62	2.23	15	5
1:B:75:ILE:HD13	1:B:126:ILE:HA	0.62	1.72	12	2
1:A:43:LEU:HD22	1:B:106:ASN:HD21	0.62	1.54	19	1
1:B:72:LEU:HD13	1:B:72:LEU:C	0.62	2.19	11	13
1:A:64:GLN:CB	1:A:65:PRO:CD	0.62	2.77	20	3
1:A:9:ILE:CD1	1:A:9:ILE:N	0.62	2.63	12	1
1:A:47:LEU:HD21	1:B:123:LEU:CB	0.62	2.25	9	1
1:A:20:LEU:CD2	1:A:31:ILE:HG21	0.62	2.24	11	6
1:A:13:LYS:NZ	1:A:53:LEU:O	0.62	2.33	13	16
1:A:13:LYS:NZ	1:A:55:THR:OG1	0.62	2.32	13	4
1:B:84:SER:OG	1:B:94:ARG:NH1	0.62	2.31	19	11
1:A:64:GLN:HB2	1:A:65:PRO:HD3	0.61	1.71	20	2
1:A:9:ILE:HG21	1:A:55:THR:HG21	0.61	1.72	15	4
1:B:90:LEU:HD11	1:B:115:ILE:HG12	0.61	1.73	12	1
1:B:76:ARG:HE	1:B:83:GLN:CD	0.61	2.04	7	1
1:A:53:LEU:C	1:A:53:LEU:HD12	0.61	2.20	10	1
1:B:75:ILE:CG2	1:B:119:LEU:HD11	0.61	2.25	1	2
1:A:13:LYS:HD2	1:A:53:LEU:HD11	0.61	1.73	4	1
1:A:32:ASN:O	1:A:36:LYS:NZ	0.61	2.33	16	4
1:B:72:LEU:HD21	1:B:83:GLN:HE22	0.61	1.54	18	1
1:A:2:ILE:O	1:A:4:ASN:N	0.60	2.31	4	2
1:B:86:LEU:H	1:B:86:LEU:CD1	0.60	2.09	7	4
1:B:75:ILE:HG21	1:B:121:THR:HG21	0.60	1.72	10	2
1:A:43:LEU:HD13	1:A:44:GLN:N	0.60	2.11	18	1
1:B:86:LEU:HD13	1:B:86:LEU:N	0.60	2.10	7	3
1:A:3:ILE:HG21	1:A:62:GLN:NE2	0.60	2.11	4	2
1:B:75:ILE:HD13	1:B:75:ILE:N	0.60	2.10	2	2
1:B:95:GLN:CD	1:B:95:GLN:C	0.60	2.69	1	1
1:B:70:ASN:ND2	1:B:100:ILE:HG22	0.60	2.11	4	1
1:A:57:LEU:HD12	1:B:109:LEU:HD21	0.60	1.74	9	1
1:B:72:LEU:HD21	1:B:119:LEU:HG	0.60	1.74	19	2
1:A:44:GLN:OE1	1:B:129:TRP:NE1	0.60	2.34	12	2
1:A:55:THR:HG23	1:A:56:PRO:HD2	0.59	1.74	17	5
1:B:73:LYS:HG3	1:B:74:LEU:HD22	0.59	1.73	14	2
1:B:76:ARG:NH1	1:B:81:ILE:O	0.59	2.35	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:79:LYS:NZ	1:B:121:THR:OG1	0.59	2.32	4	1
1:B:70:ASN:ND2	1:B:100:ILE:CG2	0.59	2.66	4	2
1:A:7:LYS:H	1:A:7:LYS:CD	0.59	2.10	7	2
1:A:23:LEU:HD13	1:A:52:TYR:CD1	0.59	2.32	17	3
1:B:75:ILE:HG22	1:B:119:LEU:HD11	0.59	1.74	15	5
1:A:53:LEU:HD13	1:A:54:ASN:ND2	0.59	2.11	16	1
1:A:57:LEU:HD13	1:A:57:LEU:O	0.59	1.97	16	2
1:A:63:TRP:CZ3	1:B:114:LYS:HG3	0.59	2.33	15	2
1:B:107:PRO:HB3	1:B:111:LEU:HD12	0.59	1.74	4	2
1:A:6:LEU:C	1:A:6:LEU:HD13	0.59	2.23	13	14
1:A:9:ILE:HD12	1:A:9:ILE:N	0.59	2.13	1	4
1:B:115:ILE:O	1:B:119:LEU:CB	0.59	2.51	4	9
1:A:20:LEU:HD13	1:A:20:LEU:N	0.58	2.13	1	4
1:B:72:LEU:HD23	1:B:126:ILE:CG2	0.58	2.28	13	2
1:A:63:TRP:NE1	1:B:113:LEU:HD13	0.58	2.12	3	3
1:B:95:GLN:H	1:B:95:GLN:CD	0.58	2.06	16	2
1:B:86:LEU:C	1:B:86:LEU:HD23	0.58	2.23	14	1
1:B:119:LEU:HD13	1:B:120:ASN:ND2	0.58	2.13	16	2
1:B:107:PRO:HG2	1:B:127:PHE:CZ	0.58	2.32	2	2
1:A:6:LEU:HD23	1:A:7:LYS:N	0.58	2.14	18	2
1:B:89:LEU:HD12	1:B:118:TYR:CG	0.58	2.34	9	1
1:A:35:GLU:HG3	1:A:36:LYS:CD	0.58	2.28	15	1
1:B:110:GLN:OE1	1:B:114:LYS:NZ	0.58	2.35	6	4
1:B:120:ASN:ND2	1:B:120:ASN:C	0.58	2.61	16	1
1:B:102:LYS:N	1:B:102:LYS:HD3	0.58	2.14	12	2
1:A:29:GLN:OE1	1:A:38:LYS:NZ	0.58	2.36	11	1
1:B:79:LYS:NZ	1:B:119:LEU:O	0.58	2.35	4	16
1:B:72:LEU:HD23	1:B:73:LYS:N	0.57	2.15	18	2
1:A:5:ASN:HD21	1:A:62:GLN:N	0.57	1.97	2	1
1:A:9:ILE:N	1:A:9:ILE:HD13	0.57	2.13	2	2
1:A:64:GLN:N	1:B:110:GLN:OE1	0.57	2.34	16	3
1:A:3:ILE:HD13	1:A:62:GLN:HG2	0.57	1.77	4	2
1:B:97:ILE:HD13	1:B:100:ILE:HD12	0.57	1.76	9	3
1:A:29:GLN:CD	1:A:29:GLN:C	0.57	2.73	1	1
1:A:53:LEU:HD22	1:A:53:LEU:C	0.57	2.22	16	1
1:A:10:ARG:NE	1:A:17:GLN:OE1	0.57	2.38	8	5
1:A:38:LYS:NZ	1:A:39:TYR:OH	0.57	2.37	1	6
1:B:123:LEU:HD13	1:B:123:LEU:O	0.57	2.00	7	12
1:A:9:ILE:CG2	1:A:53:LEU:HD21	0.57	2.30	4	1
1:B:84:SER:OG	1:B:94:ARG:NE	0.57	2.36	16	1
1:A:13:LYS:HD2	1:A:53:LEU:CD1	0.57	2.30	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:74:LEU:H	1:B:74:LEU:CD1	0.57	1.97	11	1
1:A:10:ARG:NE	1:A:15:ILE:O	0.56	2.31	18	9
1:B:75:ILE:N	1:B:75:ILE:HD12	0.56	2.15	3	2
1:A:9:ILE:HD11	1:A:59:ASP:O	0.56	1.99	5	2
1:A:21:ALA:HB1	1:A:26:VAL:O	0.56	2.00	18	4
1:A:43:LEU:C	1:A:43:LEU:CD2	0.56	2.78	18	1
1:B:76:ARG:NE	1:B:83:GLN:OE1	0.56	2.32	11	3
1:A:57:LEU:O	1:A:57:LEU:HD13	0.56	1.99	18	6
1:B:69:ILE:HG21	1:B:128:GLN:NE2	0.56	2.15	15	1
1:A:46:ALA:HB1	1:B:109:LEU:HD23	0.56	1.78	18	1
1:A:20:LEU:H	1:A:20:LEU:CD1	0.56	2.13	12	4
1:A:24:LEU:HB3	1:A:45:LEU:HD21	0.56	1.74	8	2
1:B:79:LYS:C	1:B:80:LYS:HG3	0.56	2.26	11	2
1:A:63:TRP:CZ3	1:B:110:GLN:HG2	0.56	2.36	15	1
1:B:86:LEU:N	1:B:86:LEU:HD13	0.56	2.15	16	1
1:A:7:LYS:HG3	1:A:8:LEU:HD22	0.56	1.78	4	5
1:A:53:LEU:C	1:A:53:LEU:CD1	0.56	2.79	10	2
1:B:76:ARG:HD3	1:B:77:GLU:N	0.56	2.15	11	3
1:B:67:MET:SD	1:B:68:ILE:HG12	0.56	2.41	16	1
1:B:79:LYS:NZ	1:B:120:ASN:CG	0.56	2.64	14	1
1:B:90:LEU:HD21	1:B:115:ILE:HA	0.56	1.78	1	1
1:A:1:MET:HG3	1:A:2:ILE:N	0.56	2.15	8	1
1:B:75:ILE:HD11	1:B:125:ASP:O	0.56	2.01	14	3
1:B:68:ILE:HG21	1:B:106:ASN:ND2	0.56	2.15	13	1
1:A:44:GLN:CG	1:B:129:TRP:CD1	0.56	2.89	5	2
1:A:53:LEU:HD12	1:A:54:ASN:N	0.56	2.15	10	1
1:B:86:LEU:HD13	1:B:86:LEU:H	0.56	1.61	16	1
1:A:10:ARG:NH1	1:A:15:ILE:O	0.55	2.38	13	1
1:A:45:LEU:HD13	1:A:49:ILE:HG13	0.55	1.76	14	5
1:A:44:GLN:OE1	1:A:48:LYS:NZ	0.55	2.32	13	5
1:B:119:LEU:HD13	1:B:120:ASN:HD22	0.55	1.62	14	1
1:B:90:LEU:HD22	1:B:115:ILE:HG12	0.55	1.79	3	1
1:A:24:LEU:HD21	1:A:49:ILE:HA	0.55	1.78	7	1
1:B:79:LYS:NZ	1:B:120:ASN:O	0.55	2.35	17	3
1:A:37:ASN:O	1:A:37:ASN:ND2	0.55	2.40	20	2
1:A:61:PHE:CD2	1:B:109:LEU:HD13	0.55	2.37	7	4
1:A:65:PRO:O	1:B:114:LYS:NZ	0.55	2.37	11	4
1:A:11:GLU:O	1:A:14:LYS:NZ	0.55	2.34	19	3
1:A:47:LEU:HD13	1:B:124:GLU:HG2	0.55	1.78	1	2
1:A:7:LYS:O	1:A:11:GLU:HG3	0.55	2.02	17	8
1:A:5:ASN:O	1:A:8:LEU:HD13	0.55	2.02	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:TRP:CH2	1:B:114:LYS:HG3	0.55	2.37	15	2
1:B:98:ASN:O	1:B:102:LYS:NZ	0.55	2.40	12	8
1:A:43:LEU:C	1:A:43:LEU:HD23	0.55	2.26	16	3
1:B:107:PRO:HG3	1:B:127:PHE:CZ	0.55	2.37	9	1
1:A:16:SER:H	1:A:19:GLU:CD	0.55	2.10	16	2
1:A:48:LYS:HG2	1:B:129:TRP:CZ3	0.55	2.37	16	4
1:A:48:LYS:HG3	1:B:129:TRP:CH2	0.54	2.36	15	2
1:A:64:GLN:O	1:A:66:GLU:N	0.54	2.38	10	4
1:A:10:ARG:NH2	1:A:17:GLN:OE1	0.54	2.40	8	1
1:A:50:ALA:CB	1:A:57:LEU:HD22	0.54	2.32	11	1
1:A:4:ASN:C	1:A:6:LEU:H	0.54	2.10	5	7
1:B:99:GLY:O	1:B:103:ASN:N	0.54	2.41	11	2
1:B:95:GLN:O	1:B:99:GLY:N	0.54	2.37	12	1
1:A:50:ALA:HB1	1:A:55:THR:O	0.54	2.01	16	1
1:A:44:GLN:HG3	1:B:129:TRP:CD1	0.54	2.37	5	2
1:B:75:ILE:CG2	1:B:119:LEU:HD12	0.54	2.32	8	2
1:B:121:THR:HG23	1:B:122:PRO:HD2	0.54	1.77	13	9
1:A:1:MET:H3	1:A:1:MET:CE	0.54	2.15	5	1
1:A:63:TRP:CD1	1:B:113:LEU:CD1	0.54	2.90	3	1
1:A:63:TRP:CD1	1:B:113:LEU:HD13	0.54	2.36	3	1
1:B:124:GLU:H	1:B:124:GLU:CD	0.54	2.11	14	4
1:A:49:ILE:O	1:A:53:LEU:HB2	0.54	2.03	9	5
1:A:61:PHE:CG	1:B:109:LEU:HD13	0.54	2.37	20	1
1:A:35:GLU:OE2	1:A:36:LYS:NZ	0.54	2.41	18	10
1:B:102:LYS:O	1:B:103:ASN:HB3	0.54	2.02	13	6
1:B:76:ARG:NE	1:B:83:GLN:HE22	0.54	1.99	17	2
1:A:55:THR:CG2	1:A:60:ILE:HG23	0.54	2.33	8	3
1:A:1:MET:SD	1:B:110:GLN:NE2	0.54	2.81	10	1
1:A:41:PRO:CB	1:A:45:LEU:HD12	0.54	2.33	11	2
1:B:76:ARG:NE	1:B:81:ILE:O	0.54	2.30	6	10
1:A:7:LYS:NZ	1:A:35:GLU:O	0.54	2.37	4	7
1:A:36:LYS:N	1:A:36:LYS:HD3	0.54	2.18	12	1
1:A:63:TRP:CZ2	1:B:117:TYR:CE2	0.54	2.96	15	1
1:A:63:TRP:CD1	1:A:66:GLU:HA	0.54	2.38	20	1
1:A:32:ASN:OD1	1:A:36:LYS:NZ	0.53	2.42	7	2
1:A:2:ILE:HG21	1:A:40:ASN:HB3	0.53	1.80	14	3
1:B:124:GLU:HG3	1:B:129:TRP:CD1	0.53	2.38	16	1
1:A:34:ILE:HD13	1:A:41:PRO:HD3	0.53	1.81	1	1
1:A:44:GLN:OE1	1:B:130:GLN:N	0.53	2.41	9	4
1:A:8:LEU:O	1:A:12:LYS:N	0.53	2.41	13	3
1:B:73:LYS:CD	1:B:101:GLU:HB2	0.53	2.34	18	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:HD23	1:A:21:ALA:N	0.53	2.19	20	2
1:A:13:LYS:NZ	1:A:54:ASN:CG	0.53	2.66	16	1
1:A:63:TRP:NE1	1:B:110:GLN:OE1	0.53	2.38	12	1
1:B:69:ILE:N	1:B:69:ILE:CD1	0.53	2.69	15	1
1:B:68:ILE:C	1:B:69:ILE:HG12	0.53	2.28	16	1
1:B:70:ASN:HD21	1:B:106:ASN:ND2	0.53	2.02	18	1
1:A:10:ARG:O	1:A:15:ILE:N	0.53	2.41	6	3
1:A:2:ILE:HG22	1:A:61:PHE:CD1	0.53	2.38	14	1
1:A:44:GLN:HB2	1:B:68:ILE:CD1	0.53	2.33	17	2
1:A:5:ASN:O	1:A:9:ILE:HD12	0.53	2.04	19	1
1:B:101:GLU:OE2	1:B:102:LYS:NZ	0.53	2.41	16	9
1:A:5:ASN:N	1:A:60:ILE:O	0.53	2.42	12	3
1:A:10:ARG:CD	1:A:10:ARG:C	0.53	2.82	13	2
1:A:53:LEU:C	1:A:54:ASN:HD22	0.53	2.11	14	2
1:A:50:ALA:HB2	1:A:60:ILE:CD1	0.53	2.33	16	1
1:A:53:LEU:C	1:A:53:LEU:HD13	0.53	2.28	6	1
1:A:40:ASN:OD1	1:A:40:ASN:N	0.53	2.41	11	1
1:A:49:ILE:O	1:A:53:LEU:CB	0.53	2.56	4	11
1:A:19:GLU:H	1:A:19:GLU:CD	0.53	2.06	2	1
1:B:83:GLN:CD	1:B:83:GLN:N	0.53	2.67	2	2
1:A:20:LEU:O	1:A:24:LEU:N	0.53	2.41	7	2
1:A:25:GLU:OE2	1:A:48:LYS:NZ	0.53	2.41	18	2
1:B:109:LEU:N	1:B:109:LEU:HD12	0.53	2.18	18	1
1:B:115:ILE:O	1:B:119:LEU:HB2	0.53	2.04	18	9
1:A:53:LEU:O	1:A:54:ASN:CB	0.53	2.56	16	2
1:A:54:ASN:CG	1:A:54:ASN:O	0.53	2.51	14	2
1:B:74:LEU:O	1:B:78:LYS:N	0.53	2.42	6	2
1:B:102:LYS:O	1:B:103:ASN:ND2	0.53	2.40	7	1
1:B:119:LEU:O	1:B:120:ASN:ND2	0.53	2.41	14	1
1:A:9:ILE:HG22	1:A:53:LEU:CD1	0.53	2.33	15	1
1:A:57:LEU:HG	1:B:113:LEU:HD11	0.53	1.80	15	1
1:B:76:ARG:HH21	1:B:101:GLU:CD	0.53	2.12	17	1
1:A:60:ILE:HD12	1:A:61:PHE:CE2	0.52	2.39	10	1
1:B:89:LEU:HD22	1:B:118:TYR:CZ	0.52	2.39	11	2
1:A:13:LYS:C	1:A:14:LYS:HG3	0.52	2.29	11	2
1:B:109:LEU:C	1:B:109:LEU:HD23	0.52	2.29	16	1
1:A:20:LEU:HD22	1:A:20:LEU:C	0.52	2.29	5	4
1:B:86:LEU:HD22	1:B:86:LEU:C	0.52	2.28	1	3
1:B:91:GLU:OE1	1:B:114:LYS:NZ	0.52	2.43	11	1
1:B:76:ARG:CZ	1:B:83:GLN:HE22	0.52	2.17	17	1
1:B:129:TRP:C	1:B:129:TRP:CD1	0.52	2.85	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:70:ASN:HA	1:B:127:PHE:CD1	0.52	2.40	5	2
1:A:10:ARG:NH2	1:A:35:GLU:OE2	0.52	2.41	17	2
1:B:109:LEU:H	1:B:109:LEU:HD22	0.52	1.64	11	1
1:B:95:GLN:CD	1:B:95:GLN:N	0.52	2.68	16	1
1:A:47:LEU:HD21	1:B:123:LEU:HB3	0.52	1.81	9	3
1:A:63:TRP:CH2	1:B:113:LEU:HB2	0.52	2.39	15	2
1:A:4:ASN:O	1:A:6:LEU:N	0.52	2.42	5	4
1:B:110:GLN:HE21	1:B:111:LEU:N	0.52	2.03	6	2
1:B:110:GLN:CD	1:B:111:LEU:N	0.52	2.68	2	1
1:A:66:GLU:C	1:B:114:LYS:HZ2	0.52	2.12	12	3
1:A:10:ARG:HE	1:A:17:GLN:NE2	0.52	2.03	7	1
1:A:8:LEU:N	1:A:8:LEU:CD1	0.52	2.68	11	1
1:A:9:ILE:HD13	1:A:60:ILE:HA	0.52	1.82	13	2
1:A:51:TYR:O	1:A:54:ASN:ND2	0.52	2.37	15	5
1:A:9:ILE:HG22	1:A:53:LEU:HD21	0.52	1.80	4	1
1:B:76:ARG:HG2	1:B:81:ILE:O	0.52	2.04	6	6
1:A:5:ASN:OD1	1:A:5:ASN:N	0.52	2.42	8	2
1:B:119:LEU:O	1:B:120:ASN:CB	0.52	2.57	16	2
1:A:1:MET:HE3	1:A:1:MET:H3	0.52	1.64	19	1
1:A:3:ILE:HG21	1:A:62:GLN:HE21	0.52	1.65	1	1
1:A:16:SER:O	1:A:20:LEU:CD1	0.52	2.58	5	3
1:B:104:LYS:NZ	1:B:105:TYR:OH	0.52	2.40	5	4
1:B:96:THR:OG1	1:B:104:LYS:NZ	0.52	2.39	15	1
1:B:90:LEU:CB	1:B:92:VAL:HG22	0.52	2.34	14	9
1:A:40:ASN:HD22	1:B:108:SER:CB	0.52	2.17	11	1
1:B:79:LYS:NZ	1:B:120:ASN:OD1	0.52	2.39	16	2
1:A:24:LEU:HD11	1:A:49:ILE:HG12	0.51	1.82	6	2
1:B:73:LYS:HD2	1:B:101:GLU:HB2	0.51	1.81	7	1
1:A:33:GLY:C	1:A:38:LYS:HB2	0.51	2.30	10	3
1:B:79:LYS:O	1:B:80:LYS:CD	0.51	2.57	11	1
1:A:57:LEU:CB	1:B:113:LEU:HD21	0.51	2.36	1	2
1:A:9:ILE:HG21	1:A:53:LEU:HD11	0.51	1.81	6	1
1:B:82:SER:O	1:B:86:LEU:CD1	0.51	2.59	7	3
1:B:116:ALA:O	1:B:120:ASN:N	0.51	2.43	4	6
1:A:43:LEU:HD12	1:B:109:LEU:HD23	0.51	1.81	3	1
1:B:111:LEU:HD13	1:B:111:LEU:O	0.51	2.05	7	9
1:B:101:GLU:HG3	1:B:102:LYS:N	0.51	2.21	6	1
1:A:5:ASN:ND2	1:A:59:ASP:O	0.51	2.43	20	2
1:A:13:LYS:NZ	1:A:54:ASN:O	0.51	2.44	13	8
1:A:55:THR:CG2	1:A:59:ASP:HB3	0.51	2.36	13	3
1:B:96:THR:HG23	1:B:104:LYS:NZ	0.51	2.17	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:LEU:CB	1:A:26:VAL:HG22	0.51	2.35	14	11
1:A:6:LEU:HD12	1:A:49:ILE:CG2	0.51	2.36	3	1
1:B:129:TRP:CD1	1:B:130:GLN:O	0.51	2.64	17	3
1:A:63:TRP:HE1	1:A:66:GLU:C	0.51	2.14	6	1
1:B:75:ILE:HG22	1:B:119:LEU:CD1	0.51	2.35	20	3
1:B:103:ASN:HD22	1:B:103:ASN:N	0.51	2.04	14	3
1:A:7:LYS:CD	1:A:35:GLU:HB2	0.51	2.35	20	1
1:B:119:LEU:HD12	1:B:121:THR:HB	0.51	1.83	1	1
1:B:107:PRO:CG	1:B:127:PHE:CZ	0.51	2.94	2	2
1:A:64:GLN:HB3	1:A:65:PRO:CD	0.51	2.36	9	1
1:B:119:LEU:HD22	1:B:119:LEU:C	0.51	2.30	14	1
1:A:58:GLU:CD	1:A:58:GLU:N	0.51	2.68	9	2
1:A:36:LYS:O	1:A:37:ASN:HB3	0.51	2.05	14	4
1:B:100:ILE:HD13	1:B:107:PRO:HG3	0.51	1.82	7	1
1:B:102:LYS:O	1:B:103:ASN:CB	0.51	2.59	7	1
1:A:57:LEU:C	1:A:57:LEU:CD1	0.51	2.84	16	6
1:B:75:ILE:CD1	1:B:126:ILE:HA	0.51	2.36	8	2
1:B:114:LYS:HB3	1:B:118:TYR:CE2	0.51	2.41	18	1
1:A:5:ASN:ND2	1:A:62:GLN:N	0.51	2.59	2	1
1:B:70:ASN:C	1:B:72:LEU:H	0.50	2.14	17	6
1:B:95:GLN:OE1	1:B:104:LYS:NZ	0.50	2.43	10	2
1:B:77:GLU:O	1:B:80:LYS:NZ	0.50	2.36	4	6
1:B:129:TRP:C	1:B:130:GLN:HG2	0.50	2.29	19	2
1:A:3:ILE:C	1:A:5:ASN:H	0.50	2.13	13	1
1:B:73:LYS:CD	1:B:73:LYS:H	0.50	2.19	7	2
1:A:9:ILE:HD11	1:A:59:ASP:C	0.50	2.31	16	4
1:B:75:ILE:HD13	1:B:126:ILE:CG2	0.50	2.36	7	4
1:B:86:LEU:HD12	1:B:119:LEU:HG	0.50	1.83	14	1
1:A:7:LYS:O	1:A:11:GLU:CG	0.50	2.59	12	5
1:A:25:GLU:OE1	1:A:48:LYS:NZ	0.50	2.41	8	4
1:B:119:LEU:C	1:B:120:ASN:HD22	0.50	2.14	14	1
1:A:4:ASN:HD21	1:A:40:ASN:ND2	0.50	2.04	18	1
1:A:43:LEU:HB2	1:B:68:ILE:HD12	0.50	1.83	1	1
1:B:75:ILE:O	1:B:78:LYS:HB3	0.50	2.06	15	9
1:B:106:ASN:ND2	1:B:107:PRO:HD2	0.50	2.21	13	1
1:A:47:LEU:HB2	1:B:129:TRP:CH2	0.50	2.42	2	2
1:B:90:LEU:O	1:B:91:GLU:HB2	0.50	2.07	19	6
1:B:112:ALA:HB1	1:B:123:LEU:HD21	0.50	1.83	8	2
1:A:35:GLU:HG3	1:A:36:LYS:HD3	0.50	1.82	4	4
1:B:110:GLN:CD	1:B:114:LYS:HE3	0.50	2.31	16	2
1:B:129:TRP:NE1	1:B:130:GLN:O	0.50	2.45	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:GLN:NE2	1:A:45:LEU:N	0.50	2.59	10	2
1:A:9:ILE:HD12	1:A:9:ILE:H	0.50	1.67	15	2
1:A:23:LEU:HD12	1:A:52:TYR:CE2	0.50	2.40	9	1
1:B:89:LEU:HB3	1:B:118:TYR:CD2	0.50	2.42	17	3
1:A:44:GLN:OE1	1:A:44:GLN:N	0.50	2.45	2	1
1:A:47:LEU:HB3	1:B:129:TRP:CH2	0.50	2.42	12	1
1:A:64:GLN:O	1:B:110:GLN:CD	0.49	2.55	4	1
1:A:7:LYS:O	1:A:11:GLU:N	0.49	2.41	7	2
1:B:128:GLN:OE1	1:B:130:GLN:NE2	0.49	2.42	20	1
1:B:73:LYS:O	1:B:77:GLU:CG	0.49	2.60	5	7
1:B:112:ALA:HB1	1:B:123:LEU:CD1	0.49	2.38	9	1
1:A:44:GLN:HA	1:A:47:LEU:HD12	0.49	1.84	1	2
1:A:5:ASN:C	1:A:8:LEU:CD1	0.49	2.86	11	1
1:A:17:GLN:OE1	1:A:17:GLN:N	0.49	2.45	11	1
1:B:111:LEU:CD1	1:B:115:ILE:HD11	0.49	2.37	11	2
1:B:70:ASN:HD21	1:B:100:ILE:CG2	0.49	2.20	4	1
1:A:44:GLN:CD	1:B:67:MET:SD	0.49	2.95	10	1
1:B:110:GLN:OE1	1:B:114:LYS:HE3	0.49	2.08	13	2
1:B:121:THR:HG21	1:B:126:ILE:HG23	0.49	1.85	14	1
1:B:76:ARG:NH1	1:B:77:GLU:OE2	0.49	2.43	17	1
1:A:1:MET:N	1:A:64:GLN:HB2	0.49	2.23	3	1
1:B:96:THR:O	1:B:100:ILE:HG13	0.49	2.06	12	3
1:A:3:ILE:C	1:A:4:ASN:HD22	0.49	2.15	7	1
1:A:3:ILE:HD13	1:A:62:GLN:CG	0.49	2.37	15	1
1:B:71:ASN:C	1:B:74:LEU:CD1	0.49	2.85	11	1
1:A:9:ILE:O	1:A:12:LYS:HB3	0.49	2.07	13	11
1:A:20:LEU:N	1:A:20:LEU:CD1	0.49	2.74	12	3
1:B:83:GLN:HB3	1:B:94:ARG:HG3	0.49	1.85	5	3
1:A:1:MET:H3	1:A:64:GLN:HB2	0.49	1.66	3	1
1:A:63:TRP:CE2	1:B:113:LEU:HB3	0.49	2.43	5	1
1:A:46:ALA:HB1	1:B:109:LEU:HD21	0.49	1.84	8	1
1:B:73:LYS:O	1:B:77:GLU:HG2	0.49	2.08	2	2
1:B:111:LEU:HD13	1:B:115:ILE:HG13	0.49	1.84	3	4
1:A:1:MET:C	1:A:3:ILE:H	0.49	2.16	4	1
1:B:82:SER:HB2	1:B:85:GLU:CD	0.49	2.33	5	1
1:A:65:PRO:O	1:A:66:GLU:HB2	0.49	2.08	7	2
1:A:44:GLN:NE2	1:B:130:GLN:O	0.48	2.45	1	1
1:B:121:THR:CG2	1:B:122:PRO:HD2	0.48	2.38	18	4
1:B:95:GLN:HA	1:B:98:ASN:ND2	0.48	2.23	11	11
1:B:123:LEU:O	1:B:127:PHE:N	0.48	2.40	6	1
1:A:5:ASN:O	1:A:5:ASN:ND2	0.48	2.46	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:GLN:CB	1:B:68:ILE:HD11	0.48	2.39	10	1
1:A:35:GLU:CD	1:A:36:LYS:CE	0.48	2.86	13	1
1:B:119:LEU:O	1:B:120:ASN:CG	0.48	2.56	14	1
1:B:120:ASN:CG	1:B:120:ASN:O	0.48	2.55	14	2
1:A:11:GLU:OE1	1:A:14:LYS:NZ	0.48	2.42	18	4
1:A:57:LEU:HD11	1:B:109:LEU:HD21	0.48	1.85	16	1
1:B:117:TYR:O	1:B:120:ASN:ND2	0.48	2.42	11	6
1:B:90:LEU:HD23	1:B:114:LYS:HB3	0.48	1.85	7	1
1:B:123:LEU:HD13	1:B:123:LEU:C	0.48	2.34	7	2
1:A:41:PRO:HB3	1:A:45:LEU:HD12	0.48	1.86	11	1
1:A:13:LYS:CD	1:A:54:ASN:HD21	0.48	2.21	14	1
1:A:10:ARG:HD3	1:A:11:GLU:N	0.48	2.24	11	2
1:A:2:ILE:O	1:A:2:ILE:HG22	0.48	2.09	4	1
1:B:111:LEU:HD22	1:B:114:LYS:HD2	0.48	1.84	9	1
1:A:20:LEU:HD23	1:A:20:LEU:C	0.48	2.33	20	1
1:B:123:LEU:CD1	1:B:126:ILE:HD11	0.48	2.38	1	1
1:A:32:ASN:O	1:A:36:LYS:HG2	0.48	2.08	16	1
1:A:24:LEU:HD23	1:A:48:LYS:HB3	0.48	1.85	5	1
1:A:43:LEU:HD12	1:B:106:ASN:HD22	0.48	1.68	5	1
1:B:103:ASN:O	1:B:104:LYS:C	0.48	2.56	13	1
1:A:32:ASN:O	1:A:36:LYS:CG	0.48	2.62	20	1
1:A:44:GLN:CD	1:A:45:LEU:N	0.48	2.71	2	1
1:B:123:LEU:HD22	1:B:126:ILE:HD11	0.48	1.85	14	3
1:B:71:ASN:ND2	1:B:125:ASP:O	0.48	2.47	6	3
1:A:10:ARG:CG	1:A:15:ILE:O	0.48	2.61	7	1
1:A:43:LEU:HD23	1:B:123:LEU:HD11	0.48	1.86	7	1
1:A:25:GLU:CD	1:A:48:LYS:HZ2	0.48	2.15	18	1
1:B:89:LEU:HB3	1:B:118:TYR:CD1	0.48	2.44	2	1
1:B:89:LEU:HB3	1:B:118:TYR:CG	0.48	2.43	4	3
1:B:78:LYS:NZ	1:B:125:ASP:OD2	0.48	2.47	6	4
1:B:129:TRP:CD1	1:B:130:GLN:N	0.48	2.81	4	2
1:A:53:LEU:HD12	1:A:55:THR:HB	0.48	1.86	17	2
1:B:129:TRP:CD1	1:B:129:TRP:C	0.48	2.89	5	1
1:A:10:ARG:NE	1:A:17:GLN:CD	0.48	2.71	7	1
1:A:47:LEU:HB3	1:B:129:TRP:CE2	0.48	2.43	10	1
1:A:7:LYS:O	1:A:10:ARG:N	0.48	2.47	11	1
1:A:4:ASN:ND2	1:A:34:ILE:O	0.48	2.45	12	1
1:B:95:GLN:N	1:B:95:GLN:OE1	0.48	2.46	14	1
1:B:100:ILE:HD13	1:B:107:PRO:HD3	0.48	1.86	14	2
1:A:3:ILE:HB	1:A:62:GLN:HB3	0.47	1.86	2	2
1:A:50:ALA:O	1:A:54:ASN:N	0.47	2.46	17	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:PHE:CE2	1:B:109:LEU:HD13	0.47	2.44	4	1
1:B:89:LEU:HD13	1:B:118:TYR:CE1	0.47	2.44	10	3
1:B:100:ILE:CG1	1:B:105:TYR:CE1	0.47	2.97	13	1
1:A:44:GLN:HG2	1:B:129:TRP:CZ3	0.47	2.44	15	1
1:A:7:LYS:HD2	1:A:35:GLU:HB2	0.47	1.84	7	1
1:B:100:ILE:HG12	1:B:105:TYR:CE1	0.47	2.44	13	1
1:A:47:LEU:HD21	1:B:123:LEU:CG	0.47	2.39	14	1
1:A:66:GLU:OXT	1:B:114:LYS:NZ	0.47	2.44	2	2
1:B:68:ILE:HD12	1:B:68:ILE:N	0.47	2.25	3	1
1:A:35:GLU:CG	1:A:36:LYS:HD3	0.47	2.40	15	2
1:A:13:LYS:NZ	1:A:54:ASN:OD1	0.47	2.41	16	1
1:A:4:ASN:CG	1:A:34:ILE:HG22	0.47	2.34	18	1
1:A:63:TRP:CZ2	1:B:113:LEU:HB3	0.47	2.45	6	2
1:A:63:TRP:NE1	1:B:113:LEU:HD12	0.47	2.24	7	1
1:A:40:ASN:ND2	1:A:41:PRO:HD2	0.47	2.24	13	1
1:A:55:THR:HG22	1:A:60:ILE:HG23	0.47	1.87	17	1
1:A:10:ARG:NH1	1:A:11:GLU:OE1	0.47	2.41	11	2
1:B:126:ILE:HG13	1:B:127:PHE:CD2	0.47	2.45	9	1
1:B:98:ASN:O	1:B:102:LYS:HG2	0.47	2.10	12	3
1:B:99:GLY:C	1:B:104:LYS:HB2	0.47	2.35	18	4
1:A:66:GLU:C	1:B:110:GLN:HE21	0.47	2.18	2	2
1:B:115:ILE:O	1:B:119:LEU:N	0.47	2.39	2	1
1:A:23:LEU:HB3	1:A:52:TYR:CD2	0.47	2.44	5	1
1:A:66:GLU:O	1:B:114:LYS:NZ	0.47	2.40	6	6
1:B:77:GLU:OE1	1:B:80:LYS:NZ	0.47	2.44	15	4
1:B:106:ASN:ND2	1:B:106:ASN:H	0.47	2.07	8	1
1:A:17:GLN:HB3	1:A:28:ARG:HG3	0.47	1.86	18	2
1:A:48:LYS:NZ	1:B:130:GLN:O	0.47	2.39	14	2
1:A:34:ILE:HG21	1:A:41:PRO:HD3	0.47	1.86	19	3
1:A:6:LEU:HD22	1:A:6:LEU:C	0.47	2.34	17	1
1:A:55:THR:CG2	1:A:56:PRO:HD2	0.47	2.40	2	2
1:B:119:LEU:O	1:B:120:ASN:HB2	0.47	2.10	4	3
1:B:89:LEU:HB2	1:B:118:TYR:CZ	0.47	2.45	9	1
1:B:75:ILE:CD1	1:B:75:ILE:N	0.47	2.77	11	1
1:B:124:GLU:CD	1:B:129:TRP:HB2	0.47	2.35	12	1
1:A:45:LEU:HD13	1:A:45:LEU:O	0.47	2.10	5	5
1:A:19:GLU:O	1:A:22:ALA:HB3	0.47	2.09	5	1
1:A:47:LEU:HD13	1:B:129:TRP:NE1	0.47	2.25	14	2
1:A:43:LEU:HD12	1:B:107:PRO:O	0.47	2.10	15	1
1:A:63:TRP:HE1	1:B:113:LEU:HD12	0.46	1.70	7	1
1:B:76:ARG:HH21	1:B:83:GLN:NE2	0.46	2.07	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:ILE:CD1	1:B:108:SER:HB3	0.46	2.40	8	1
1:A:45:LEU:C	1:A:45:LEU:HD13	0.46	2.35	12	2
1:B:104:LYS:HE2	1:B:105:TYR:CE2	0.46	2.44	8	3
1:A:47:LEU:HB3	1:B:129:TRP:CZ3	0.46	2.45	6	2
1:B:83:GLN:HA	1:B:86:LEU:HD11	0.46	1.86	7	1
1:B:86:LEU:N	1:B:86:LEU:CD1	0.46	2.78	12	3
1:A:19:GLU:O	1:A:23:LEU:HG	0.46	2.10	2	3
1:B:69:ILE:HD11	1:B:130:GLN:OE1	0.46	2.11	3	1
1:A:7:LYS:NZ	1:A:35:GLU:OE1	0.46	2.45	13	2
1:A:3:ILE:O	1:A:5:ASN:N	0.46	2.41	13	1
1:B:76:ARG:CD	1:B:76:ARG:C	0.46	2.88	13	1
1:A:29:GLN:HG2	1:A:30:THR:N	0.46	2.26	18	2
1:A:10:ARG:HG2	1:A:15:ILE:O	0.46	2.11	2	4
1:A:40:ASN:HB2	1:B:109:LEU:HD12	0.46	1.88	3	1
1:B:71:ASN:CB	1:B:74:LEU:HD23	0.46	2.41	14	1
1:B:98:ASN:O	1:B:102:LYS:HD2	0.46	2.10	3	2
1:B:101:GLU:HG3	1:B:102:LYS:HD3	0.46	1.88	12	2
1:B:73:LYS:NZ	1:B:101:GLU:O	0.46	2.41	16	1
1:A:1:MET:O	1:A:64:GLN:N	0.46	2.49	3	1
1:B:75:ILE:HG22	1:B:119:LEU:CD2	0.46	2.37	4	1
1:A:1:MET:CG	1:A:2:ILE:H	0.46	2.24	5	1
1:A:1:MET:CG	1:A:2:ILE:N	0.46	2.77	8	1
1:A:23:LEU:HD23	1:A:23:LEU:N	0.46	2.26	9	1
1:B:110:GLN:NE2	1:B:114:LYS:HE3	0.46	2.26	9	2
1:A:4:ASN:ND2	1:A:61:PHE:CE1	0.46	2.84	10	1
1:A:47:LEU:HB3	1:B:129:TRP:CZ2	0.46	2.45	12	5
1:B:106:ASN:OD1	1:B:107:PRO:HD2	0.46	2.11	10	1
1:A:35:GLU:CD	1:A:36:LYS:HE2	0.46	2.35	13	1
1:B:75:ILE:HD11	1:B:125:ASP:C	0.46	2.36	14	2
1:A:48:LYS:O	1:A:52:TYR:HB3	0.46	2.11	16	1
1:A:53:LEU:O	1:A:54:ASN:CG	0.46	2.59	16	1
1:B:76:ARG:NH1	1:B:77:GLU:HG2	0.46	2.26	1	3
1:B:69:ILE:HG12	1:B:130:GLN:CG	0.46	2.41	2	1
1:B:121:THR:CG2	1:B:125:ASP:HB3	0.46	2.41	7	1
1:B:112:ALA:HB1	1:B:123:LEU:HD11	0.46	1.87	9	1
1:B:69:ILE:HD11	1:B:130:GLN:HG3	0.46	1.83	15	1
1:A:24:LEU:O	1:A:25:GLU:HB2	0.46	2.10	7	6
1:A:44:GLN:HE21	1:A:45:LEU:N	0.46	2.08	4	1
1:B:110:GLN:CD	1:B:114:LYS:HZ3	0.46	2.17	6	1
1:A:13:LYS:O	1:A:14:LYS:CD	0.46	2.64	11	1
1:A:9:ILE:HG21	1:A:60:ILE:HG22	0.45	1.87	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:68:ILE:CG2	1:B:106:ASN:ND2	0.45	2.79	7	1
1:A:13:LYS:HZ2	1:A:54:ASN:CG	0.45	2.19	16	1
1:A:57:LEU:HD11	1:B:109:LEU:CD2	0.45	2.41	16	1
1:A:44:GLN:CB	1:B:68:ILE:CD1	0.45	2.94	17	1
1:A:43:LEU:CB	1:B:112:ALA:CB	0.45	2.93	18	1
1:B:116:ALA:HB2	1:B:123:LEU:HD22	0.45	1.87	19	1
1:A:17:GLN:NE2	1:A:17:GLN:HA	0.45	2.26	7	1
1:A:29:GLN:NE2	1:A:30:THR:OG1	0.45	2.50	4	2
1:A:14:LYS:HD3	1:A:14:LYS:C	0.45	2.36	11	1
1:A:37:ASN:HD22	1:A:37:ASN:N	0.45	2.09	12	2
1:A:1:MET:SD	1:A:2:ILE:HG12	0.45	2.52	16	2
1:A:2:ILE:HG22	1:A:61:PHE:HB3	0.45	1.87	16	1
1:B:74:LEU:O	1:B:78:LYS:HB3	0.45	2.12	17	1
1:B:76:ARG:NH1	1:B:77:GLU:OE1	0.45	2.49	1	2
1:A:30:THR:O	1:A:34:ILE:N	0.45	2.45	4	3
1:A:10:ARG:HE	1:A:17:GLN:CD	0.45	2.20	7	1
1:B:119:LEU:C	1:B:120:ASN:ND2	0.45	2.74	14	1
1:A:13:LYS:O	1:A:14:LYS:HD3	0.45	2.12	11	1
1:A:23:LEU:HD22	1:A:52:TYR:CZ	0.45	2.47	11	1
1:A:61:PHE:O	1:A:62:GLN:C	0.45	2.60	11	1
1:B:79:LYS:O	1:B:80:LYS:HD3	0.45	2.12	11	1
1:B:83:GLN:HE22	1:B:101:GLU:CD	0.45	2.19	12	1
1:A:2:ILE:CD1	1:B:108:SER:CB	0.45	2.94	14	1
1:B:104:LYS:NZ	1:B:105:TYR:CE2	0.45	2.84	19	1
1:A:12:LYS:NZ	1:A:59:ASP:OD2	0.45	2.40	14	2
1:A:64:GLN:C	1:A:66:GLU:H	0.45	2.20	12	2
1:B:107:PRO:CB	1:B:111:LEU:HD12	0.45	2.42	6	1
1:A:23:LEU:HD12	1:A:52:TYR:CG	0.45	2.44	9	1
1:B:89:LEU:N	1:B:89:LEU:CD2	0.45	2.79	9	1
1:A:32:ASN:O	1:A:35:GLU:HG2	0.45	2.12	14	1
1:A:60:ILE:HG13	1:A:61:PHE:CD2	0.45	2.47	19	2
1:A:20:LEU:O	1:A:24:LEU:HG	0.45	2.11	8	11
1:B:70:ASN:O	1:B:72:LEU:N	0.45	2.48	17	6
1:B:86:LEU:O	1:B:90:LEU:HG	0.45	2.12	10	10
1:A:63:TRP:CH2	1:B:113:LEU:HB3	0.45	2.46	20	3
1:A:47:LEU:HD13	1:B:129:TRP:HE1	0.45	1.72	14	1
1:B:71:ASN:N	1:B:126:ILE:O	0.45	2.50	2	1
1:B:94:ARG:NH1	1:B:95:GLN:OE1	0.45	2.50	16	1
1:A:38:LYS:HG3	1:A:39:TYR:CE1	0.45	2.47	7	2
1:B:69:ILE:HB	1:B:128:GLN:HG2	0.45	1.89	9	1
1:B:93:SER:OG	1:B:96:THR:OG1	0.45	2.33	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:113:LEU:O	1:B:117:TYR:N	0.45	2.43	18	2
1:A:1:MET:HE3	1:A:2:ILE:HG12	0.45	1.89	1	1
1:A:9:ILE:CD1	1:A:60:ILE:HA	0.45	2.42	7	1
1:A:21:ALA:O	1:A:25:GLU:N	0.45	2.50	10	3
1:A:37:ASN:O	1:A:37:ASN:CG	0.45	2.60	14	2
1:A:43:LEU:HD13	1:B:127:PHE:CE2	0.45	2.47	14	1
1:B:95:GLN:NE2	1:B:96:THR:HG23	0.44	2.27	8	1
1:A:8:LEU:O	1:A:12:LYS:HB3	0.44	2.12	17	2
1:A:15:ILE:HG21	1:A:20:LEU:HD13	0.44	1.89	10	1
1:B:80:LYS:HD3	1:B:80:LYS:C	0.44	2.37	11	1
1:A:46:ALA:HB2	1:B:109:LEU:HD22	0.44	1.88	13	1
1:A:35:GLU:HG3	1:A:36:LYS:HG3	0.44	1.88	3	1
1:A:66:GLU:C	1:B:110:GLN:NE2	0.44	2.75	9	1
1:B:98:ASN:O	1:B:101:GLU:HG2	0.44	2.13	16	2
1:A:38:LYS:HE2	1:A:39:TYR:CE2	0.44	2.47	8	4
1:A:41:PRO:HG3	1:A:61:PHE:CZ	0.44	2.48	12	2
1:A:23:LEU:HB3	1:A:52:TYR:CG	0.44	2.47	6	1
1:A:3:ILE:O	1:A:4:ASN:ND2	0.44	2.49	14	1
1:A:18:SER:HA	1:A:28:ARG:NE	0.44	2.28	14	1
1:A:10:ARG:HG3	1:A:17:GLN:NE2	0.44	2.26	18	1
1:B:104:LYS:O	1:B:105:TYR:C	0.44	2.60	18	5
1:A:40:ASN:OD1	1:B:109:LEU:N	0.44	2.42	8	1
1:B:93:SER:OG	1:B:95:GLN:NE2	0.44	2.48	8	1
1:B:110:GLN:CD	1:B:110:GLN:C	0.44	2.85	13	1
1:A:43:LEU:HD21	1:B:112:ALA:CB	0.44	2.43	6	1
1:B:71:ASN:O	1:B:75:ILE:HD12	0.44	2.13	7	2
1:A:66:GLU:C	1:B:114:LYS:HZ1	0.44	2.19	13	1
1:A:13:LYS:HE3	1:A:54:ASN:ND2	0.44	2.27	14	1
1:A:36:LYS:O	1:A:37:ASN:ND2	0.44	2.40	15	1
1:B:126:ILE:HD12	1:B:127:PHE:CE2	0.44	2.48	15	1
1:A:45:LEU:O	1:A:49:ILE:N	0.44	2.46	19	1
1:A:10:ARG:NH2	1:A:35:GLU:OE1	0.44	2.50	20	1
1:A:57:LEU:HB3	1:B:113:LEU:HD11	0.44	1.88	2	1
1:B:95:GLN:NE2	1:B:96:THR:OG1	0.44	2.39	9	2
1:A:63:TRP:CE2	1:B:117:TYR:CE2	0.44	3.06	15	1
1:B:75:ILE:N	1:B:75:ILE:CD1	0.44	2.81	2	2
1:B:83:GLN:CB	1:B:94:ARG:HG3	0.44	2.43	5	1
1:A:19:GLU:OE1	1:A:19:GLU:N	0.44	2.50	10	1
1:B:69:ILE:HG13	1:B:128:GLN:CG	0.44	2.43	11	1
1:B:124:GLU:O	1:B:128:GLN:HA	0.44	2.13	5	1
1:A:35:GLU:HG3	1:A:36:LYS:HE2	0.44	1.89	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LYS:HD3	1:A:36:LYS:N	0.44	2.27	15	1
1:A:46:ALA:CB	1:B:109:LEU:HD21	0.44	2.42	17	1
1:B:70:ASN:HB2	1:B:101:GLU:HA	0.44	1.89	18	1
1:A:2:ILE:HD11	1:B:108:SER:HB3	0.43	1.90	1	1
1:B:70:ASN:O	1:B:73:LYS:HE2	0.43	2.13	4	2
1:A:9:ILE:HG21	1:A:60:ILE:CG2	0.43	2.42	3	1
1:A:29:GLN:HA	1:A:32:ASN:ND2	0.43	2.28	8	6
1:A:16:SER:O	1:A:19:GLU:HG2	0.43	2.13	17	4
1:A:1:MET:CA	1:A:64:GLN:HB2	0.43	2.43	7	1
1:B:71:ASN:ND2	1:B:126:ILE:O	0.43	2.51	12	2
1:A:43:LEU:HD22	1:A:43:LEU:H	0.43	1.72	11	1
1:A:30:THR:O	1:A:34:ILE:HG13	0.43	2.13	15	1
1:A:38:LYS:HG2	1:A:39:TYR:CD2	0.43	2.48	16	1
1:A:53:LEU:C	1:A:53:LEU:CD2	0.43	2.91	16	1
1:A:64:GLN:H	1:B:110:GLN:CD	0.43	2.18	16	1
1:B:72:LEU:HD21	1:B:83:GLN:NE2	0.43	2.26	18	1
1:B:67:MET:C	1:B:68:ILE:HD12	0.43	2.37	3	1
1:A:9:ILE:CD1	1:A:59:ASP:C	0.43	2.91	6	1
1:A:36:LYS:O	1:A:38:LYS:N	0.43	2.51	15	1
1:B:89:LEU:HD13	1:B:118:TYR:HB3	0.43	1.90	4	1
1:A:61:PHE:CB	1:B:109:LEU:HD13	0.43	2.43	6	1
1:B:92:VAL:HG21	1:B:97:ILE:HD11	0.43	1.89	6	1
1:A:3:ILE:C	1:A:5:ASN:N	0.43	2.77	13	1
1:A:13:LYS:CE	1:A:54:ASN:HD21	0.43	2.27	14	1
1:A:57:LEU:HD13	1:A:57:LEU:C	0.43	2.38	20	3
1:B:115:ILE:O	1:B:119:LEU:HB3	0.43	2.12	7	2
1:A:49:ILE:O	1:A:53:LEU:HB3	0.43	2.13	11	1
1:A:40:ASN:HD21	1:B:108:SER:CB	0.43	2.25	12	1
1:A:27:SER:OG	1:A:30:THR:OG1	0.43	2.31	14	1
1:A:2:ILE:CD1	1:B:110:GLN:HB2	0.43	2.43	15	1
1:A:64:GLN:O	1:B:114:LYS:NZ	0.43	2.39	15	1
1:B:119:LEU:O	1:B:120:ASN:HB3	0.43	2.12	16	1
1:B:79:LYS:O	1:B:81:ILE:HD12	0.43	2.14	17	1
1:A:2:ILE:HG21	1:A:40:ASN:HD21	0.43	1.73	19	2
1:A:9:ILE:N	1:A:9:ILE:CD1	0.43	2.81	1	1
1:B:95:GLN:OE1	1:B:95:GLN:N	0.43	2.45	6	2
1:A:45:LEU:CD1	1:A:49:ILE:HD11	0.43	2.44	11	1
1:A:51:TYR:CE2	1:B:129:TRP:CZ2	0.43	3.06	15	1
1:B:79:LYS:HB2	1:B:81:ILE:HG12	0.43	1.91	5	3
1:B:111:LEU:HD13	1:B:111:LEU:C	0.43	2.39	7	6
1:A:58:GLU:HG3	1:B:113:LEU:HD22	0.43	1.89	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:81:ILE:CG2	1:B:86:LEU:HD12	0.43	2.44	7	1
1:B:73:LYS:HB3	1:B:101:GLU:CD	0.43	2.37	10	1
1:A:5:ASN:O	1:A:8:LEU:CD1	0.43	2.66	11	1
1:A:42:SER:O	1:A:46:ALA:N	0.43	2.39	18	1
1:A:13:LYS:HB2	1:A:15:ILE:HG12	0.43	1.90	6	5
1:A:43:LEU:HD13	1:B:127:PHE:CG	0.43	2.49	4	1
1:A:53:LEU:O	1:A:53:LEU:HD13	0.43	2.14	5	1
1:A:57:LEU:O	1:A:61:PHE:N	0.43	2.44	5	3
1:A:4:ASN:HA	1:A:61:PHE:CD2	0.43	2.48	8	1
1:A:20:LEU:HD21	1:A:24:LEU:HD11	0.43	1.91	13	1
1:B:72:LEU:CD2	1:B:126:ILE:HG22	0.43	2.37	13	1
1:A:13:LYS:CE	1:A:54:ASN:ND2	0.43	2.82	14	1
1:B:124:GLU:CD	1:B:124:GLU:H	0.43	2.22	9	1
1:B:70:ASN:OD1	1:B:106:ASN:ND2	0.43	2.47	10	2
1:A:43:LEU:HD23	1:B:109:LEU:CD2	0.43	2.44	14	1
1:A:7:LYS:HD3	1:A:35:GLU:HB2	0.43	1.90	20	1
1:B:72:LEU:O	1:B:75:ILE:N	0.43	2.52	3	1
1:B:76:ARG:NE	1:B:83:GLN:CD	0.43	2.75	7	1
1:A:55:THR:HG23	1:A:59:ASP:HB3	0.43	1.89	8	1
1:A:63:TRP:O	1:A:64:GLN:NE2	0.43	2.51	14	3
1:A:53:LEU:C	1:A:54:ASN:ND2	0.43	2.77	16	1
1:A:45:LEU:HD13	1:A:45:LEU:C	0.43	2.38	5	4
1:A:33:GLY:O	1:A:38:LYS:N	0.43	2.39	8	1
1:B:103:ASN:O	1:B:103:ASN:ND2	0.43	2.52	11	1
1:A:10:ARG:HG2	1:A:15:ILE:HB	0.43	1.91	16	1
1:A:38:LYS:O	1:A:39:TYR:C	0.42	2.61	9	3
1:B:119:LEU:O	1:B:119:LEU:HD13	0.42	2.13	1	1
1:B:111:LEU:C	1:B:111:LEU:HD13	0.42	2.39	8	3
1:A:46:ALA:HB1	1:A:57:LEU:HD11	0.42	1.90	4	2
1:B:72:LEU:C	1:B:72:LEU:CD1	0.42	2.91	11	1
1:A:32:ASN:C	1:A:32:ASN:OD1	0.42	2.61	19	2
1:A:36:LYS:CD	1:A:36:LYS:N	0.42	2.82	15	1
1:A:57:LEU:CD1	1:A:61:PHE:HB2	0.42	2.44	15	1
1:A:2:ILE:C	1:A:3:ILE:HG12	0.42	2.38	18	2
1:A:61:PHE:CD2	1:B:109:LEU:CD2	0.42	3.02	18	1
1:B:81:ILE:N	1:B:81:ILE:CD1	0.42	2.82	19	1
1:B:76:ARG:CD	1:B:81:ILE:O	0.42	2.67	20	1
1:A:63:TRP:CZ3	1:B:110:GLN:HB2	0.42	2.49	2	1
1:A:64:GLN:HB3	1:A:65:PRO:HD2	0.42	1.90	9	1
1:A:29:GLN:OE1	1:A:29:GLN:N	0.42	2.41	13	2
1:A:1:MET:CE	1:A:2:ILE:H	0.42	2.27	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:GLN:H	1:A:29:GLN:CD	0.42	2.17	13	1
1:A:23:LEU:HB3	1:A:52:TYR:CD1	0.42	2.49	16	1
1:A:12:LYS:HD2	1:A:12:LYS:C	0.42	2.40	17	1
1:A:19:GLU:O	1:A:23:LEU:N	0.42	2.48	2	1
1:A:6:LEU:O	1:A:9:ILE:N	0.42	2.52	3	1
1:A:1:MET:SD	1:A:40:ASN:ND2	0.42	2.92	4	1
1:A:8:LEU:N	1:A:8:LEU:HD13	0.42	2.30	12	1
1:B:90:LEU:O	1:B:91:GLU:HG2	0.42	2.15	12	1
1:B:120:ASN:C	1:B:120:ASN:HD22	0.42	2.22	16	1
1:B:73:LYS:HG2	1:B:74:LEU:HD22	0.42	1.91	19	1
1:B:124:GLU:CD	1:B:129:TRP:HE1	0.42	2.22	19	1
1:B:76:ARG:NH2	1:B:101:GLU:OE1	0.42	2.50	20	1
1:B:85:GLU:O	1:B:89:LEU:HG	0.42	2.14	13	4
1:A:9:ILE:N	1:A:9:ILE:HD12	0.42	2.29	12	1
1:B:106:ASN:CG	1:B:107:PRO:HD2	0.42	2.39	13	1
1:B:79:LYS:NZ	1:B:120:ASN:ND2	0.42	2.67	14	1
1:B:85:GLU:O	1:B:88:ALA:HB3	0.42	2.14	16	1
1:A:63:TRP:CZ3	1:B:114:LYS:HG2	0.42	2.49	1	3
1:B:67:MET:O	1:B:130:GLN:HG2	0.42	2.14	4	1
1:B:82:SER:O	1:B:85:GLU:HG2	0.42	2.14	9	1
1:B:79:LYS:C	1:B:80:LYS:CG	0.42	2.92	11	1
1:B:79:LYS:O	1:B:81:ILE:CD1	0.42	2.67	17	1
1:B:98:ASN:O	1:B:102:LYS:CG	0.42	2.68	20	1
1:B:72:LEU:HD22	1:B:72:LEU:C	0.42	2.39	1	3
1:A:16:SER:HB2	1:A:19:GLU:CD	0.42	2.39	10	1
1:B:85:GLU:CG	1:B:86:LEU:N	0.42	2.83	15	1
1:A:36:LYS:O	1:A:37:ASN:CB	0.42	2.68	14	3
1:A:17:GLN:HB2	1:A:28:ARG:HG3	0.42	1.91	8	1
1:A:3:ILE:HG13	1:A:62:GLN:CD	0.42	2.40	11	1
1:A:44:GLN:OE1	1:A:48:LYS:HE3	0.42	2.14	12	2
1:B:129:TRP:HA	1:B:129:TRP:CE3	0.42	2.50	15	1
1:A:3:ILE:HG12	1:A:64:GLN:CG	0.42	2.44	17	1
1:B:103:ASN:CG	1:B:103:ASN:O	0.42	2.62	17	1
1:B:110:GLN:CD	1:B:111:LEU:H	0.42	2.23	2	1
1:A:10:ARG:HH21	1:A:35:GLU:CD	0.42	2.23	4	1
1:A:44:GLN:NE2	1:B:67:MET:SD	0.42	2.93	5	1
1:A:24:LEU:O	1:A:25:GLU:HG2	0.42	2.15	12	1
1:A:8:LEU:O	1:A:12:LYS:HB2	0.42	2.15	13	2
1:A:64:GLN:O	1:B:110:GLN:NE2	0.42	2.46	16	1
1:B:109:LEU:CD1	1:B:110:GLN:H	0.42	2.27	18	1
1:B:124:GLU:HG2	1:B:129:TRP:HE1	0.42	1.73	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:79:LYS:CG	1:B:81:ILE:HD13	0.42	2.45	10	1
1:B:96:THR:CG2	1:B:104:LYS:NZ	0.42	2.83	15	1
1:B:83:GLN:HB2	1:B:94:ARG:HG3	0.42	1.92	17	1
1:B:79:LYS:HB2	1:B:81:ILE:CD1	0.41	2.45	5	1
1:B:123:LEU:C	1:B:123:LEU:CD1	0.41	2.93	7	2
1:A:28:ARG:O	1:A:29:GLN:C	0.41	2.63	20	1
1:A:13:LYS:HE3	1:A:53:LEU:CD1	0.41	2.45	3	1
1:A:2:ILE:C	1:A:3:ILE:CD1	0.41	2.91	4	1
1:B:96:THR:O	1:B:100:ILE:N	0.41	2.48	6	1
1:B:83:GLN:OE1	1:B:83:GLN:N	0.41	2.53	11	2
1:A:47:LEU:O	1:A:51:TYR:N	0.41	2.47	9	1
1:A:20:LEU:C	1:A:20:LEU:CD2	0.41	2.89	14	2
1:A:1:MET:HB3	1:A:2:ILE:HG23	0.41	1.91	18	1
1:A:38:LYS:HG3	1:A:39:TYR:CD2	0.41	2.50	20	1
1:A:44:GLN:NE2	1:A:48:LYS:HE3	0.41	2.31	1	1
1:B:74:LEU:O	1:B:78:LYS:HB2	0.41	2.16	2	1
1:A:1:MET:O	1:A:64:GLN:HB2	0.41	2.14	6	1
1:A:32:ASN:O	1:A:36:LYS:HG3	0.41	2.16	20	2
1:A:63:TRP:CD1	1:B:110:GLN:HA	0.41	2.49	8	1
1:B:95:GLN:HG2	1:B:96:THR:N	0.41	2.30	13	1
1:B:83:GLN:HB2	1:B:94:ARG:CD	0.41	2.45	16	1
1:A:15:ILE:CG2	1:A:20:LEU:HD12	0.41	2.45	5	2
1:B:71:ASN:C	1:B:74:LEU:HD13	0.41	2.41	11	1
1:B:121:THR:HG22	1:B:125:ASP:HB3	0.41	1.92	12	1
1:B:79:LYS:HE3	1:B:119:LEU:CD1	0.41	2.45	18	1
1:A:5:ASN:HB3	1:A:8:LEU:HD23	0.41	1.90	2	2
1:A:45:LEU:HD22	1:A:45:LEU:HA	0.41	1.77	3	1
1:A:43:LEU:HB3	1:B:112:ALA:CB	0.41	2.45	18	1
1:B:95:GLN:HG3	1:B:96:THR:N	0.41	2.31	18	1
1:A:5:ASN:HD21	1:A:62:GLN:H	0.41	1.56	2	1
1:A:60:ILE:HG13	1:A:61:PHE:N	0.41	2.30	6	1
1:A:53:LEU:HD13	1:A:53:LEU:C	0.41	2.38	7	2
1:B:86:LEU:CD1	1:B:86:LEU:N	0.41	2.78	7	1
1:B:70:ASN:ND2	1:B:100:ILE:O	0.41	2.53	13	2
1:B:71:ASN:OD1	1:B:128:GLN:NE2	0.41	2.47	8	1
1:A:53:LEU:O	1:A:53:LEU:HD22	0.41	2.16	14	1
1:B:77:GLU:C	1:B:80:LYS:H	0.41	2.24	18	1
1:B:121:THR:CG2	1:B:122:PRO:CD	0.41	2.99	18	1
1:A:3:ILE:O	1:A:4:ASN:CG	0.41	2.63	19	1
1:A:6:LEU:C	1:A:6:LEU:CD1	0.41	2.94	1	1
1:A:57:LEU:HB3	1:B:113:LEU:HD21	0.41	1.92	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LEU:HA	1:B:109:LEU:CD2	0.41	2.46	2	1
1:A:6:LEU:O	1:A:10:ARG:N	0.41	2.40	3	1
1:A:33:GLY:O	1:A:37:ASN:N	0.41	2.42	8	1
1:A:7:LYS:HD3	1:A:35:GLU:CG	0.41	2.46	10	1
1:A:2:ILE:HG21	1:A:40:ASN:HB2	0.41	1.93	12	1
1:B:94:ARG:O	1:B:95:GLN:C	0.41	2.63	18	1
1:B:95:GLN:HA	1:B:98:ASN:HD21	0.41	1.75	11	1
1:B:89:LEU:CD1	1:B:118:TYR:CE2	0.41	3.03	12	1
1:B:123:LEU:HD13	1:B:123:LEU:HA	0.41	1.79	1	1
1:B:110:GLN:N	1:B:110:GLN:OE1	0.41	2.54	2	1
1:B:75:ILE:H	1:B:75:ILE:HD12	0.41	1.76	6	1
1:B:101:GLU:HG3	1:B:102:LYS:H	0.41	1.76	6	1
1:A:53:LEU:HD12	1:A:55:THR:OG1	0.41	2.16	7	1
1:A:44:GLN:CD	1:B:130:GLN:O	0.41	2.64	11	1
1:A:24:LEU:C	1:A:25:GLU:HG2	0.41	2.41	12	1
1:B:67:MET:HG3	1:B:68:ILE:H	0.41	1.75	13	1
1:A:46:ALA:HB1	1:A:57:LEU:HD21	0.41	1.92	14	1
1:A:66:GLU:CD	1:B:110:GLN:HE22	0.41	2.23	15	1
1:B:96:THR:CG2	1:B:104:LYS:HZ2	0.41	2.22	15	1
1:A:12:LYS:HG3	1:A:13:LYS:N	0.41	2.31	17	1
1:B:98:ASN:O	1:B:102:LYS:HG3	0.41	2.15	20	1
1:A:47:LEU:CB	1:B:129:TRP:CH2	0.41	3.04	2	1
1:A:5:ASN:ND2	1:A:60:ILE:O	0.41	2.54	5	1
1:A:43:LEU:HD11	1:B:107:PRO:O	0.41	2.16	14	1
1:B:93:SER:HB3	1:B:95:GLN:OE1	0.41	2.16	14	1
1:B:120:ASN:ND2	1:B:120:ASN:O	0.41	2.54	14	1
1:A:57:LEU:HD11	1:B:109:LEU:HD22	0.41	1.92	17	1
1:B:79:LYS:HE3	1:B:119:LEU:O	0.41	2.15	19	1
1:A:38:LYS:HD2	1:A:39:TYR:CE2	0.40	2.51	1	1
1:A:3:ILE:CD1	1:A:62:GLN:HG2	0.40	2.46	4	1
1:A:36:LYS:C	1:A:37:ASN:HD22	0.40	2.24	14	1
1:A:3:ILE:HG22	1:A:4:ASN:H	0.40	1.76	16	1
1:A:37:ASN:ND2	1:A:38:LYS:N	0.40	2.69	16	1
1:A:13:LYS:O	1:A:15:ILE:CD1	0.40	2.69	17	1
1:B:73:LYS:CB	1:B:76:ARG:NH2	0.40	2.84	20	1
1:A:47:LEU:HD21	1:B:123:LEU:HB2	0.40	1.93	9	1
1:B:76:ARG:CG	1:B:81:ILE:O	0.40	2.68	14	1
1:B:119:LEU:HD13	1:B:119:LEU:C	0.40	2.41	16	1
1:B:68:ILE:HG12	1:B:106:ASN:ND2	0.40	2.30	18	1
1:B:70:ASN:ND2	1:B:106:ASN:OD1	0.40	2.55	20	1
1:A:63:TRP:CD1	1:B:113:LEU:HD12	0.40	2.51	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:HD22	1:A:6:LEU:O	0.40	2.16	10	1
1:A:65:PRO:C	1:B:114:LYS:HZ1	0.40	2.21	12	1
1:B:76:ARG:HD2	1:B:77:GLU:N	0.40	2.32	13	1
1:A:16:SER:HB3	1:A:19:GLU:CD	0.40	2.41	14	1
1:B:89:LEU:HB3	1:B:118:TYR:HB3	0.40	1.94	14	1
1:B:67:MET:O	1:B:130:GLN:HG3	0.40	2.17	1	1
1:A:35:GLU:CG	1:A:36:LYS:N	0.40	2.84	3	1
1:B:70:ASN:O	1:B:73:LYS:CE	0.40	2.69	4	1
1:B:75:ILE:O	1:B:78:LYS:CB	0.40	2.70	15	1
1:B:90:LEU:HB3	1:B:92:VAL:HG22	0.40	1.93	17	1
1:B:87:ALA:O	1:B:91:GLU:N	0.40	2.55	1	1
1:A:65:PRO:HA	1:B:110:GLN:HE22	0.40	1.77	4	1
1:A:35:GLU:HG3	1:A:36:LYS:N	0.40	2.32	6	1
1:A:51:TYR:CD1	1:B:129:TRP:CH2	0.40	3.10	12	1
1:A:27:SER:HB3	1:A:29:GLN:NE2	0.40	2.32	13	1
1:B:94:ARG:HB3	1:B:94:ARG:CZ	0.40	2.46	16	1
1:A:50:ALA:HB2	1:A:60:ILE:HD11	0.40	1.93	17	1
1:B:100:ILE:HA	1:B:104:LYS:HB3	0.40	1.93	17	1
1:A:6:LEU:HD23	1:A:6:LEU:C	0.40	2.41	18	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	64/66 (97%)	58±2 (91±3%)	4±2 (6±2%)	2±1 (4±2%)	4	32
1	B	63/66 (95%)	58±2 (92±2%)	3±1 (5±2%)	2±1 (3±2%)	5	38
All	All	2540/2640 (96%)	2319 (91%)	137 (5%)	84 (3%)	5	35

All 17 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	37	ASN	19
1	B	103	ASN	18

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Mol	Chain	Res	Type	Models (Total)
1	A	3	ILE	6
1	A	5	ASN	6
1	B	71	ASN	6
1	B	69	ILE	5
1	B	130	GLN	4
1	A	64	GLN	3
1	A	4	ASN	3
1	A	38	LYS	3
1	A	65	PRO	2
1	B	104	LYS	2
1	A	54	ASN	2
1	B	120	ASN	2
1	A	2	ILE	1
1	A	63	TRP	1
1	B	129	TRP	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	61/61 (100%)	48±2 (79±3%)	13±2 (21±3%)	3	30
1	B	59/61 (97%)	47±2 (79±4%)	12±2 (21±4%)	3	31
All	All	2400/2440 (98%)	1892 (79%)	508 (21%)	3	31

All 85 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	8	LEU	20
1	B	74	LEU	19
1	B	119	LEU	17
1	A	53	LEU	16
1	A	30	THR	15
1	B	77	GLU	13
1	B	123	LEU	13
1	A	36	LYS	12
1	A	45	LEU	12

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Mol	Chain	Res	Type	Models (Total)
1	A	37	ASN	12
1	A	44	GLN	12
1	B	111	LEU	12
1	B	72	LEU	11
1	B	110	GLN	11
1	A	11	GLU	11
1	B	103	ASN	11
1	B	96	THR	10
1	B	102	LYS	10
1	A	20	LEU	9
1	B	71	ASN	9
1	B	76	ARG	9
1	A	40	ASN	9
1	A	5	ASN	8
1	B	86	LEU	8
1	B	95	GLN	8
1	A	6	LEU	8
1	B	67	MET	8
1	A	10	ARG	7
1	A	29	GLN	7
1	B	83	GLN	7
1	B	120	ASN	7
1	A	18	SER	7
1	A	57	LEU	7
1	B	73	LYS	7
1	A	27	SER	6
1	B	98	ASN	6
1	A	1	MET	6
1	B	84	SER	5
1	A	43	LEU	5
1	A	54	ASN	5
1	A	15	ILE	4
1	B	106	ASN	4
1	A	39	TYR	4
1	A	42	SER	4
1	A	55	THR	4
1	B	109	LEU	4
1	A	16	SER	3
1	A	38	LYS	3
1	A	58	GLU	3
1	A	51	TYR	3
1	A	3	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	17	GLN	3
1	B	69	ILE	3
1	B	81	ILE	3
1	B	82	SER	3
1	A	66	GLU	3
1	A	7	LYS	3
1	A	35	GLU	3
1	A	12	LYS	3
1	A	13	LYS	3
1	A	62	GLN	3
1	B	79	LYS	3
1	B	124	GLU	3
1	A	14	LYS	3
1	A	9	ILE	2
1	A	19	GLU	2
1	B	75	ILE	2
1	A	63	TRP	2
1	A	64	GLN	2
1	B	68	ILE	2
1	B	93	SER	2
1	B	105	TYR	2
1	B	78	LYS	2
1	B	91	GLU	2
1	B	80	LYS	2
1	A	25	GLU	2
1	A	4	ASN	2
1	B	130	GLN	2
1	B	117	TYR	1
1	B	85	GLU	1
1	A	23	LEU	1
1	B	89	LEU	1
1	B	118	TYR	1
1	B	108	SER	1
1	B	121	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 [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 37% for the well-defined parts and 37% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

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

Total number of shifts	717
Number of shifts mapped to atoms	717
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	56	-1.23 ± 0.18	Should be checked
$^{13}\text{C}_\beta$	40	-0.12 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	61	1.27 ± 0.35	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 37%, i.e. 717 atoms were assigned a chemical shift out of a possible 1926. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	234/642 (36%)	117/257 (46%)	56/260 (22%)	61/125 (49%)
Sidechain	443/1186 (37%)	306/770 (40%)	126/368 (34%)	11/48 (23%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	40/98 (41%)	20/46 (43%)	20/50 (40%)	0/2 (0%)
Overall	717/1926 (37%)	443/1073 (41%)	202/678 (30%)	72/175 (41%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 37%, i.e. 717 atoms were assigned a chemical shift out of a possible 1950. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	234/650 (36%)	117/260 (45%)	56/264 (21%)	61/126 (48%)
Sidechain	443/1202 (37%)	306/780 (39%)	126/374 (34%)	11/48 (23%)
Aromatic	40/98 (41%)	20/46 (43%)	20/50 (40%)	0/2 (0%)
Overall	717/1950 (37%)	443/1086 (41%)	202/688 (29%)	72/176 (41%)

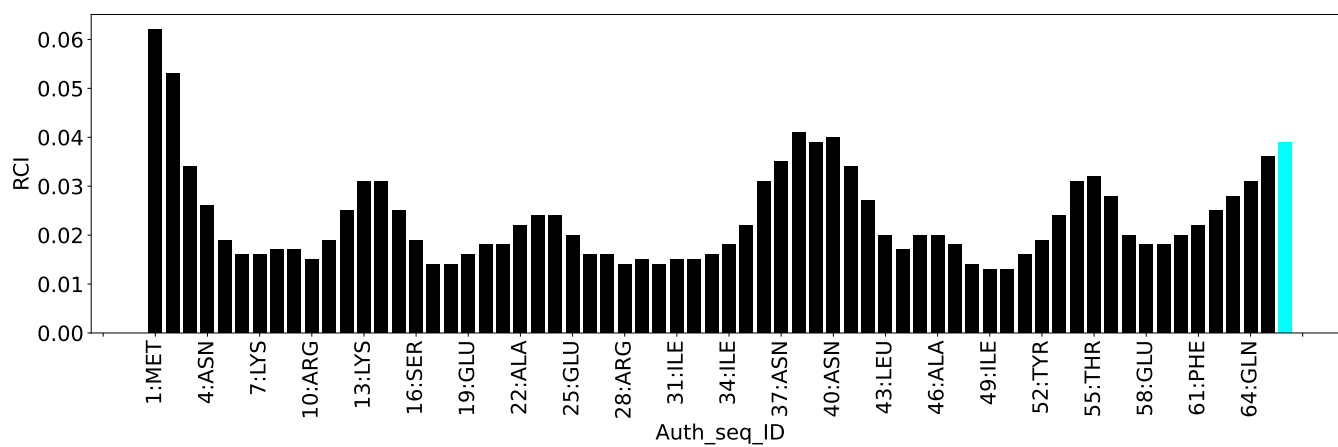
7.1.4 Statistically unusual chemical shifts [i](#)

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	2180
Intra-residue ($ i-j =0$)	518
Sequential ($ i-j =1$)	460
Medium range ($ i-j >1$ and $ i-j <5$)	513
Long range ($ i-j \geq 5$)	554
Inter-chain	135
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	96
Number of unmapped restraints	0
Number of restraints per residue	17.2
Number of long range restraints per residue ¹	4.2

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	42.3	0.2
0.2-0.5 (Medium)	26.5	0.5
>0.5 (Large)	49.4	27.54

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)	5.5	9.96
10.0-20.0 (Medium)	3.4	18.37
>20.0 (Large)	0.3	29.76

9 Distance violation analysis ⓘ

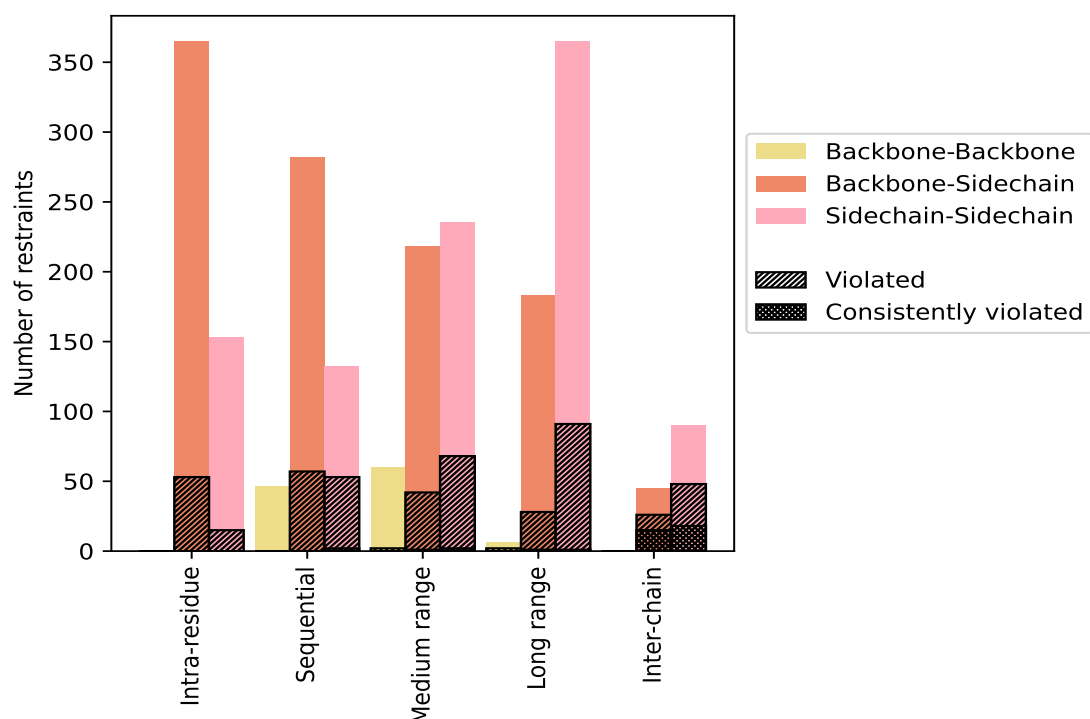
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	518	23.8	68	13.1	3.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	365	16.7	53	14.5	2.4	0	0.0	0.0
Sidechain-Sidechain	153	7.0	15	9.8	0.7	0	0.0	0.0
Sequential (i-j =1)	460	21.1	110	23.9	5.0	2	0.4	0.1
Backbone-Backbone	46	2.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	282	12.9	57	20.2	2.6	0	0.0	0.0
Sidechain-Sidechain	132	6.1	53	40.2	2.4	2	1.5	0.1
Medium range (i-j >1 & i-j <5)	513	23.5	112	21.8	5.1	3	0.6	0.1
Backbone-Backbone	60	2.8	2	3.3	0.1	0	0.0	0.0
Backbone-Sidechain	218	10.0	42	19.3	1.9	1	0.5	0.0
Sidechain-Sidechain	235	10.8	68	28.9	3.1	2	0.9	0.1
Long range (i-j ≥5)	554	25.4	121	21.8	5.6	2	0.4	0.1
Backbone-Backbone	6	0.3	2	33.3	0.1	0	0.0	0.0
Backbone-Sidechain	183	8.4	28	15.3	1.3	1	0.5	0.0
Sidechain-Sidechain	365	16.7	91	24.9	4.2	1	0.3	0.0
Inter-chain	135	6.2	74	54.8	3.4	33	24.4	1.5
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	45	2.1	26	57.8	1.2	15	33.3	0.7
Sidechain-Sidechain	90	4.1	48	53.3	2.2	18	20.0	0.8
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	2180	100.0	485	22.2	22.2	40	1.8	1.8
Backbone-Backbone	112	5.1	4	3.6	0.2	0	0.0	0.0
Backbone-Sidechain	1093	50.1	206	18.8	9.4	17	1.6	0.8
Sidechain-Sidechain	975	44.7	275	28.2	12.6	23	2.4	1.1

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	11	22	22	25	43	123	5.48	26.94	8.58	0.31
2	13	22	23	34	42	134	4.96	27.01	8.26	0.28
3	5	28	25	30	41	129	5.15	25.48	8.27	0.32
4	7	26	28	36	35	132	4.95	25.99	8.02	0.26
5	8	21	17	18	38	102	6.41	26.22	8.93	0.28
6	10	24	25	27	40	126	5.41	26.61	8.65	0.26
7	9	31	25	32	36	133	5.26	27.54	8.57	0.42
8	9	20	15	23	35	102	6.07	24.91	8.55	0.26
9	12	25	20	28	39	124	5.45	26.71	8.72	0.22
10	5	22	17	25	37	106	6.51	25.81	9.31	0.31

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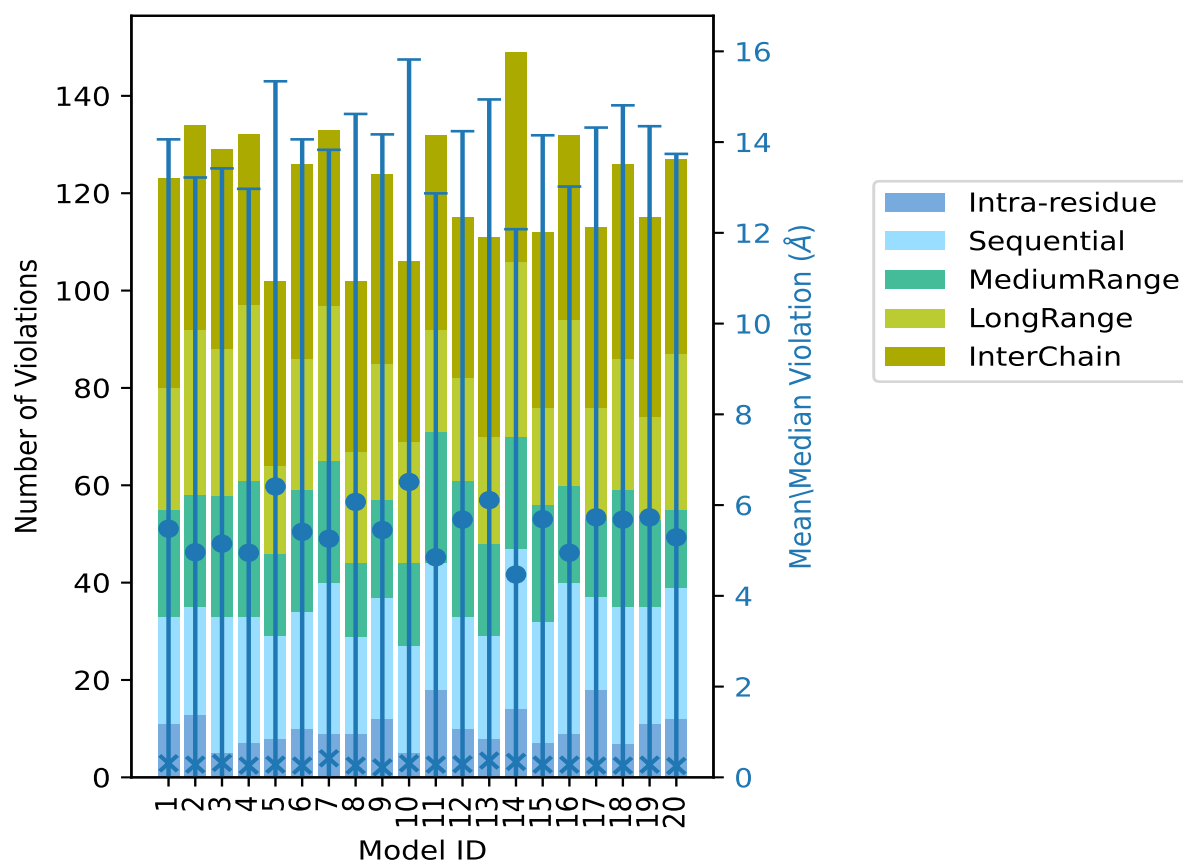
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	18	26	27	21	40	132	4.85	26.35	8.02	0.28
12	10	23	28	21	33	115	5.68	26.15	8.56	0.29
13	8	21	19	22	41	111	6.11	25.18	8.83	0.37
14	14	33	23	36	43	149	4.47	25.87	7.61	0.34
15	7	25	24	20	36	112	5.69	26.97	8.46	0.28
16	9	31	20	34	38	132	4.95	26.22	8.07	0.28
17	18	19	16	23	37	113	5.73	25.87	8.59	0.26
18	7	28	24	27	40	126	5.68	27.5	9.13	0.26
19	11	24	18	21	41	115	5.73	26.32	8.62	0.28
20	12	27	16	32	40	127	5.29	25.31	8.45	0.25

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

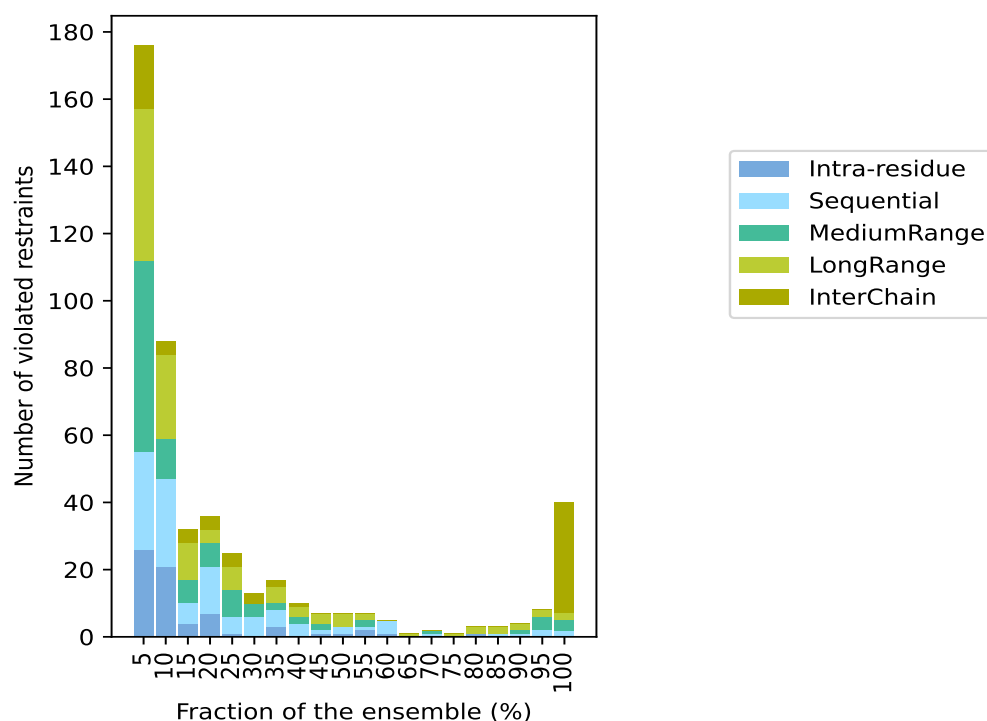
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1695(IR:450, SQ:350, MR:401, LR:433, IC:61) restraints are 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	%
26	29	57	45	19	176	1	5.0
21	26	12	25	4	88	2	10.0
4	6	7	11	4	32	3	15.0
7	14	7	4	4	36	4	20.0
1	5	8	7	4	25	5	25.0
0	6	4	0	3	13	6	30.0
3	5	2	5	2	17	7	35.0
0	4	2	3	1	10	8	40.0
1	1	2	3	0	7	9	45.0
1	2	0	4	0	7	10	50.0
2	1	2	2	0	7	11	55.0
1	4	0	0	0	5	12	60.0
0	0	0	1	0	1	13	65.0
0	1	1	0	0	2	14	70.0
0	0	0	1	0	1	15	75.0
1	0	0	2	0	3	16	80.0
0	1	0	2	0	3	17	85.0
0	1	1	2	0	4	18	90.0
0	2	4	2	0	8	19	95.0
0	2	3	2	33	40	20	100.0

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

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

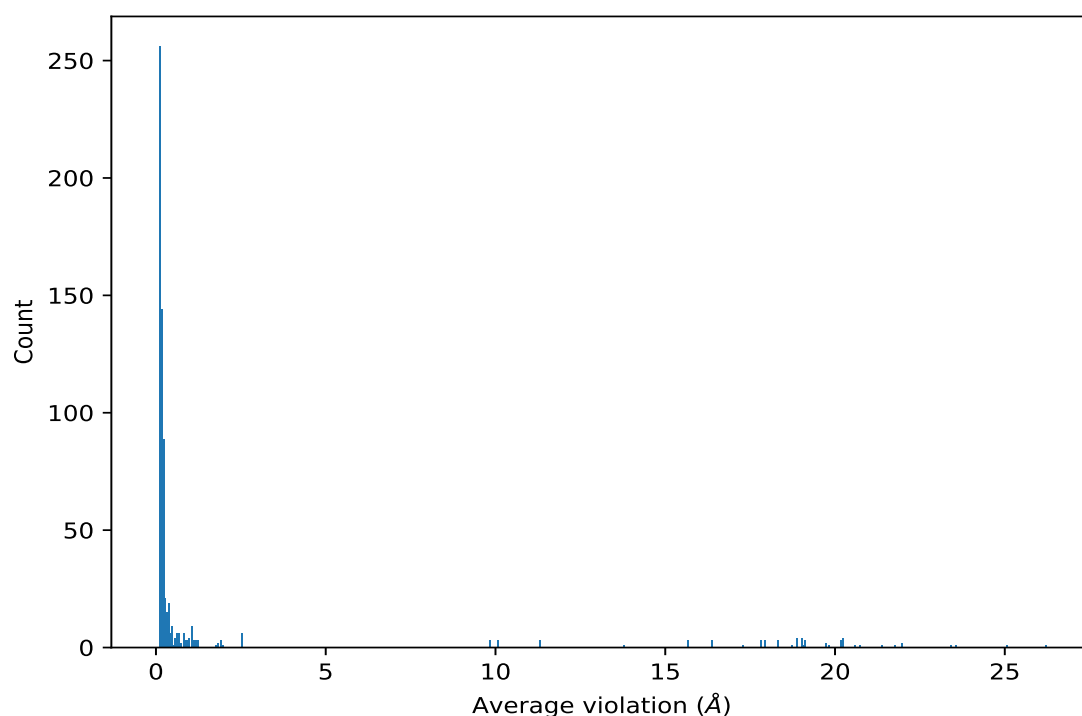
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	20	26.22	0.77	26.22
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	20	25.07	0.73	24.88
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	20	23.59	0.76	23.48
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	20	23.43	1.06	23.54
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	20	21.97	0.7	21.83
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	20	21.96	0.71	21.83
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	20	21.75	0.98	21.49
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	20	21.4	2.08	21.05
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	20	20.71	0.73	20.6
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	20	20.55	0.7	20.68
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	20	20.23	0.63	20.16
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	20	20.21	1.07	20.34
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	20	20.21	1.07	20.34
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	20	20.21	1.07	20.34
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	20	20.16	0.95	19.84
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	20	20.16	0.95	19.84

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	20	20.16	0.95	19.84
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	20	19.8	0.64	19.65
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	20	19.74	0.97	19.75
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	20	19.72	1.99	19.35
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	20	19.11	0.83	18.93
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	20	19.11	0.83	18.93
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	20	19.11	0.83	18.93
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	20	19.06	0.74	18.97
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	20	19.04	0.97	19.01
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	20	19.01	1.12	19.04
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	20	19.01	1.12	19.04
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	20	19.01	1.12	19.04
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	20	18.88	0.75	18.82
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	20	18.87	1.29	18.94
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	20	18.87	1.29	18.94
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	20	18.87	1.29	18.94
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	20	18.7	1.11	18.71
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	20	18.34	0.89	18.2
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	20	18.34	0.89	18.2
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	20	18.34	0.89	18.2
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	20	17.93	0.79	17.73
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	20	17.93	0.79	17.73
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	20	17.93	0.79	17.73
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	20	17.81	1.2	17.77
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	20	17.81	1.2	17.77
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	20	17.81	1.2	17.77
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	20	17.25	1.13	17.1
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	20	16.4	1.26	16.35
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	20	16.4	1.26	16.35
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	20	16.4	1.26	16.35
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	20	15.68	1.11	15.77
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	20	15.68	1.11	15.77
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	20	15.68	1.11	15.77
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	20	13.76	1.09	13.82
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	20	11.31	0.86	11.16
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	20	11.31	0.86	11.16
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	20	11.31	0.86	11.16
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	20	10.09	0.9	10.08
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	20	10.09	0.9	10.08
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	20	10.09	0.9	10.08
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	20	9.8	0.98	9.91
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	20	9.8	0.98	9.91

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	20	9.8	0.98	9.91
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	20	2.5	0.67	2.3
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	20	2.5	0.67	2.3
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	20	2.5	0.67	2.3
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	20	1.99	0.41	2.16
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	20	1.84	0.41	1.76
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	20	1.17	0.38	1.14
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	20	1.17	0.38	1.14
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	20	1.17	0.38	1.14
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	20	0.92	0.38	0.97
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	20	0.92	0.38	0.97
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	20	0.92	0.38	0.97
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	20	0.65	0.31	0.59
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	20	0.65	0.31	0.59
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	20	0.65	0.31	0.59
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	20	0.21	0.04	0.2
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	19	2.52	0.87	3.05
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	19	2.52	0.87	3.05
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	19	2.52	0.87	3.05
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	19	1.8	0.59	1.64
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	19	1.75	0.41	1.75
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	19	1.07	0.52	1.03
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	19	1.07	0.52	1.03
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	19	1.07	0.52	1.03
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	19	1.06	0.36	0.94
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	19	1.06	0.36	0.94
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	19	1.06	0.36	0.94
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	19	0.67	0.3	0.71
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	19	0.67	0.3	0.71
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	19	0.67	0.3	0.71
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	19	0.22	0.05	0.22
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	19	0.22	0.05	0.22
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	19	0.22	0.05	0.22
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	19	0.22	0.04	0.21
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	18	1.07	0.71	1.1
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	18	1.07	0.71	1.1
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	18	1.07	0.71	1.1
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	18	0.82	0.65	0.44
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	18	0.82	0.65	0.44
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	18	0.82	0.65	0.44
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	18	0.26	0.05	0.27
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	18	0.26	0.05	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	18	0.26	0.05	0.27
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	18	0.24	0.04	0.25
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	18	0.24	0.04	0.25
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	18	0.24	0.04	0.25
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	17	0.45	0.23	0.42
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	17	0.45	0.23	0.42
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	17	0.45	0.23	0.42
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	17	0.25	0.05	0.23
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	17	0.25	0.05	0.23
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	17	0.25	0.05	0.23
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	17	0.21	0.08	0.2
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	17	0.21	0.08	0.2
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	17	0.21	0.08	0.2
(1,1998)	1:102:B:LYS:HA	1:102:B:LYS:HE2	16	0.21	0.07	0.2
(1,385)	1:20:A:LEU:HD21	1:28:A:ARG:HB2	16	0.21	0.08	0.18
(1,385)	1:20:A:LEU:HD22	1:28:A:ARG:HB2	16	0.21	0.08	0.18
(1,385)	1:20:A:LEU:HD23	1:28:A:ARG:HB2	16	0.21	0.08	0.18
(1,165)	1:5:A:ASN:HA	1:35:A:GLU:HA	16	0.19	0.07	0.19
(1,212)	1:34:A:ILE:HD11	1:61:A:PHE:HE2	15	0.64	0.28	0.63
(1,212)	1:34:A:ILE:HD12	1:61:A:PHE:HE2	15	0.64	0.28	0.63
(1,212)	1:34:A:ILE:HD13	1:61:A:PHE:HE2	15	0.64	0.28	0.63
(1,1499)	1:109:B:LEU:HD11	1:110:B:GLN:HA	14	0.36	0.06	0.37
(1,1499)	1:109:B:LEU:HD12	1:110:B:GLN:HA	14	0.36	0.06	0.37
(1,1499)	1:109:B:LEU:HD13	1:110:B:GLN:HA	14	0.36	0.06	0.37
(1,1499)	1:109:B:LEU:HD21	1:110:B:GLN:HA	14	0.36	0.06	0.37
(1,1499)	1:109:B:LEU:HD22	1:110:B:GLN:HA	14	0.36	0.06	0.37
(1,1499)	1:109:B:LEU:HD23	1:110:B:GLN:HA	14	0.36	0.06	0.37
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG21	14	0.3	0.09	0.31
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG22	14	0.3	0.09	0.31
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG23	14	0.3	0.09	0.31
(1,182)	1:23:A:LEU:HD21	1:52:A:TYR:HE2	13	1.13	0.7	1.37
(1,182)	1:23:A:LEU:HD22	1:52:A:TYR:HE2	13	1.13	0.7	1.37
(1,182)	1:23:A:LEU:HD23	1:52:A:TYR:HE2	13	1.13	0.7	1.37
(1,1267)	1:43:A:LEU:HD11	1:44:A:GLN:HA	12	0.37	0.07	0.38
(1,1267)	1:43:A:LEU:HD12	1:44:A:GLN:HA	12	0.37	0.07	0.38
(1,1267)	1:43:A:LEU:HD13	1:44:A:GLN:HA	12	0.37	0.07	0.38
(1,1267)	1:43:A:LEU:HD21	1:44:A:GLN:HA	12	0.37	0.07	0.38
(1,1267)	1:43:A:LEU:HD22	1:44:A:GLN:HA	12	0.37	0.07	0.38
(1,1267)	1:43:A:LEU:HD23	1:44:A:GLN:HA	12	0.37	0.07	0.38
(1,1399)	1:81:B:ILE:HG13	1:82:B:SER:H	12	0.35	0.04	0.34
(1,1167)	1:15:A:ILE:HG13	1:16:A:SER:H	12	0.34	0.06	0.36
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD11	12	0.19	0.04	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD12	12	0.19	0.04	0.2
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD13	12	0.19	0.04	0.2
(1,1872)	1:78:B:LYS:H	1:78:B:LYS:HD2	12	0.15	0.04	0.15
(1,191)	1:89:B:LEU:HD21	1:118:B:TYR:HE2	11	0.98	0.58	1.03
(1,191)	1:89:B:LEU:HD22	1:118:B:TYR:HE2	11	0.98	0.58	1.03
(1,191)	1:89:B:LEU:HD23	1:118:B:TYR:HE2	11	0.98	0.58	1.03
(1,260)	1:107:B:PRO:HB3	1:127:B:PHE:HE1	11	0.49	0.34	0.36
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG21	11	0.32	0.05	0.32
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG22	11	0.32	0.05	0.32
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG23	11	0.32	0.05	0.32
(1,1730)	1:36:A:LYS:HA	1:36:A:LYS:HE2	11	0.19	0.09	0.16
(1,1098)	1:6:A:LEU:H	1:7:A:LYS:HE3	11	0.19	0.05	0.19
(1,1042)	1:79:B:LYS:HG3	1:81:B:ILE:HA	11	0.15	0.05	0.13
(1,1899)	1:80:B:LYS:HA	1:80:B:LYS:HE2	11	0.15	0.05	0.14
(1,177)	1:23:A:LEU:HG	1:52:A:TYR:HD2	10	0.97	0.46	0.93
(1,186)	1:89:B:LEU:HG	1:118:B:TYR:HD2	10	0.55	0.26	0.6
(1,1372)	1:77:B:GLU:HG3	1:78:B:LYS:HB3	10	0.29	0.09	0.28
(1,86)	1:9:A:ILE:HG13	1:59:A:ASP:HB2	10	0.2	0.06	0.22
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD11	10	0.2	0.04	0.19
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD12	10	0.2	0.04	0.19
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD13	10	0.2	0.04	0.19
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG21	10	0.16	0.04	0.15
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG22	10	0.16	0.04	0.15
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG23	10	0.16	0.04	0.15
(1,1904)	1:80:B:LYS:HB2	1:80:B:LYS:HE2	10	0.12	0.02	0.11
(1,180)	1:23:A:LEU:HD11	1:52:A:TYR:HD2	9	0.63	0.24	0.54
(1,180)	1:23:A:LEU:HD12	1:52:A:TYR:HD2	9	0.63	0.24	0.54
(1,180)	1:23:A:LEU:HD13	1:52:A:TYR:HD2	9	0.63	0.24	0.54
(1,170)	1:71:B:ASN:HA	1:101:B:GLU:HA	9	0.23	0.08	0.22
(1,1150)	1:12:A:LYS:HE3	1:13:A:LYS:H	9	0.2	0.05	0.21
(1,689)	1:81:B:ILE:HG13	1:85:B:GLU:HG2	9	0.18	0.05	0.18
(1,583)	1:7:A:LYS:HG2	1:11:A:GLU:HG2	9	0.18	0.04	0.17
(1,1631)	1:14:A:LYS:HA	1:14:A:LYS:HE2	9	0.13	0.03	0.13
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG21	9	0.13	0.03	0.14
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG22	9	0.13	0.03	0.14
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG23	9	0.13	0.03	0.14
(1,189)	1:89:B:LEU:HD11	1:118:B:TYR:HD2	8	0.38	0.19	0.33
(1,189)	1:89:B:LEU:HD12	1:118:B:TYR:HD2	8	0.38	0.19	0.33
(1,189)	1:89:B:LEU:HD13	1:118:B:TYR:HD2	8	0.38	0.19	0.33
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD11	8	0.36	0.07	0.34
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD12	8	0.36	0.07	0.34
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD13	8	0.36	0.07	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD11	8	0.2	0.04	0.2
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD12	8	0.2	0.04	0.2
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD13	8	0.2	0.04	0.2
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD11	8	0.18	0.03	0.18
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD12	8	0.18	0.03	0.18
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD13	8	0.18	0.03	0.18
(1,1545)	1:128:B:GLN:HG2	1:129:B:TRP:H	8	0.18	0.03	0.19
(1,1330)	1:72:B:LEU:H	1:73:B:LYS:HE3	8	0.17	0.04	0.16
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG21	8	0.17	0.02	0.18
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG22	8	0.17	0.02	0.18
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG23	8	0.17	0.02	0.18
(1,971)	1:13:A:LYS:HG3	1:15:A:ILE:HA	8	0.16	0.06	0.14
(1,780)	1:9:A:ILE:HA	1:12:A:LYS:HE3	8	0.15	0.03	0.16
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD21	8	0.15	0.04	0.14
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD22	8	0.15	0.04	0.14
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD23	8	0.15	0.04	0.14
(1,299)	1:115:B:ILE:HG21	1:127:B:PHE:HE1	7	0.58	0.42	0.51
(1,299)	1:115:B:ILE:HG22	1:127:B:PHE:HE1	7	0.58	0.42	0.51
(1,299)	1:115:B:ILE:HG23	1:127:B:PHE:HE1	7	0.58	0.42	0.51
(1,257)	1:41:A:PRO:HB3	1:61:A:PHE:HE1	7	0.52	0.37	0.31
(1,261)	1:107:B:PRO:HG2	1:127:B:PHE:HD1	7	0.49	0.24	0.45
(1,2109)	1:47:A:LEU:HD11	1:129:B:TRP:HZ3	7	0.34	0.05	0.35
(1,2109)	1:47:A:LEU:HD12	1:129:B:TRP:HZ3	7	0.34	0.05	0.35
(1,2109)	1:47:A:LEU:HD13	1:129:B:TRP:HZ3	7	0.34	0.05	0.35
(1,1140)	1:11:A:GLU:HG3	1:12:A:LYS:HB3	7	0.32	0.12	0.29
(1,1146)	1:12:A:LYS:HD2	1:13:A:LYS:H	7	0.24	0.06	0.23
(1,1731)	1:36:A:LYS:HA	1:36:A:LYS:HE3	7	0.23	0.02	0.23
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD11	7	0.19	0.05	0.21
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD12	7	0.19	0.05	0.21
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD13	7	0.19	0.05	0.21
(1,95)	1:75:B:ILE:HG13	1:125:B:ASP:HB2	7	0.19	0.04	0.19
(1,1018)	1:68:B:ILE:HG21	1:70:B:ASN:HD21	7	0.19	0.05	0.18
(1,1018)	1:68:B:ILE:HG22	1:70:B:ASN:HD21	7	0.19	0.05	0.18
(1,1018)	1:68:B:ILE:HG23	1:70:B:ASN:HD21	7	0.19	0.05	0.18
(1,2156)	1:63:A:TRP:HE1	1:114:B:LYS:HA	7	0.17	0.04	0.18
(1,1651)	1:17:A:GLN:H	1:17:A:GLN:HE21	7	0.16	0.04	0.17
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD11	7	0.16	0.04	0.16
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD12	7	0.16	0.04	0.16
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD13	7	0.16	0.04	0.16
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD11	7	0.16	0.04	0.16
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD12	7	0.16	0.04	0.16
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD13	7	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1604)	1:12:A:LYS:H	1:12:A:LYS:HD2	7	0.16	0.04	0.16
(1,593)	1:15:A:ILE:HG13	1:19:A:GLU:HG2	7	0.15	0.03	0.13
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG21	7	0.13	0.03	0.12
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG22	7	0.13	0.03	0.12
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG23	7	0.13	0.03	0.12
(1,1255)	1:38:A:LYS:HD2	1:39:A:TYR:HD2	6	0.72	0.83	0.16
(1,2105)	1:43:A:LEU:HD21	1:127:B:PHE:HD1	6	0.32	0.13	0.28
(1,2105)	1:43:A:LEU:HD22	1:127:B:PHE:HD1	6	0.32	0.13	0.28
(1,2105)	1:43:A:LEU:HD23	1:127:B:PHE:HD1	6	0.32	0.13	0.28
(1,2111)	1:48:A:LYS:HG3	1:129:B:TRP:HE1	6	0.27	0.14	0.2
(1,1228)	1:35:A:GLU:H	1:36:A:LYS:HD2	6	0.25	0.12	0.18
(1,874)	1:75:B:ILE:HA	1:78:B:LYS:HE3	6	0.24	0.05	0.22
(1,1381)	1:78:B:LYS:HD3	1:79:B:LYS:HA	6	0.2	0.07	0.18
(1,1313)	1:62:A:GLN:HG2	1:63:A:TRP:H	6	0.19	0.07	0.18
(1,1134)	1:10:A:ARG:HD2	1:11:A:GLU:HA	6	0.16	0.05	0.15
(1,1221)	1:31:A:ILE:HG21	1:32:A:ASN:HD21	6	0.15	0.03	0.15
(1,1221)	1:31:A:ILE:HG22	1:32:A:ASN:HD21	6	0.15	0.03	0.15
(1,1221)	1:31:A:ILE:HG23	1:32:A:ASN:HD21	6	0.15	0.03	0.15
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD11	6	0.14	0.03	0.14
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD12	6	0.14	0.03	0.14
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD13	6	0.14	0.03	0.14
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD11	6	0.14	0.03	0.14
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD12	6	0.14	0.03	0.14
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD13	6	0.14	0.03	0.14
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD11	6	0.14	0.03	0.14
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD12	6	0.14	0.03	0.14
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD13	6	0.14	0.03	0.14
(1,637)	1:44:A:GLN:HA	1:48:A:LYS:HD2	6	0.13	0.01	0.12
(1,848)	1:57:A:LEU:HD11	1:60:A:ILE:H	6	0.12	0.02	0.12
(1,848)	1:57:A:LEU:HD12	1:60:A:ILE:H	6	0.12	0.02	0.12
(1,848)	1:57:A:LEU:HD13	1:60:A:ILE:H	6	0.12	0.02	0.12
(1,2103)	1:44:A:GLN:HG2	1:130:B:GLN:H	6	0.12	0.02	0.12
(1,258)	1:41:A:PRO:HG2	1:61:A:PHE:HD1	5	0.73	0.34	0.82
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD21	5	0.45	0.18	0.47
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD22	5	0.45	0.18	0.47
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD23	5	0.45	0.18	0.47
(1,1460)	1:101:B:GLU:H	1:102:B:LYS:HD2	5	0.29	0.05	0.27
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD11	5	0.22	0.11	0.18
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD12	5	0.22	0.11	0.18
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD13	5	0.22	0.11	0.18
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD21	5	0.2	0.04	0.23
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD22	5	0.2	0.04	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD23	5	0.2	0.04	0.23
(1,1453)	1:97:B:ILE:HG21	1:98:B:ASN:HD21	5	0.2	0.13	0.15
(1,1453)	1:97:B:ILE:HG22	1:98:B:ASN:HD21	5	0.2	0.13	0.15
(1,1453)	1:97:B:ILE:HG23	1:98:B:ASN:HD21	5	0.2	0.13	0.15
(1,1693)	1:29:A:GLN:H	1:29:A:GLN:HE22	5	0.17	0.09	0.13
(1,913)	1:95:B:GLN:HB3	1:98:B:ASN:HD22	5	0.17	0.07	0.14
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD21	5	0.16	0.02	0.15
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD22	5	0.16	0.02	0.15
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD23	5	0.16	0.02	0.15
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD11	5	0.16	0.04	0.14
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD12	5	0.16	0.04	0.14
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD13	5	0.16	0.04	0.14
(1,1149)	1:12:A:LYS:HD3	1:13:A:LYS:HA	5	0.16	0.03	0.16
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD21	5	0.15	0.02	0.15
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD22	5	0.15	0.02	0.15
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD23	5	0.15	0.02	0.15
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD21	5	0.15	0.02	0.15
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD22	5	0.15	0.02	0.15
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD23	5	0.15	0.02	0.15
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD21	5	0.15	0.02	0.15
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD22	5	0.15	0.02	0.15
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD23	5	0.15	0.02	0.15
(1,1329)	1:72:B:LEU:H	1:73:B:LYS:HE2	5	0.15	0.04	0.14
(1,2087)	1:2:A:ILE:HD11	1:110:B:GLN:H	5	0.15	0.02	0.14
(1,2087)	1:2:A:ILE:HD12	1:110:B:GLN:H	5	0.15	0.02	0.14
(1,2087)	1:2:A:ILE:HD13	1:110:B:GLN:H	5	0.15	0.02	0.14
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD11	5	0.15	0.04	0.14
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD12	5	0.15	0.04	0.14
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD13	5	0.15	0.04	0.14
(1,172)	1:71:B:ASN:HA	1:101:B:GLU:HB3	5	0.15	0.03	0.14
(1,2086)	1:129:B:TRP:HE3	1:51:A:TYR:HD1	5	0.14	0.03	0.15
(1,2086)	1:129:B:TRP:HE3	1:51:A:TYR:HD2	5	0.14	0.03	0.15
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD21	5	0.14	0.04	0.12
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD22	5	0.14	0.04	0.12
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD23	5	0.14	0.04	0.12
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD21	5	0.14	0.04	0.12
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD22	5	0.14	0.04	0.12
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD23	5	0.14	0.04	0.12
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD21	5	0.14	0.04	0.12
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD22	5	0.14	0.04	0.12
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD23	5	0.14	0.04	0.12
(1,679)	1:73:B:LYS:HG2	1:77:B:GLU:HG2	5	0.14	0.04	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD11	5	0.14	0.02	0.13
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD12	5	0.14	0.02	0.13
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD13	5	0.14	0.02	0.13
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD11	5	0.14	0.02	0.13
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD12	5	0.14	0.02	0.13
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD13	5	0.14	0.02	0.13
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD11	5	0.14	0.02	0.13
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD12	5	0.14	0.02	0.13
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD13	5	0.14	0.02	0.13
(1,641)	1:44:A:GLN:HE21	1:48:A:LYS:HB2	5	0.13	0.01	0.13
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD11	5	0.13	0.03	0.13
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD12	5	0.13	0.03	0.13
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD13	5	0.13	0.03	0.13
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD21	5	0.13	0.03	0.13
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD22	5	0.13	0.03	0.13
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD23	5	0.13	0.03	0.13
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD11	5	0.13	0.03	0.13
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD12	5	0.13	0.03	0.13
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD13	5	0.13	0.03	0.13
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD21	5	0.13	0.03	0.13
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD22	5	0.13	0.03	0.13
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD23	5	0.13	0.03	0.13
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD11	5	0.13	0.03	0.13
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD12	5	0.13	0.03	0.13
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD13	5	0.13	0.03	0.13
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD21	5	0.13	0.03	0.13
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD22	5	0.13	0.03	0.13
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD23	5	0.13	0.03	0.13
(1,207)	1:73:B:LYS:HE2	1:101:B:GLU:HG2	5	0.13	0.02	0.12
(1,675)	1:72:B:LEU:HD21	1:76:B:ARG:HD2	5	0.12	0.01	0.12
(1,675)	1:72:B:LEU:HD22	1:76:B:ARG:HD2	5	0.12	0.01	0.12
(1,675)	1:72:B:LEU:HD23	1:76:B:ARG:HD2	5	0.12	0.01	0.12
(1,229)	1:24:A:LEU:HD21	1:49:A:ILE:HA	5	0.12	0.01	0.12
(1,229)	1:24:A:LEU:HD22	1:49:A:ILE:HA	5	0.12	0.01	0.12
(1,229)	1:24:A:LEU:HD23	1:49:A:ILE:HA	5	0.12	0.01	0.12
(1,297)	1:49:A:ILE:HG21	1:61:A:PHE:HE1	4	0.84	0.61	0.63
(1,297)	1:49:A:ILE:HG22	1:61:A:PHE:HE1	4	0.84	0.61	0.63
(1,297)	1:49:A:ILE:HG23	1:61:A:PHE:HE1	4	0.84	0.61	0.63
(1,2104)	1:43:A:LEU:HD11	1:127:B:PHE:HD1	4	0.44	0.2	0.34
(1,2104)	1:43:A:LEU:HD12	1:127:B:PHE:HD1	4	0.44	0.2	0.34
(1,2104)	1:43:A:LEU:HD13	1:127:B:PHE:HD1	4	0.44	0.2	0.34
(1,2157)	1:63:A:TRP:HE1	1:114:B:LYS:HG3	4	0.35	0.15	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1378)	1:78:B:LYS:HD2	1:79:B:LYS:H	4	0.3	0.09	0.26
(1,1156)	1:13:A:LYS:HB2	1:14:A:LYS:HG2	4	0.23	0.11	0.2
(1,1961)	1:95:B:GLN:H	1:95:B:GLN:HE22	4	0.21	0.08	0.22
(1,1388)	1:79:B:LYS:HB2	1:80:B:LYS:HG2	4	0.21	0.08	0.21
(1,735)	1:110:B:GLN:HB2	1:114:B:LYS:HD2	4	0.2	0.03	0.22
(1,1919)	1:83:B:GLN:H	1:83:B:GLN:HE21	4	0.19	0.12	0.12
(1,1999)	1:102:B:LYS:HA	1:102:B:LYS:HE3	4	0.19	0.06	0.2
(1,3)	1:2:A:ILE:HD11	1:64:A:GLN:HB2	4	0.18	0.05	0.17
(1,3)	1:2:A:ILE:HD12	1:64:A:GLN:HB2	4	0.18	0.05	0.17
(1,3)	1:2:A:ILE:HD13	1:64:A:GLN:HB2	4	0.18	0.05	0.17
(1,1442)	1:95:B:GLN:HG2	1:96:B:THR:HG21	4	0.18	0.06	0.18
(1,1442)	1:95:B:GLN:HG2	1:96:B:THR:HG22	4	0.18	0.06	0.18
(1,1442)	1:95:B:GLN:HG2	1:96:B:THR:HG23	4	0.18	0.06	0.18
(1,2110)	1:48:A:LYS:HA	1:129:B:TRP:HE1	4	0.18	0.03	0.18
(1,1504)	1:110:B:GLN:HE22	1:111:B:LEU:HD21	4	0.18	0.04	0.16
(1,1504)	1:110:B:GLN:HE22	1:111:B:LEU:HD22	4	0.18	0.04	0.16
(1,1504)	1:110:B:GLN:HE22	1:111:B:LEU:HD23	4	0.18	0.04	0.16
(1,699)	1:85:B:GLU:HG2	1:89:B:LEU:HD21	4	0.18	0.03	0.19
(1,699)	1:85:B:GLU:HG2	1:89:B:LEU:HD22	4	0.18	0.03	0.19
(1,699)	1:85:B:GLU:HG2	1:89:B:LEU:HD23	4	0.18	0.03	0.19
(1,1172)	1:18:A:SER:H	1:19:A:GLU:HB3	4	0.18	0.04	0.19
(1,2029)	1:110:B:GLN:H	1:110:B:GLN:HE21	4	0.18	0.05	0.18
(1,2100)	1:2:A:ILE:HG21	1:109:B:LEU:HD21	4	0.17	0.04	0.18
(1,2100)	1:2:A:ILE:HG21	1:109:B:LEU:HD22	4	0.17	0.04	0.18
(1,2100)	1:2:A:ILE:HG21	1:109:B:LEU:HD23	4	0.17	0.04	0.18
(1,2100)	1:2:A:ILE:HG22	1:109:B:LEU:HD21	4	0.17	0.04	0.18
(1,2100)	1:2:A:ILE:HG22	1:109:B:LEU:HD22	4	0.17	0.04	0.18
(1,2100)	1:2:A:ILE:HG22	1:109:B:LEU:HD23	4	0.17	0.04	0.18
(1,2100)	1:2:A:ILE:HG23	1:109:B:LEU:HD21	4	0.17	0.04	0.18
(1,2100)	1:2:A:ILE:HG23	1:109:B:LEU:HD22	4	0.17	0.04	0.18
(1,2100)	1:2:A:ILE:HG23	1:109:B:LEU:HD23	4	0.17	0.04	0.18
(1,1210)	1:29:A:GLN:HG2	1:30:A:THR:HG21	4	0.17	0.06	0.16
(1,1210)	1:29:A:GLN:HG2	1:30:A:THR:HG22	4	0.17	0.06	0.16
(1,1210)	1:29:A:GLN:HG2	1:30:A:THR:HG23	4	0.17	0.06	0.16
(1,1097)	1:6:A:LEU:H	1:7:A:LYS:HE2	4	0.16	0.06	0.14
(1,603)	1:19:A:GLU:HG2	1:23:A:LEU:HD21	4	0.16	0.04	0.18
(1,603)	1:19:A:GLU:HG2	1:23:A:LEU:HD22	4	0.16	0.04	0.18
(1,603)	1:19:A:GLU:HG2	1:23:A:LEU:HD23	4	0.16	0.04	0.18
(1,947)	1:2:A:ILE:HG21	1:4:A:ASN:HD21	4	0.16	0.04	0.16
(1,947)	1:2:A:ILE:HG22	1:4:A:ASN:HD21	4	0.16	0.04	0.16
(1,947)	1:2:A:ILE:HG23	1:4:A:ASN:HD21	4	0.16	0.04	0.16
(1,1305)	1:54:A:ASN:HD21	1:55:A:THR:H	4	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1049)	1:86:B:LEU:HD21	1:88:B:ALA:H	4	0.16	0.02	0.15
(1,1049)	1:86:B:LEU:HD22	1:88:B:ALA:H	4	0.16	0.02	0.15
(1,1049)	1:86:B:LEU:HD23	1:88:B:ALA:H	4	0.16	0.02	0.15
(1,1260)	1:38:A:LYS:HG3	1:39:A:TYR:H	4	0.15	0.03	0.14
(1,1404)	1:84:B:SER:H	1:85:B:GLU:HB3	4	0.14	0.04	0.12
(1,1632)	1:14:A:LYS:HA	1:14:A:LYS:HE3	4	0.14	0.03	0.15
(1,1112)	1:7:A:LYS:HG2	1:8:A:LEU:HA	4	0.14	0.04	0.13
(1,1761)	1:44:A:GLN:H	1:44:A:GLN:HE21	4	0.14	0.02	0.15
(1,1147)	1:12:A:LYS:HD2	1:13:A:LYS:HE2	4	0.14	0.01	0.14
(1,1055)	1:90:B:LEU:HG	1:92:B:VAL:HG11	4	0.13	0.02	0.13
(1,1055)	1:90:B:LEU:HG	1:92:B:VAL:HG12	4	0.13	0.02	0.13
(1,1055)	1:90:B:LEU:HG	1:92:B:VAL:HG13	4	0.13	0.02	0.13
(1,1366)	1:76:B:ARG:HD2	1:77:B:GLU:HA	4	0.12	0.02	0.12
(1,1040)	1:79:B:LYS:HD3	1:81:B:ILE:HG13	4	0.12	0.01	0.12
(1,154)	1:68:B:ILE:HB	1:106:B:ASN:HD21	4	0.12	0.0	0.12
(1,1636)	1:14:A:LYS:HB2	1:14:A:LYS:HE2	4	0.12	0.01	0.12
(1,239)	1:90:B:LEU:HD21	1:115:B:ILE:HA	4	0.12	0.01	0.12
(1,239)	1:90:B:LEU:HD22	1:115:B:ILE:HA	4	0.12	0.01	0.12
(1,239)	1:90:B:LEU:HD23	1:115:B:ILE:HA	4	0.12	0.01	0.12
(1,466)	1:100:B:ILE:HG21	1:106:B:ASN:HB3	3	0.22	0.03	0.21
(1,466)	1:100:B:ILE:HG22	1:106:B:ASN:HB3	3	0.22	0.03	0.21
(1,466)	1:100:B:ILE:HG23	1:106:B:ASN:HB3	3	0.22	0.03	0.21
(1,1015)	1:64:A:GLN:HB3	1:66:A:GLU:H	3	0.21	0.02	0.21
(1,1382)	1:78:B:LYS:HE3	1:79:B:LYS:H	3	0.18	0.03	0.17
(1,2085)	1:63:A:TRP:HE3	1:117:B:TYR:HD1	3	0.18	0.04	0.2
(1,2085)	1:63:A:TRP:HE3	1:117:B:TYR:HD2	3	0.18	0.04	0.2
(1,733)	1:110:B:GLN:HA	1:114:B:LYS:HD2	3	0.17	0.04	0.17
(1,1487)	1:104:B:LYS:HD2	1:105:B:TYR:HD2	3	0.17	0.05	0.18
(1,127)	1:79:B:LYS:HE2	1:120:B:ASN:HB2	3	0.17	0.04	0.18
(1,786)	1:10:A:ARG:HA	1:13:A:LYS:HE3	3	0.17	0.04	0.19
(1,1397)	1:80:B:LYS:HG2	1:81:B:ILE:HD11	3	0.17	0.04	0.15
(1,1397)	1:80:B:LYS:HG2	1:81:B:ILE:HD12	3	0.17	0.04	0.15
(1,1397)	1:80:B:LYS:HG2	1:81:B:ILE:HD13	3	0.17	0.04	0.15
(1,1569)	1:7:A:LYS:H	1:7:A:LYS:HD3	3	0.16	0.0	0.16
(1,1869)	1:77:B:GLU:H	1:77:B:GLU:HG2	3	0.15	0.04	0.18
(1,2177)	1:44:A:GLN:HB2	1:68:B:ILE:HG21	3	0.15	0.05	0.13
(1,2177)	1:44:A:GLN:HB2	1:68:B:ILE:HG22	3	0.15	0.05	0.13
(1,2177)	1:44:A:GLN:HB2	1:68:B:ILE:HG23	3	0.15	0.05	0.13
(1,1165)	1:14:A:LYS:HG2	1:15:A:ILE:HD11	3	0.15	0.05	0.11
(1,1165)	1:14:A:LYS:HG2	1:15:A:ILE:HD12	3	0.15	0.05	0.11
(1,1165)	1:14:A:LYS:HG2	1:15:A:ILE:HD13	3	0.15	0.05	0.11
(1,1652)	1:17:A:GLN:HA	1:17:A:GLN:HE22	3	0.15	0.03	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1968)	1:95:B:GLN:HB3	1:95:B:GLN:HE21	3	0.15	0.04	0.15
(1,108)	1:75:B:ILE:HG21	1:121:B:THR:HG21	3	0.14	0.03	0.15
(1,108)	1:75:B:ILE:HG21	1:121:B:THR:HG22	3	0.14	0.03	0.15
(1,108)	1:75:B:ILE:HG21	1:121:B:THR:HG23	3	0.14	0.03	0.15
(1,108)	1:75:B:ILE:HG22	1:121:B:THR:HG21	3	0.14	0.03	0.15
(1,108)	1:75:B:ILE:HG22	1:121:B:THR:HG22	3	0.14	0.03	0.15
(1,108)	1:75:B:ILE:HG22	1:121:B:THR:HG23	3	0.14	0.03	0.15
(1,108)	1:75:B:ILE:HG23	1:121:B:THR:HG21	3	0.14	0.03	0.15
(1,108)	1:75:B:ILE:HG23	1:121:B:THR:HG22	3	0.14	0.03	0.15
(1,108)	1:75:B:ILE:HG23	1:121:B:THR:HG23	3	0.14	0.03	0.15
(1,84)	1:9:A:ILE:HG12	1:59:A:ASP:HB2	3	0.14	0.01	0.14
(1,247)	1:25:A:GLU:HG3	1:48:A:LYS:HD3	3	0.14	0.02	0.15
(1,2)	1:2:A:ILE:HD11	1:64:A:GLN:H	3	0.14	0.03	0.12
(1,2)	1:2:A:ILE:HD12	1:64:A:GLN:H	3	0.14	0.03	0.12
(1,2)	1:2:A:ILE:HD13	1:64:A:GLN:H	3	0.14	0.03	0.12
(1,639)	1:44:A:GLN:HB2	1:48:A:LYS:HD2	3	0.14	0.01	0.15
(1,156)	1:68:B:ILE:HD11	1:106:B:ASN:HD21	3	0.14	0.02	0.13
(1,156)	1:68:B:ILE:HD12	1:106:B:ASN:HD21	3	0.14	0.02	0.13
(1,156)	1:68:B:ILE:HD13	1:106:B:ASN:HD21	3	0.14	0.02	0.13
(1,198)	1:7:A:LYS:HE2	1:35:A:GLU:HG2	3	0.14	0.0	0.14
(1,740)	1:110:B:GLN:HG2	1:114:B:LYS:HE2	3	0.14	0.02	0.13
(1,104)	1:9:A:ILE:HG21	1:55:A:THR:HG21	3	0.13	0.02	0.14
(1,104)	1:9:A:ILE:HG21	1:55:A:THR:HG22	3	0.13	0.02	0.14
(1,104)	1:9:A:ILE:HG21	1:55:A:THR:HG23	3	0.13	0.02	0.14
(1,104)	1:9:A:ILE:HG22	1:55:A:THR:HG21	3	0.13	0.02	0.14
(1,104)	1:9:A:ILE:HG22	1:55:A:THR:HG22	3	0.13	0.02	0.14
(1,104)	1:9:A:ILE:HG22	1:55:A:THR:HG23	3	0.13	0.02	0.14
(1,104)	1:9:A:ILE:HG23	1:55:A:THR:HG21	3	0.13	0.02	0.14
(1,104)	1:9:A:ILE:HG23	1:55:A:THR:HG22	3	0.13	0.02	0.14
(1,104)	1:9:A:ILE:HG23	1:55:A:THR:HG23	3	0.13	0.02	0.14
(1,1208)	1:29:A:GLN:HE21	1:30:A:THR:H	3	0.13	0.02	0.12
(1,330)	1:86:B:LEU:HD21	1:97:B:ILE:HG12	3	0.13	0.03	0.11
(1,330)	1:86:B:LEU:HD22	1:97:B:ILE:HG12	3	0.13	0.03	0.11
(1,330)	1:86:B:LEU:HD23	1:97:B:ILE:HG12	3	0.13	0.03	0.11
(1,737)	1:110:B:GLN:HE21	1:114:B:LYS:HB2	3	0.13	0.02	0.14
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD11	3	0.13	0.02	0.12
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD12	3	0.13	0.02	0.12
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD13	3	0.13	0.02	0.12
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD21	3	0.13	0.02	0.12
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD22	3	0.13	0.02	0.12
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD23	3	0.13	0.02	0.12
(1,1396)	1:80:B:LYS:HD2	1:81:B:ILE:H	3	0.12	0.0	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2125)	1:43:A:LEU:HD11	1:112:B:ALA:HB1	3	0.12	0.02	0.13
(1,2125)	1:43:A:LEU:HD11	1:112:B:ALA:HB2	3	0.12	0.02	0.13
(1,2125)	1:43:A:LEU:HD11	1:112:B:ALA:HB3	3	0.12	0.02	0.13
(1,2125)	1:43:A:LEU:HD12	1:112:B:ALA:HB1	3	0.12	0.02	0.13
(1,2125)	1:43:A:LEU:HD12	1:112:B:ALA:HB2	3	0.12	0.02	0.13
(1,2125)	1:43:A:LEU:HD12	1:112:B:ALA:HB3	3	0.12	0.02	0.13
(1,2125)	1:43:A:LEU:HD13	1:112:B:ALA:HB1	3	0.12	0.02	0.13
(1,2125)	1:43:A:LEU:HD13	1:112:B:ALA:HB2	3	0.12	0.02	0.13
(1,2125)	1:43:A:LEU:HD13	1:112:B:ALA:HB3	3	0.12	0.02	0.13
(1,2125)	1:43:A:LEU:HD21	1:112:B:ALA:HB1	3	0.12	0.02	0.13
(1,2125)	1:43:A:LEU:HD21	1:112:B:ALA:HB2	3	0.12	0.02	0.13
(1,2125)	1:43:A:LEU:HD21	1:112:B:ALA:HB3	3	0.12	0.02	0.13
(1,2125)	1:43:A:LEU:HD22	1:112:B:ALA:HB1	3	0.12	0.02	0.13
(1,2125)	1:43:A:LEU:HD22	1:112:B:ALA:HB2	3	0.12	0.02	0.13
(1,2125)	1:43:A:LEU:HD22	1:112:B:ALA:HB3	3	0.12	0.02	0.13
(1,2125)	1:43:A:LEU:HD23	1:112:B:ALA:HB1	3	0.12	0.02	0.13
(1,2125)	1:43:A:LEU:HD23	1:112:B:ALA:HB2	3	0.12	0.02	0.13
(1,2125)	1:43:A:LEU:HD23	1:112:B:ALA:HB3	3	0.12	0.02	0.13
(1,5)	1:68:B:ILE:HD11	1:130:B:GLN:H	3	0.12	0.0	0.12
(1,5)	1:68:B:ILE:HD12	1:130:B:GLN:H	3	0.12	0.0	0.12
(1,5)	1:68:B:ILE:HD13	1:130:B:GLN:H	3	0.12	0.0	0.12
(1,981)	1:21:A:ALA:HA	1:23:A:LEU:HG	3	0.12	0.01	0.12
(1,499)	1:34:A:ILE:HD11	1:39:A:TYR:HE1	2	1.92	0.1	1.92
(1,499)	1:34:A:ILE:HD12	1:39:A:TYR:HE1	2	1.92	0.1	1.92
(1,499)	1:34:A:ILE:HD13	1:39:A:TYR:HE1	2	1.92	0.1	1.92
(1,498)	1:34:A:ILE:HD11	1:39:A:TYR:HD1	2	1.23	0.11	1.23
(1,498)	1:34:A:ILE:HD12	1:39:A:TYR:HD1	2	1.23	0.11	1.23
(1,498)	1:34:A:ILE:HD13	1:39:A:TYR:HD1	2	1.23	0.11	1.23
(1,501)	1:34:A:ILE:HG21	1:39:A:TYR:HD1	2	0.86	0.32	0.86
(1,501)	1:34:A:ILE:HG22	1:39:A:TYR:HD1	2	0.86	0.32	0.86
(1,501)	1:34:A:ILE:HG23	1:39:A:TYR:HD1	2	0.86	0.32	0.86
(1,1258)	1:38:A:LYS:HE2	1:39:A:TYR:HD2	2	0.45	0.06	0.45
(1,1629)	1:14:A:LYS:HA	1:14:A:LYS:HD2	2	0.44	0.02	0.44
(1,1897)	1:80:B:LYS:HA	1:80:B:LYS:HD2	2	0.42	0.01	0.42
(1,1252)	1:38:A:LYS:HA	1:39:A:TYR:HD2	2	0.4	0.21	0.4
(1,1256)	1:38:A:LYS:HD2	1:39:A:TYR:HE2	2	0.37	0.17	0.37
(1,1791)	1:54:A:ASN:HA	1:54:A:ASN:HD22	2	0.34	0.05	0.34
(1,1627)	1:14:A:LYS:H	1:14:A:LYS:HD2	2	0.32	0.04	0.32
(1,1309)	1:59:A:ASP:HB3	1:60:A:ILE:HG21	2	0.3	0.14	0.3
(1,1309)	1:59:A:ASP:HB3	1:60:A:ILE:HG22	2	0.3	0.14	0.3
(1,1309)	1:59:A:ASP:HB3	1:60:A:ILE:HG23	2	0.3	0.14	0.3
(1,2059)	1:120:B:ASN:HA	1:120:B:ASN:HD22	2	0.26	0.04	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1895)	1:80:B:LYS:H	1:80:B:LYS:HD2	2	0.26	0.03	0.26
(1,1900)	1:80:B:LYS:HA	1:80:B:LYS:HE3	2	0.26	0.03	0.26
(1,1789)	1:54:A:ASN:H	1:54:A:ASN:HD22	2	0.25	0.14	0.25
(1,469)	1:6:A:LEU:HD11	1:11:A:GLU:H	2	0.22	0.0	0.22
(1,469)	1:6:A:LEU:HD12	1:11:A:GLU:H	2	0.22	0.0	0.22
(1,469)	1:6:A:LEU:HD13	1:11:A:GLU:H	2	0.22	0.0	0.22
(1,1880)	1:78:B:LYS:HB3	1:78:B:LYS:HE2	2	0.22	0.11	0.22
(1,2142)	1:43:A:LEU:HD11	1:106:B:ASN:H	2	0.22	0.11	0.22
(1,2142)	1:43:A:LEU:HD12	1:106:B:ASN:H	2	0.22	0.11	0.22
(1,2142)	1:43:A:LEU:HD13	1:106:B:ASN:H	2	0.22	0.11	0.22
(1,2142)	1:43:A:LEU:HD21	1:106:B:ASN:H	2	0.22	0.11	0.22
(1,2142)	1:43:A:LEU:HD22	1:106:B:ASN:H	2	0.22	0.11	0.22
(1,2142)	1:43:A:LEU:HD23	1:106:B:ASN:H	2	0.22	0.11	0.22
(1,517)	1:72:B:LEU:HD11	1:77:B:GLU:H	2	0.22	0.04	0.22
(1,517)	1:72:B:LEU:HD12	1:77:B:GLU:H	2	0.22	0.04	0.22
(1,517)	1:72:B:LEU:HD13	1:77:B:GLU:H	2	0.22	0.04	0.22
(1,44)	1:3:A:ILE:HG13	1:62:A:GLN:HE22	2	0.22	0.04	0.22
(1,1300)	1:53:A:LEU:HD21	1:54:A:ASN:HB2	2	0.22	0.07	0.22
(1,1300)	1:53:A:LEU:HD22	1:54:A:ASN:HB2	2	0.22	0.07	0.22
(1,1300)	1:53:A:LEU:HD23	1:54:A:ASN:HB2	2	0.22	0.07	0.22
(1,123)	1:13:A:LYS:HE2	1:54:A:ASN:HB2	2	0.21	0.08	0.21
(1,1319)	1:67:B:MET:HB3	1:68:B:ILE:HD11	2	0.21	0.1	0.21
(1,1319)	1:67:B:MET:HB3	1:68:B:ILE:HD12	2	0.21	0.1	0.21
(1,1319)	1:67:B:MET:HB3	1:68:B:ILE:HD13	2	0.21	0.1	0.21
(1,1879)	1:78:B:LYS:HB3	1:78:B:LYS:HD2	2	0.21	0.0	0.21
(1,1344)	1:73:B:LYS:HG2	1:74:B:LEU:HA	2	0.2	0.02	0.2
(1,1472)	1:102:B:LYS:HB3	1:103:B:ASN:HB3	2	0.2	0.06	0.2
(1,732)	1:109:B:LEU:HD11	1:113:B:LEU:HD21	2	0.2	0.06	0.2
(1,732)	1:109:B:LEU:HD11	1:113:B:LEU:HD22	2	0.2	0.06	0.2
(1,732)	1:109:B:LEU:HD11	1:113:B:LEU:HD23	2	0.2	0.06	0.2
(1,732)	1:109:B:LEU:HD12	1:113:B:LEU:HD21	2	0.2	0.06	0.2
(1,732)	1:109:B:LEU:HD12	1:113:B:LEU:HD22	2	0.2	0.06	0.2
(1,732)	1:109:B:LEU:HD12	1:113:B:LEU:HD23	2	0.2	0.06	0.2
(1,732)	1:109:B:LEU:HD13	1:113:B:LEU:HD21	2	0.2	0.06	0.2
(1,732)	1:109:B:LEU:HD13	1:113:B:LEU:HD22	2	0.2	0.06	0.2
(1,732)	1:109:B:LEU:HD13	1:113:B:LEU:HD23	2	0.2	0.06	0.2
(1,732)	1:109:B:LEU:HD21	1:113:B:LEU:HD21	2	0.2	0.06	0.2
(1,732)	1:109:B:LEU:HD21	1:113:B:LEU:HD22	2	0.2	0.06	0.2
(1,732)	1:109:B:LEU:HD21	1:113:B:LEU:HD23	2	0.2	0.06	0.2
(1,732)	1:109:B:LEU:HD22	1:113:B:LEU:HD21	2	0.2	0.06	0.2
(1,732)	1:109:B:LEU:HD22	1:113:B:LEU:HD22	2	0.2	0.06	0.2
(1,732)	1:109:B:LEU:HD22	1:113:B:LEU:HD23	2	0.2	0.06	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,732)	1:109:B:LEU:HD23	1:113:B:LEU:HD21	2	0.2	0.06	0.2
(1,732)	1:109:B:LEU:HD23	1:113:B:LEU:HD22	2	0.2	0.06	0.2
(1,732)	1:109:B:LEU:HD23	1:113:B:LEU:HD23	2	0.2	0.06	0.2
(1,1601)	1:11:A:GLU:H	1:11:A:GLU:HG2	2	0.2	0.02	0.2
(1,1611)	1:12:A:LYS:HB3	1:12:A:LYS:HD2	2	0.2	0.02	0.2
(1,460)	1:34:A:ILE:HG21	1:40:A:ASN:HB3	2	0.19	0.0	0.19
(1,460)	1:34:A:ILE:HG22	1:40:A:ASN:HB3	2	0.19	0.0	0.19
(1,460)	1:34:A:ILE:HG23	1:40:A:ASN:HB3	2	0.19	0.0	0.19
(1,571)	1:6:A:LEU:HD11	1:10:A:ARG:HD2	2	0.19	0.06	0.19
(1,571)	1:6:A:LEU:HD12	1:10:A:ARG:HD2	2	0.19	0.06	0.19
(1,571)	1:6:A:LEU:HD13	1:10:A:ARG:HD2	2	0.19	0.06	0.19
(1,1531)	1:119:B:LEU:HD11	1:120:B:ASN:HB2	2	0.19	0.07	0.19
(1,1531)	1:119:B:LEU:HD12	1:120:B:ASN:HB2	2	0.19	0.07	0.19
(1,1531)	1:119:B:LEU:HD13	1:120:B:ASN:HB2	2	0.19	0.07	0.19
(1,1800)	1:62:A:GLN:H	1:62:A:GLN:HE21	2	0.19	0.04	0.19
(1,1321)	1:67:B:MET:HG2	1:68:B:ILE:HD11	2	0.18	0.02	0.18
(1,1321)	1:67:B:MET:HG2	1:68:B:ILE:HD12	2	0.18	0.02	0.18
(1,1321)	1:67:B:MET:HG2	1:68:B:ILE:HD13	2	0.18	0.02	0.18
(1,143)	1:2:A:ILE:HB	1:40:A:ASN:HD21	2	0.18	0.07	0.18
(1,864)	1:72:B:LEU:HD21	1:75:B:ILE:HB	2	0.18	0.04	0.18
(1,864)	1:72:B:LEU:HD22	1:75:B:ILE:HB	2	0.18	0.04	0.18
(1,864)	1:72:B:LEU:HD23	1:75:B:ILE:HB	2	0.18	0.04	0.18
(1,978)	1:20:A:LEU:HD21	1:22:A:ALA:H	2	0.18	0.01	0.18
(1,978)	1:20:A:LEU:HD22	1:22:A:ALA:H	2	0.18	0.01	0.18
(1,978)	1:20:A:LEU:HD23	1:22:A:ALA:H	2	0.18	0.01	0.18
(1,1320)	1:67:B:MET:HG2	1:68:B:ILE:HB	2	0.18	0.06	0.18
(1,2174)	1:44:A:GLN:H	1:68:B:ILE:HD11	2	0.18	0.08	0.18
(1,2174)	1:44:A:GLN:H	1:68:B:ILE:HD12	2	0.18	0.08	0.18
(1,2174)	1:44:A:GLN:H	1:68:B:ILE:HD13	2	0.18	0.08	0.18
(1,216)	1:74:B:LEU:HD21	1:101:B:GLU:HB2	2	0.18	0.08	0.18
(1,216)	1:74:B:LEU:HD22	1:101:B:GLU:HB2	2	0.18	0.08	0.18
(1,216)	1:74:B:LEU:HD23	1:101:B:GLU:HB2	2	0.18	0.08	0.18
(1,1101)	1:6:A:LEU:HD11	1:7:A:LYS:HB3	2	0.18	0.08	0.18
(1,1101)	1:6:A:LEU:HD12	1:7:A:LYS:HB3	2	0.18	0.08	0.18
(1,1101)	1:6:A:LEU:HD13	1:7:A:LYS:HB3	2	0.18	0.08	0.18
(1,2057)	1:120:B:ASN:H	1:120:B:ASN:HD22	2	0.18	0.03	0.18
(1,213)	1:34:A:ILE:HD11	1:61:A:PHE:HZ	2	0.17	0.06	0.17
(1,213)	1:34:A:ILE:HD12	1:61:A:PHE:HZ	2	0.17	0.06	0.17
(1,213)	1:34:A:ILE:HD13	1:61:A:PHE:HZ	2	0.17	0.06	0.17
(1,93)	1:75:B:ILE:HG12	1:125:B:ASP:HB2	2	0.17	0.04	0.17
(1,1492)	1:104:B:LYS:HG3	1:105:B:TYR:H	2	0.17	0.05	0.17
(1,98)	1:75:B:ILE:HD11	1:125:B:ASP:HB2	2	0.16	0.01	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,98)	1:75:B:ILE:HD12	1:125:B:ASP:HB2	2	0.16	0.01	0.16
(1,98)	1:75:B:ILE:HD13	1:125:B:ASP:HB2	2	0.16	0.01	0.16
(1,1248)	1:37:A:ASN:HD21	1:38:A:LYS:HD3	2	0.16	0.02	0.16
(1,891)	1:83:B:GLN:HE21	1:86:B:LEU:HD21	2	0.16	0.02	0.16
(1,891)	1:83:B:GLN:HE21	1:86:B:LEU:HD22	2	0.16	0.02	0.16
(1,891)	1:83:B:GLN:HE21	1:86:B:LEU:HD23	2	0.16	0.02	0.16
(1,557)	1:116:B:ALA:HA	1:121:B:THR:HG21	2	0.16	0.02	0.16
(1,557)	1:116:B:ALA:HA	1:121:B:THR:HG22	2	0.16	0.02	0.16
(1,557)	1:116:B:ALA:HA	1:121:B:THR:HG23	2	0.16	0.02	0.16
(1,1698)	1:29:A:GLN:HB2	1:29:A:GLN:HE21	2	0.15	0.01	0.15
(1,1206)	1:28:A:ARG:HG2	1:29:A:GLN:HB3	2	0.15	0.03	0.15
(1,1253)	1:38:A:LYS:HB3	1:39:A:TYR:H	2	0.15	0.0	0.15
(1,1139)	1:11:A:GLU:HG2	1:12:A:LYS:H	2	0.15	0.02	0.15
(1,1465)	1:101:B:GLU:HG2	1:102:B:LYS:HD2	2	0.15	0.03	0.15
(1,208)	1:73:B:LYS:HG2	1:101:B:GLU:HB2	2	0.14	0.01	0.14
(1,708)	1:94:B:ARG:HD2	1:98:B:ASN:HD22	2	0.14	0.02	0.14
(1,942)	1:123:B:LEU:HD11	1:126:B:ILE:H	2	0.14	0.01	0.14
(1,942)	1:123:B:LEU:HD12	1:126:B:ILE:H	2	0.14	0.01	0.14
(1,942)	1:123:B:LEU:HD13	1:126:B:ILE:H	2	0.14	0.01	0.14
(1,1246)	1:37:A:ASN:HD21	1:38:A:LYS:H	2	0.14	0.01	0.14
(1,1333)	1:72:B:LEU:HD11	1:73:B:LYS:HB3	2	0.14	0.04	0.14
(1,1333)	1:72:B:LEU:HD12	1:73:B:LYS:HB3	2	0.14	0.04	0.14
(1,1333)	1:72:B:LEU:HD13	1:73:B:LYS:HB3	2	0.14	0.04	0.14
(1,1995)	1:102:B:LYS:H	1:102:B:LYS:HE3	2	0.14	0.0	0.14
(1,199)	1:7:A:LYS:HG2	1:35:A:GLU:HB2	2	0.14	0.02	0.14
(1,962)	1:13:A:LYS:H	1:15:A:ILE:HD11	2	0.14	0.02	0.14
(1,962)	1:13:A:LYS:H	1:15:A:ILE:HD12	2	0.14	0.02	0.14
(1,962)	1:13:A:LYS:H	1:15:A:ILE:HD13	2	0.14	0.02	0.14
(1,1343)	1:73:B:LYS:HG2	1:74:B:LEU:H	2	0.14	0.02	0.14
(1,1489)	1:104:B:LYS:HE2	1:105:B:TYR:H	2	0.14	0.02	0.14
(1,1727)	1:36:A:LYS:H	1:36:A:LYS:HE3	2	0.14	0.02	0.14
(1,363)	1:76:B:ARG:HG2	1:86:B:LEU:HD11	2	0.13	0.02	0.13
(1,363)	1:76:B:ARG:HG2	1:86:B:LEU:HD12	2	0.13	0.02	0.13
(1,363)	1:76:B:ARG:HG2	1:86:B:LEU:HD13	2	0.13	0.02	0.13
(1,425)	1:50:A:ALA:HB1	1:57:A:LEU:HD21	2	0.13	0.01	0.13
(1,425)	1:50:A:ALA:HB1	1:57:A:LEU:HD22	2	0.13	0.01	0.13
(1,425)	1:50:A:ALA:HB1	1:57:A:LEU:HD23	2	0.13	0.01	0.13
(1,425)	1:50:A:ALA:HB2	1:57:A:LEU:HD21	2	0.13	0.01	0.13
(1,425)	1:50:A:ALA:HB2	1:57:A:LEU:HD22	2	0.13	0.01	0.13
(1,425)	1:50:A:ALA:HB2	1:57:A:LEU:HD23	2	0.13	0.01	0.13
(1,425)	1:50:A:ALA:HB3	1:57:A:LEU:HD21	2	0.13	0.01	0.13
(1,425)	1:50:A:ALA:HB3	1:57:A:LEU:HD22	2	0.13	0.01	0.13

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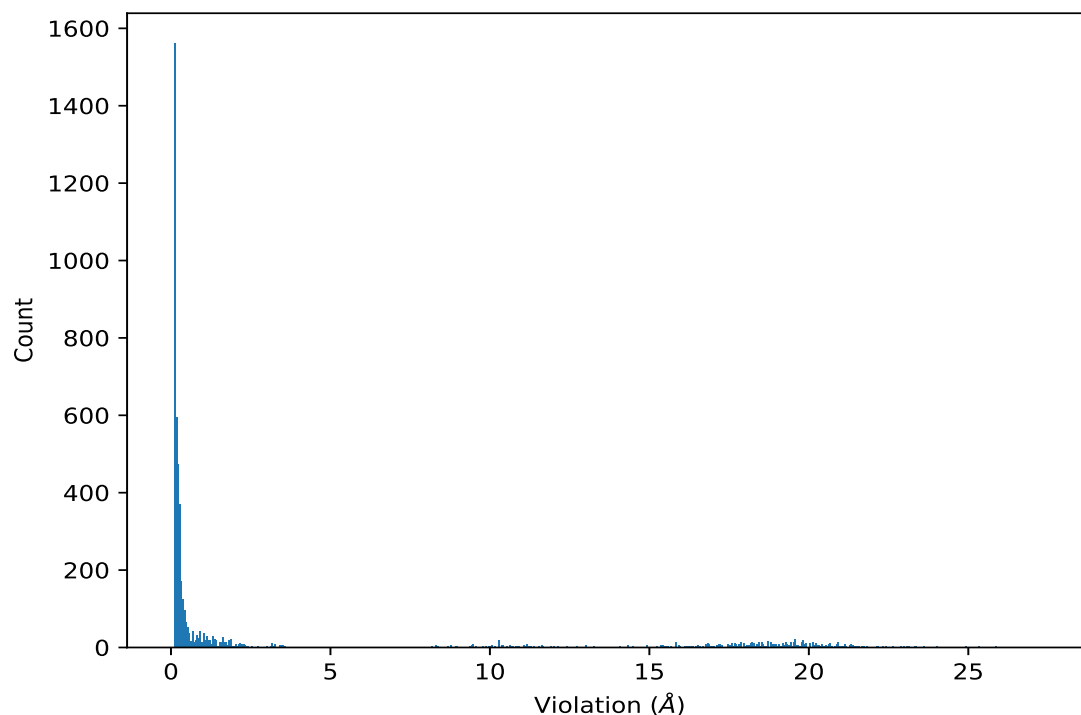
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,425)	1:50:A:ALA:HB3	1:57:A:LEU:HD23	2	0.13	0.01	0.13
(1,685)	1:76:B:ARG:HD3	1:80:B:LYS:HA	2	0.13	0.02	0.13
(1,770)	1:6:A:LEU:HD21	1:9:A:ILE:HB	2	0.13	0.0	0.13
(1,770)	1:6:A:LEU:HD22	1:9:A:ILE:HB	2	0.13	0.0	0.13
(1,770)	1:6:A:LEU:HD23	1:9:A:ILE:HB	2	0.13	0.0	0.13
(1,1921)	1:83:B:GLN:HB2	1:83:B:GLN:HE21	2	0.13	0.0	0.13
(1,160)	1:81:B:ILE:H	1:119:B:LEU:HD21	2	0.12	0.01	0.12
(1,160)	1:81:B:ILE:H	1:119:B:LEU:HD22	2	0.12	0.01	0.12
(1,160)	1:81:B:ILE:H	1:119:B:LEU:HD23	2	0.12	0.01	0.12
(1,1211)	1:29:A:GLN:HG3	1:30:A:THR:H	2	0.12	0.01	0.12
(1,1476)	1:102:B:LYS:HG3	1:103:B:ASN:HD21	2	0.12	0.02	0.12
(1,396)	1:115:B:ILE:H	1:123:B:LEU:HD21	2	0.12	0.0	0.12
(1,396)	1:115:B:ILE:H	1:123:B:LEU:HD22	2	0.12	0.0	0.12
(1,396)	1:115:B:ILE:H	1:123:B:LEU:HD23	2	0.12	0.0	0.12
(1,2170)	1:43:A:LEU:HD21	1:68:B:ILE:HG21	2	0.12	0.01	0.12
(1,2170)	1:43:A:LEU:HD21	1:68:B:ILE:HG22	2	0.12	0.01	0.12
(1,2170)	1:43:A:LEU:HD21	1:68:B:ILE:HG23	2	0.12	0.01	0.12
(1,2170)	1:43:A:LEU:HD22	1:68:B:ILE:HG21	2	0.12	0.01	0.12
(1,2170)	1:43:A:LEU:HD22	1:68:B:ILE:HG22	2	0.12	0.01	0.12
(1,2170)	1:43:A:LEU:HD22	1:68:B:ILE:HG23	2	0.12	0.01	0.12
(1,2170)	1:43:A:LEU:HD23	1:68:B:ILE:HG21	2	0.12	0.01	0.12
(1,2170)	1:43:A:LEU:HD23	1:68:B:ILE:HG22	2	0.12	0.01	0.12
(1,2170)	1:43:A:LEU:HD23	1:68:B:ILE:HG23	2	0.12	0.01	0.12
(1,2069)	1:128:B:GLN:H	1:128:B:GLN:HG2	2	0.12	0.02	0.12
(1,1362)	1:76:B:ARG:H	1:77:B:GLU:HG3	2	0.12	0.0	0.12
(1,1)	1:2:A:ILE:H	1:64:A:GLN:HB2	2	0.11	0.01	0.11
(1,4)	1:2:A:ILE:H	1:64:A:GLN:HB2	2	0.11	0.01	0.11
(1,135)	1:79:B:LYS:HD2	1:119:B:LEU:HD21	2	0.11	0.0	0.11
(1,135)	1:79:B:LYS:HD2	1:119:B:LEU:HD22	2	0.11	0.0	0.11
(1,135)	1:79:B:LYS:HD2	1:119:B:LEU:HD23	2	0.11	0.0	0.11
(1,1922)	1:83:B:GLN:HB3	1:83:B:GLN:HE21	2	0.11	0.01	0.11
(1,233)	1:90:B:LEU:HA	1:115:B:ILE:HG12	2	0.11	0.0	0.11
(1,951)	1:3:A:ILE:HG12	1:5:A:ASN:HD22	2	0.11	0.0	0.11
(1,965)	1:13:A:LYS:HB2	1:15:A:ILE:HG12	2	0.11	0.0	0.11
(1,1164)	1:14:A:LYS:HD2	1:15:A:ILE:H	2	0.11	0.0	0.11
(1,1755)	1:40:A:ASN:H	1:40:A:ASN:HD21	2	0.11	0.0	0.11
(1,2165)	1:64:A:GLN:H	1:110:B:GLN:HG2	2	0.11	0.0	0.11
(1,193)	1:7:A:LYS:HD2	1:35:A:GLU:HG3	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	7	27.54
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	18	27.5
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	2	27.01
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	15	26.97
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	1	26.94
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	9	26.71
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	18	26.69
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	6	26.61
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	9	26.44
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	11	26.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	19	26.32
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	5	26.22
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	16	26.22
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	12	26.15
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	4	25.99
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	7	25.88
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	14	25.87
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	17	25.87
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	12	25.83
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	10	25.81
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	18	25.7
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	10	25.55
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	2	25.54
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	3	25.48
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	6	25.4
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	6	25.32
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	9	25.32
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	20	25.31
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	18	25.29
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	13	25.18
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	11	25.17
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	1	24.95
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	9	24.94
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	8	24.91
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	7	24.86
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	5	24.81
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	3	24.76
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	17	24.75
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	1	24.71
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	19	24.7
(1,1079)	1:128:B:GLN:HE22	1:64:A:GLN:HE22	13	24.59
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	16	24.57
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	18	24.54
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	7	24.53
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	4	24.49
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	8	24.41
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	12	24.38
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	10	24.37
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	15	24.22
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	19	24.2
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	20	24.04
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	6	24.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	2	24.0
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	10	23.99
(1,56)	1:3:A:ILE:HG13	1:128:B:GLN:HE22	14	23.98
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	10	23.91
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	14	23.88
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	20	23.85
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	15	23.83
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	11	23.78
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	3	23.64
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	13	23.64
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	18	23.63
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	17	23.5
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	5	23.45
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	9	23.43
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	18	23.39
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	13	23.36
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	1	23.35
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	2	23.32
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	19	23.31
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	10	23.3
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	2	23.28
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	9	23.23
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	18	23.19
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	9	23.18
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	7	23.14
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	2	23.13
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	7	23.1
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	3	23.09
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	16	23.09
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	17	23.05
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	16	23.02
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	7	22.99
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	1	22.98
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	4	22.97
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	4	22.9
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	8	22.9
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	5	22.88
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	20	22.83
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	3	22.8
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	18	22.74
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	2	22.72
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	15	22.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	1	22.65
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	13	22.62
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	10	22.61
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	20	22.61
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	12	22.52
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	14	22.51
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	15	22.48
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	18	22.44
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	18	22.44
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	18	22.44
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	10	22.43
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	17	22.42
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	11	22.4
(1,55)	1:3:A:ILE:HG13	1:128:B:GLN:HE21	14	22.36
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	18	22.34
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	3	22.32
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	6	22.3
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	12	22.29
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	7	22.25
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	9	22.24
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	6	22.19
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	6	22.17
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	15	22.16
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	18	22.14
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	18	22.14
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	18	22.14
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	5	22.08
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	16	22.01
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	1	21.98
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	9	21.87
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	11	21.83
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	19	21.83
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	18	21.8
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	10	21.72
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	16	21.71
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	4	21.71
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	12	21.67
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	5	21.67
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	4	21.66
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	11	21.6
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	19	21.6
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	14	21.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	3	21.57
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	5	21.55
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	17	21.54
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	4	21.52
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	6	21.51
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	2	21.51
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	4	21.5
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	15	21.48
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	13	21.46
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	13	21.46
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	13	21.46
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	13	21.45
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	17	21.43
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	3	21.43
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	13	21.41
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	10	21.4
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	10	21.4
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	10	21.4
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	7	21.37
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	7	21.37
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	7	21.37
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	9	21.34
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	2	21.33
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	9	21.32
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	9	21.32
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	9	21.32
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	20	21.32
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	20	21.32
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	20	21.32
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	10	21.31
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	9	21.31
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	7	21.29
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	2	21.27
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	4	21.27
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	8	21.27
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	20	21.26
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	12	21.26
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	6	21.2
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	6	21.2
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	6	21.2
(1,2075)	1:130:B:GLN:HA	1:64:A:GLN:HE21	8	21.15
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	20	21.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	14	21.13
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	6	21.12
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	19	21.11
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	15	21.11
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	18	21.1
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	18	21.1
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	18	21.1
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	10	21.1
(1,58)	1:3:A:ILE:HG13	1:128:B:GLN:HG3	16	21.07
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	18	21.05
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	13	21.05
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	17	21.04
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	2	21.04
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	7	21.02
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	16	20.99
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	12	20.99
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	4	20.98
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	7	20.95
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	10	20.94
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	10	20.94
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	10	20.94
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	6	20.93
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	6	20.93
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	6	20.93
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	1	20.92
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	6	20.92
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	10	20.92
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	18	20.92
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	18	20.92
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	18	20.92
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	2	20.89
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	12	20.87
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	17	20.87
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	13	20.86
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	10	20.86
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	19	20.85
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	10	20.85
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	10	20.85
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	10	20.85
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	1	20.84
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	7	20.84
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	7	20.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	7	20.84
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	18	20.81
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	7	20.76
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	6	20.72
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	1	20.71
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	1	20.71
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	1	20.71
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	7	20.69
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	20	20.69
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	20	20.69
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	20	20.69
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	13	20.68
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	18	20.67
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	5	20.67
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	13	20.67
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	2	20.66
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	19	20.66
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	19	20.66
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	19	20.66
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	3	20.63
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	12	20.61
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	7	20.61
(1,1080)	1:128:B:GLN:HG2	1:64:A:GLN:HE22	8	20.61
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	10	20.6
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	18	20.6
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	18	20.6
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	18	20.6
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	10	20.6
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	11	20.58
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	5	20.58
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	5	20.58
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	5	20.58
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	3	20.55
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	11	20.54
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	1	20.54
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	5	20.54
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	13	20.53
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	13	20.53
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	13	20.53
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	15	20.5
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	10	20.49
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	9	20.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	9	20.48
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	9	20.48
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	3	20.46
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	20	20.44
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	5	20.44
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	20	20.43
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	20	20.43
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	20	20.43
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	18	20.42
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	18	20.41
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	18	20.41
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	18	20.41
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	20	20.4
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	6	20.36
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	6	20.36
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	6	20.36
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	1	20.35
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	7	20.34
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	20	20.34
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	19	20.34
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	9	20.32
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	3	20.31
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	5	20.31
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	1	20.3
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	19	20.28
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	19	20.28
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	19	20.28
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	13	20.26
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	13	20.26
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	13	20.26
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	10	20.23
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	3	20.23
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	12	20.22
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	12	20.22
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	12	20.22
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	13	20.22
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	13	20.22
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	13	20.22
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	17	20.21
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	17	20.21
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	17	20.21
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	9	20.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	16	20.2
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	17	20.18
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	18	20.17
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	18	20.17
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	18	20.17
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	14	20.16
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	10	20.15
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	10	20.15
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	10	20.15
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	20	20.15
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	19	20.14
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	1	20.13
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	7	20.13
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	7	20.13
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	7	20.13
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	19	20.12
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	19	20.12
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	19	20.12
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	16	20.12
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	11	20.1
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	1	20.05
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	16	20.04
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	16	20.04
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	16	20.04
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	14	20.03
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	13	20.03
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	20	20.03
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	4	20.03
(1,2076)	1:130:B:GLN:HA	1:64:A:GLN:HG2	8	20.02
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	15	20.02
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	15	20.01
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	3	20.0
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	12	19.96
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	8	19.95
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	9	19.94
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	9	19.94
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	9	19.94
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	20	19.94
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	20	19.94
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	20	19.94
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	5	19.93
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	2	19.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	2	19.91
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	2	19.91
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	11	19.88
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	11	19.88
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	11	19.88
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	18	19.86
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	5	19.85
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	5	19.85
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	5	19.85
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	16	19.85
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	1	19.82
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	1	19.82
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	1	19.82
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	19	19.82
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	3	19.81
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	18	19.81
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	17	19.8
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	17	19.8
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	17	19.8
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	6	19.8
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	6	19.8
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	6	19.8
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	12	19.8
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	5	19.8
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	5	19.8
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	5	19.8
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	8	19.8
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	8	19.8
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	8	19.8
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	8	19.79
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	8	19.79
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	8	19.79
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	18	19.78
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	18	19.78
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	18	19.78
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	14	19.78
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	14	19.78
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	14	19.78
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	17	19.77
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	15	19.77
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	20	19.77
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	1	19.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	19	19.76
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	17	19.75
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	9	19.73
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	12	19.73
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	12	19.73
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	12	19.73
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	2	19.69
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	6	19.69
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	11	19.68
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	14	19.67
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	9	19.67
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	4	19.66
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	17	19.65
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	15	19.64
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	7	19.63
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	11	19.62
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	11	19.62
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	11	19.62
(1,57)	1:3:A:ILE:HG13	1:128:B:GLN:HG2	14	19.6
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	4	19.59
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	4	19.59
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	4	19.59
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	16	19.58
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	16	19.58
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	16	19.58
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	10	19.58
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	10	19.58
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	10	19.58
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	20	19.57
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	7	19.57
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	7	19.57
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	7	19.57
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	3	19.56
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	3	19.56
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	3	19.56
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	2	19.55
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	3	19.55
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	13	19.55
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	3	19.55
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	3	19.55
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	3	19.55
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	2	19.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	2	19.54
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	2	19.54
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	13	19.54
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	13	19.54
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	13	19.54
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	7	19.54
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	11	19.53
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	7	19.53
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	8	19.52
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	5	19.51
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	3	19.51
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	3	19.51
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	3	19.51
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	20	19.49
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	6	19.47
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	6	19.47
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	6	19.47
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	5	19.47
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	7	19.45
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	7	19.45
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	7	19.45
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	1	19.45
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	1	19.45
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	1	19.45
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	14	19.44
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	15	19.43
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	15	19.43
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	15	19.43
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	17	19.43
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	4	19.42
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	6	19.41
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	1	19.41
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	14	19.4
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	15	19.39
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	12	19.39
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	6	19.38
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	16	19.37
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	15	19.35
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	13	19.34
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	13	19.34
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	13	19.34
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	19	19.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	9	19.31
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	9	19.31
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	9	19.31
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	18	19.3
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	11	19.3
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	8	19.3
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	6	19.28
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	6	19.28
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	6	19.28
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	13	19.27
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	19	19.27
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	19	19.27
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	19	19.27
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	20	19.25
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	20	19.25
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	20	19.25
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	4	19.25
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	5	19.25
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	5	19.25
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	5	19.25
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	20	19.24
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	20	19.24
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	20	19.24
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	20	19.24
(1,53)	1:3:A:ILE:HG12	1:128:B:GLN:HG2	14	19.24
(1,1084)	1:128:B:GLN:HG3	1:64:A:GLN:HG2	8	19.23
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	10	19.21
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	20	19.19
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	20	19.19
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	20	19.19
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	16	19.18
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	16	19.17
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	6	19.17
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	6	19.17
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	6	19.17
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	13	19.17
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	13	19.17
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	13	19.17
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	6	19.13
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	6	19.13
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	6	19.13
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	6	19.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	6	19.1
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	12	19.09
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	19	19.08
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	19	19.08
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	19	19.08
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	19	19.08
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	1	19.08
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	1	19.08
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	1	19.08
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	5	19.07
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	13	19.06
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	4	19.04
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	4	19.04
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	4	19.04
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	7	19.04
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	5	18.97
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	12	18.96
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	12	18.96
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	12	18.96
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	18	18.95
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	18	18.95
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	18	18.95
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	7	18.95
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	7	18.95
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	7	18.95
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	6	18.94
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	17	18.94
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	11	18.92
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	10	18.91
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	10	18.91
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	10	18.91
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	16	18.91
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	16	18.91
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	16	18.91
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	19	18.9
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	19	18.9
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	19	18.9
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	17	18.9
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	17	18.9
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	17	18.9
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	19	18.88
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	1	18.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	13	18.85
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	2	18.85
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	14	18.83
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	14	18.83
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	14	18.83
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	1	18.83
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	5	18.82
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	5	18.82
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	5	18.82
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	4	18.81
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	4	18.81
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	4	18.81
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	3	18.81
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	8	18.8
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	8	18.8
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	8	18.8
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	3	18.78
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	2	18.75
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	17	18.74
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	17	18.74
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	17	18.74
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	2	18.74
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	2	18.74
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	2	18.74
(1,1081)	1:128:B:GLN:HG2	1:64:A:GLN:HG2	8	18.72
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	11	18.72
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	11	18.72
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	11	18.72
(1,1829)	1:69:B:ILE:HG21	1:3:A:ILE:HG13	15	18.7
(1,1829)	1:69:B:ILE:HG22	1:3:A:ILE:HG13	15	18.7
(1,1829)	1:69:B:ILE:HG23	1:3:A:ILE:HG13	15	18.7
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	1	18.7
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	1	18.7
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	1	18.7
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	17	18.69
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	17	18.69
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	17	18.69
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	14	18.69
(1,1023)	1:3:A:ILE:HG13	1:71:B:ASN:HD22	14	18.69
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	9	18.61
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	13	18.61
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	10	18.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	10	18.6
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	10	18.6
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	9	18.59
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	9	18.59
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	9	18.59
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	12	18.58
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	15	18.58
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	17	18.57
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	1	18.57
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	1	18.57
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	1	18.57
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	16	18.55
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	19	18.53
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	19	18.53
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	19	18.53
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	9	18.53
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	14	18.52
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	14	18.52
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	14	18.52
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	5	18.51
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	9	18.51
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	9	18.51
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	9	18.51
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	8	18.5
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	8	18.5
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	8	18.5
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	4	18.49
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	11	18.46
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	15	18.45
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	3	18.44
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	3	18.44
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	3	18.44
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	4	18.42
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	14	18.42
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	14	18.42
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	14	18.42
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	8	18.42
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	8	18.42
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	8	18.42
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	12	18.42
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	12	18.42
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	12	18.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	1	18.41
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	16	18.4
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	16	18.4
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	16	18.4
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	4	18.38
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	6	18.37
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	19	18.37
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	12	18.36
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	10	18.36
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	8	18.36
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	13	18.33
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	11	18.3
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	11	18.3
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	11	18.3
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	10	18.29
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	10	18.29
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	10	18.29
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	20	18.27
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	20	18.27
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	20	18.27
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	16	18.25
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	16	18.25
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	16	18.25
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	9	18.25
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	9	18.25
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	9	18.25
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	15	18.24
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	3	18.23
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	3	18.23
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	3	18.23
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	2	18.22
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	2	18.22
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	2	18.22
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	20	18.22
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	1	18.22
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	1	18.22
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	1	18.22
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	18	18.21
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	8	18.21
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	19	18.19
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	19	18.19
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	19	18.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	16	18.17
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	15	18.17
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	12	18.17
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	12	18.17
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	12	18.17
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	12	18.16
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	12	18.16
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	12	18.16
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	17	18.16
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	5	18.14
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	5	18.14
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	5	18.14
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	7	18.13
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	7	18.13
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	7	18.13
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	2	18.11
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	1	18.09
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	1	18.09
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	1	18.09
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	17	18.09
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	5	18.07
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	5	18.07
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	5	18.07
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	9	18.03
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	9	18.03
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	9	18.03
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	11	18.03
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	19	18.0
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	14	17.99
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	2	17.99
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	2	17.99
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	2	17.99
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	19	17.97
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	6	17.97
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	6	17.97
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	6	17.97
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	16	17.97
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	16	17.97
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	16	17.97
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	5	17.96
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	14	17.91
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	11	17.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	11	17.9
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	11	17.9
(1,1082)	1:128:B:GLN:HG2	1:64:A:GLN:HG3	16	17.89
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	16	17.87
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	16	17.87
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	16	17.87
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	15	17.87
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	15	17.87
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	15	17.87
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	13	17.85
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	13	17.85
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	13	17.85
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	4	17.84
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	8	17.82
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	8	17.82
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	8	17.82
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	20	17.82
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	20	17.82
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	20	17.82
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	2	17.8
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	9	17.79
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	11	17.78
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	11	17.78
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	11	17.78
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	13	17.74
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	13	17.74
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	13	17.74
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	17	17.73
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	17	17.73
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	17	17.73
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	15	17.72
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	15	17.72
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	15	17.72
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	12	17.69
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	11	17.69
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	12	17.68
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	12	17.68
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	12	17.68
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	7	17.67
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	7	17.67
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	7	17.67
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	8	17.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	8	17.67
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	8	17.67
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	9	17.66
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	3	17.64
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	5	17.61
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	5	17.61
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	5	17.61
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	11	17.59
(1,1828)	1:69:B:ILE:HG21	1:3:A:ILE:HG12	14	17.58
(1,1828)	1:69:B:ILE:HG22	1:3:A:ILE:HG12	14	17.58
(1,1828)	1:69:B:ILE:HG23	1:3:A:ILE:HG12	14	17.58
(1,54)	1:3:A:ILE:HG13	1:128:B:GLN:H	20	17.58
(1,2072)	1:130:B:GLN:H	1:64:A:GLN:HE21	8	17.57
(1,36)	1:69:B:ILE:HD11	1:64:A:GLN:HE22	4	17.57
(1,36)	1:69:B:ILE:HD12	1:64:A:GLN:HE22	4	17.57
(1,36)	1:69:B:ILE:HD13	1:64:A:GLN:HE22	4	17.57
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	16	17.56
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	16	17.56
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	16	17.56
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	11	17.5
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	11	17.5
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	11	17.5
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	11	17.5
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	11	17.5
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	11	17.5
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	17	17.48
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	17	17.48
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	17	17.48
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	2	17.47
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	2	17.47
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	2	17.47
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	17	17.47
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	17	17.47
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	17	17.47
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	8	17.37
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	12	17.36
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	8	17.34
(1,2073)	1:130:B:GLN:H	1:64:A:GLN:HG2	8	17.32
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	16	17.29
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	10	17.29
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	10	17.29
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	10	17.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	13	17.28
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	13	17.28
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	13	17.28
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	14	17.22
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	14	17.22
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	14	17.22
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	14	17.21
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	14	17.21
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	14	17.21
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	12	17.21
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	12	17.21
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	12	17.21
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	2	17.18
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	2	17.18
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	2	17.18
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	15	17.18
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	15	17.18
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	15	17.18
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	20	17.17
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	18	17.16
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	18	17.16
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	18	17.16
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	10	17.13
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	10	17.13
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	10	17.13
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	9	17.11
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	9	17.11
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	9	17.11
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG21	3	17.03
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG22	3	17.03
(1,1826)	1:3:A:ILE:HA	1:69:B:ILE:HG23	3	17.03
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	16	17.03
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	3	16.98
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	3	16.98
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	3	16.98
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	8	16.92
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	8	16.92
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	8	16.92
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	20	16.9
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	20	16.9
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	20	16.9
(1,38)	1:69:B:ILE:HG21	1:64:A:GLN:HE21	4	16.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,38)	1:69:B:ILE:HG22	1:64:A:GLN:HE21	4	16.89
(1,38)	1:69:B:ILE:HG23	1:64:A:GLN:HE21	4	16.89
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	12	16.88
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	19	16.87
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	6	16.84
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	6	16.84
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	6	16.84
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	14	16.83
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	14	16.83
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	14	16.83
(1,2074)	1:130:B:GLN:H	1:64:A:GLN:HG3	11	16.82
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	2	16.82
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	2	16.82
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	2	16.82
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	6	16.8
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	5	16.79
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	5	16.79
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	5	16.79
(1,1022)	1:3:A:ILE:HG12	1:71:B:ASN:HD22	14	16.79
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	3	16.78
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	3	16.78
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	3	16.78
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	11	16.78
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	1	16.66
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	1	16.66
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	1	16.66
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	16	16.58
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	16	16.58
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	16	16.58
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	4	16.53
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	4	16.53
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	4	16.53
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	19	16.5
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	19	16.5
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	19	16.5
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	15	16.48
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	15	16.48
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	15	16.48
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	5	16.42
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	7	16.38
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	7	16.38
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	7	16.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	5	16.33
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	5	16.33
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	5	16.33
(1,35)	1:69:B:ILE:HD11	1:64:A:GLN:HE21	4	16.26
(1,35)	1:69:B:ILE:HD12	1:64:A:GLN:HE21	4	16.26
(1,35)	1:69:B:ILE:HD13	1:64:A:GLN:HE21	4	16.26
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	4	16.22
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	4	16.22
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	4	16.22
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	12	16.19
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	12	16.19
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	12	16.19
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	8	16.11
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	8	16.11
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	8	16.11
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	7	15.98
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	7	15.98
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	7	15.98
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	17	15.91
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	17	15.91
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	17	15.91
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	19	15.9
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	19	15.9
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	19	15.9
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	11	15.85
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	11	15.85
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	11	15.85
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	12	15.85
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	12	15.85
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	12	15.85
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	17	15.85
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	17	15.85
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	17	15.85
(1,37)	1:69:B:ILE:HD11	1:64:A:GLN:HG3	15	15.83
(1,37)	1:69:B:ILE:HD12	1:64:A:GLN:HG3	15	15.83
(1,37)	1:69:B:ILE:HD13	1:64:A:GLN:HG3	15	15.83
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	13	15.81
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	4	15.79
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	17	15.71
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	8	15.7
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	8	15.7
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	8	15.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	1	15.58
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	1	15.58
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	1	15.58
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	4	15.54
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	4	15.54
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	4	15.54
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	3	15.49
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	3	15.49
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	3	15.49
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	3	15.44
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	3	15.44
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	3	15.44
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	14	15.43
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	14	15.43
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	14	15.43
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	13	15.39
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	2	15.38
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	2	15.38
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	2	15.38
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	10	15.37
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	18	15.37
(1,1547)	1:129:B:TRP:H	1:64:A:GLN:HG2	8	15.22
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	9	15.22
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	9	15.22
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	9	15.22
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	16	14.92
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	16	14.92
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	16	14.92
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	11	14.91
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	11	14.91
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	11	14.91
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	6	14.81
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	20	14.64
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD11	15	14.47
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD12	15	14.47
(1,1825)	1:3:A:ILE:HA	1:69:B:ILE:HD13	15	14.47
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	14	14.35
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	14	14.35
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	14	14.35
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	2	14.33
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	2	14.33
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	2	14.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	4	14.27
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	5	14.27
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	4	14.1
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	4	14.1
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	4	14.1
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	8	13.92
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	12	13.88
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	17	13.86
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	15	13.79
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	1	13.69
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	7	13.59
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD11	15	13.26
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD12	15	13.26
(1,1323)	1:2:A:ILE:H	1:69:B:ILE:HD13	15	13.26
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	19	13.24
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	18	13.02
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	18	13.02
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	18	13.02
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	13	13.0
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	13	13.0
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	13	13.0
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	3	12.91
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD11	15	12.73
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD12	15	12.73
(1,1822)	1:3:A:ILE:H	1:69:B:ILE:HD13	15	12.73
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	9	12.64
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	16	12.59
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	14	12.56
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	6	12.4
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	6	12.4
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	6	12.4
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	11	12.28
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	10	12.12
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	10	12.12
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	10	12.12
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	20	12.0
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	20	12.0
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	20	12.0
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	13	11.92
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	13	11.92
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	13	11.92
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	4	11.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	4	11.68
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	4	11.68
(1,1816)	1:2:A:ILE:H	1:68:B:ILE:HB	2	11.64
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	9	11.63
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	9	11.63
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	9	11.63
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	19	11.62
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	19	11.62
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	19	11.62
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	10	11.52
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	10	11.52
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	10	11.52
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	13	11.38
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	13	11.38
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	13	11.38
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	7	11.28
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	7	11.28
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	7	11.28
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	20	11.22
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	20	11.22
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	20	11.22
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	10	11.2
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	10	11.2
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	10	11.2
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	1	11.17
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	1	11.17
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	1	11.17
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	12	11.15
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	12	11.15
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	12	11.15
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	18	11.14
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	18	11.14
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	18	11.14
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	5	11.08
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	5	11.08
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	5	11.08
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	8	11.07
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	8	11.07
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	8	11.07
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	16	10.9
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	16	10.9
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	16	10.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	6	10.88
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	6	10.88
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	6	10.88
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	6	10.85
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	6	10.85
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	6	10.85
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	11	10.73
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	11	10.73
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	11	10.73
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	20	10.69
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	20	10.69
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	20	10.69
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	17	10.63
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	17	10.63
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	17	10.63
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	5	10.61
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	5	10.61
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	5	10.61
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	7	10.51
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	7	10.51
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	7	10.51
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	3	10.42
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	3	10.42
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	3	10.42
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	5	10.4
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	5	10.4
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	5	10.4
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	19	10.39
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	19	10.39
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	19	10.39
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	19	10.38
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	19	10.38
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	19	10.38
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	17	10.28
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	17	10.28
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	17	10.28
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	18	10.27
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	18	10.27
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	18	10.27
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	12	10.26
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	12	10.26
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	12	10.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	15	10.26
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	15	10.26
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	15	10.26
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	12	10.25
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	12	10.25
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	12	10.25
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	7	10.25
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	7	10.25
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	7	10.25
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	2	10.17
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	2	10.17
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	2	10.17
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	8	10.09
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	8	10.09
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	8	10.09
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	17	10.07
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	17	10.07
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	17	10.07
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	9	10.02
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	9	10.02
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	9	10.02
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	3	9.97
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	3	9.97
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	3	9.97
(1,1324)	1:68:B:ILE:HG21	1:3:A:ILE:HA	14	9.89
(1,1324)	1:68:B:ILE:HG22	1:3:A:ILE:HA	14	9.89
(1,1324)	1:68:B:ILE:HG23	1:3:A:ILE:HA	14	9.89
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	4	9.76
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	4	9.76
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	4	9.76
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	15	9.56
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	15	9.56
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	15	9.56
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	15	9.49
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	15	9.49
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	15	9.49
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	1	9.47
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	1	9.47
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	1	9.47
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	4	9.46
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	4	9.46
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	4	9.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	1	9.41
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	1	9.41
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	1	9.41
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	3	9.41
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	3	9.41
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	3	9.41
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	8	9.37
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	8	9.37
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	8	9.37
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	16	8.96
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	16	8.96
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	16	8.96
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	11	8.93
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	11	8.93
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	11	8.93
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	2	8.77
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	2	8.77
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	2	8.77
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	11	8.77
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	11	8.77
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	11	8.77
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	14	8.67
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	14	8.67
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	14	8.67
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	16	8.37
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	16	8.37
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	16	8.37
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG21	14	8.34
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG22	14	8.34
(1,1818)	1:2:A:ILE:H	1:68:B:ILE:HG23	14	8.34
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	2	8.31
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	2	8.31
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	2	8.31
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD11	9	8.18
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD12	9	8.18
(1,1817)	1:2:A:ILE:H	1:68:B:ILE:HD13	9	8.18
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	1	3.57
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	1	3.57
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	1	3.57
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	16	3.5
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	16	3.5
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	16	3.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	19	3.5
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	19	3.5
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	19	3.5
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	9	3.49
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	9	3.49
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	9	3.49
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	11	3.47
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	11	3.47
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	11	3.47
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	14	3.47
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	15	3.41
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	15	3.41
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	15	3.41
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	20	3.41
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	20	3.41
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	20	3.41
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	1	3.27
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	1	3.27
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	1	3.27
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	9	3.25
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	9	3.25
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	9	3.25
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	12	3.25
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	12	3.25
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	12	3.25
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	5	3.24
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	5	3.24
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	5	3.24
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	4	3.19
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	4	3.19
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	4	3.19
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	2	3.17
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	2	3.17
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	2	3.17
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	7	3.16
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	7	3.16
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	7	3.16
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	10	3.16
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	10	3.16
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	10	3.16
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	6	3.13
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	6	3.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	6	3.13
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	11	3.05
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	11	3.05
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	11	3.05
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	4	2.91
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	1	2.8
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	14	2.74
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	14	2.74
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	14	2.74
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	10	2.67
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	4	2.54
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	13	2.51
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	13	2.51
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	13	2.51
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	14	2.48
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	1	2.44
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	14	2.44
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	19	2.43
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	13	2.41
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	4	2.37
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	18	2.35
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	18	2.35
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	18	2.35
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	4	2.33
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	4	2.33
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	4	2.33
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	4	2.31
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	4	2.31
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	4	2.31
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	19	2.29
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	19	2.29
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	19	2.29
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	10	2.28
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	14	2.28
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	6	2.27
(1,182)	1:23:A:LEU:HD21	1:52:A:TYR:HE2	14	2.27
(1,182)	1:23:A:LEU:HD22	1:52:A:TYR:HE2	14	2.27
(1,182)	1:23:A:LEU:HD23	1:52:A:TYR:HE2	14	2.27
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	3	2.26
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	3	2.24
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	3	2.24
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	3	2.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	13	2.24
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	13	2.24
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	13	2.24
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	8	2.23
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	18	2.21
(1,182)	1:23:A:LEU:HD21	1:52:A:TYR:HE2	13	2.19
(1,182)	1:23:A:LEU:HD22	1:52:A:TYR:HE2	13	2.19
(1,182)	1:23:A:LEU:HD23	1:52:A:TYR:HE2	13	2.19
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	2	2.18
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	3	2.18
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	12	2.18
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	15	2.18
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	19	2.17
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	5	2.16
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	17	2.16
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	16	2.15
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	14	2.14
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	14	2.14
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	14	2.14
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	12	2.13
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	12	2.13
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	12	2.13
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	16	2.12
(1,1255)	1:38:A:LYS:HD2	1:39:A:TYR:HD2	7	2.1
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	18	2.1
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	14	2.06
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	14	2.06
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	14	2.06
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	2	2.05
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	2	2.05
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	2	2.05
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	17	2.05
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	15	2.04
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	15	2.04
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	15	2.04
(1,499)	1:34:A:ILE:HD11	1:39:A:TYR:HE1	7	2.02
(1,499)	1:34:A:ILE:HD12	1:39:A:TYR:HE1	7	2.02
(1,499)	1:34:A:ILE:HD13	1:39:A:TYR:HE1	7	2.02
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	10	1.96
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	10	1.96
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	10	1.96
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	20	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	13	1.95
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	8	1.94
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	8	1.94
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	8	1.94
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	15	1.94
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	7	1.9
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	3	1.9
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	13	1.89
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	13	1.89
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	13	1.89
(1,191)	1:89:B:LEU:HD21	1:118:B:TYR:HE2	14	1.89
(1,191)	1:89:B:LEU:HD22	1:118:B:TYR:HE2	14	1.89
(1,191)	1:89:B:LEU:HD23	1:118:B:TYR:HE2	14	1.89
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	17	1.88
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	17	1.88
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	17	1.88
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	18	1.88
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	2	1.88
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	2	1.88
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	2	1.88
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	8	1.87
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	20	1.87
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	20	1.87
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	20	1.87
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	14	1.85
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	14	1.85
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	14	1.85
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	5	1.84
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	5	1.84
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	5	1.84
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	14	1.84
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	14	1.84
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	14	1.84
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	18	1.82
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	18	1.82
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	18	1.82
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	5	1.82
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	19	1.82
(1,499)	1:34:A:ILE:HD11	1:39:A:TYR:HE1	14	1.81
(1,499)	1:34:A:ILE:HD12	1:39:A:TYR:HE1	14	1.81
(1,499)	1:34:A:ILE:HD13	1:39:A:TYR:HE1	14	1.81
(1,297)	1:49:A:ILE:HG21	1:61:A:PHE:HE1	14	1.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,297)	1:49:A:ILE:HG22	1:61:A:PHE:HE1	14	1.81
(1,297)	1:49:A:ILE:HG23	1:61:A:PHE:HE1	14	1.81
(1,177)	1:23:A:LEU:HG	1:52:A:TYR:HD2	16	1.8
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	9	1.79
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	20	1.78
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	11	1.77
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	9	1.75
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	3	1.75
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	3	1.75
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	3	1.75
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	15	1.74
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	17	1.74
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	17	1.74
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	17	1.74
(1,182)	1:23:A:LEU:HD21	1:52:A:TYR:HE2	20	1.74
(1,182)	1:23:A:LEU:HD22	1:52:A:TYR:HE2	20	1.74
(1,182)	1:23:A:LEU:HD23	1:52:A:TYR:HE2	20	1.74
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	2	1.71
(1,191)	1:89:B:LEU:HD21	1:118:B:TYR:HE2	7	1.71
(1,191)	1:89:B:LEU:HD22	1:118:B:TYR:HE2	7	1.71
(1,191)	1:89:B:LEU:HD23	1:118:B:TYR:HE2	7	1.71
(1,191)	1:89:B:LEU:HD21	1:118:B:TYR:HE2	16	1.71
(1,191)	1:89:B:LEU:HD22	1:118:B:TYR:HE2	16	1.71
(1,191)	1:89:B:LEU:HD23	1:118:B:TYR:HE2	16	1.71
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	3	1.7
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	3	1.7
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	3	1.7
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	11	1.7
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	7	1.7
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	7	1.7
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	7	1.7
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	3	1.69
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	3	1.69
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	3	1.69
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	9	1.67
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	15	1.67
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	7	1.67
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	7	1.67
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	7	1.67
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	1	1.65
(1,1255)	1:38:A:LYS:HD2	1:39:A:TYR:HD2	14	1.64
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	17	1.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	20	1.64
(1,182)	1:23:A:LEU:HD21	1:52:A:TYR:HE2	2	1.64
(1,182)	1:23:A:LEU:HD22	1:52:A:TYR:HE2	2	1.64
(1,182)	1:23:A:LEU:HD23	1:52:A:TYR:HE2	2	1.64
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	5	1.63
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	5	1.63
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	5	1.63
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	20	1.63
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	12	1.63
(1,177)	1:23:A:LEU:HG	1:52:A:TYR:HD2	13	1.63
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	14	1.62
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	14	1.62
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	14	1.62
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	3	1.61
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	3	1.61
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	3	1.61
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	12	1.61
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	4	1.61
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	4	1.61
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	4	1.61
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	13	1.61
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	13	1.61
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	13	1.61
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	16	1.6
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	7	1.6
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	16	1.59
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	7	1.59
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	12	1.59
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	2	1.59
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	2	1.59
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	2	1.59
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	13	1.58
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	7	1.57
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	7	1.57
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	7	1.57
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	18	1.57
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	18	1.57
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	18	1.57
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	9	1.54
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	16	1.53
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	16	1.53
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	16	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	6	1.51
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	4	1.51
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	6	1.51
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	6	1.51
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	6	1.51
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	12	1.51
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	12	1.51
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	12	1.51
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	15	1.5
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	15	1.5
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	15	1.5
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	1	1.46
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	1	1.46
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	1	1.46
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	17	1.45
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	17	1.45
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	17	1.45
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	5	1.45
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	19	1.45
(1,299)	1:115:B:ILE:HG21	1:127:B:PHE:HE1	4	1.43
(1,299)	1:115:B:ILE:HG22	1:127:B:PHE:HE1	4	1.43
(1,299)	1:115:B:ILE:HG23	1:127:B:PHE:HE1	4	1.43
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	6	1.42
(1,182)	1:23:A:LEU:HD21	1:52:A:TYR:HE2	7	1.42
(1,182)	1:23:A:LEU:HD22	1:52:A:TYR:HE2	7	1.42
(1,182)	1:23:A:LEU:HD23	1:52:A:TYR:HE2	7	1.42
(1,756)	1:123:B:LEU:HD21	1:127:B:PHE:HD1	7	1.41
(1,756)	1:123:B:LEU:HD22	1:127:B:PHE:HD1	7	1.41
(1,756)	1:123:B:LEU:HD23	1:127:B:PHE:HD1	7	1.41
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	4	1.41
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	4	1.41
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	4	1.41
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	6	1.39
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	6	1.39
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	6	1.39
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	2	1.38
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	2	1.38
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	2	1.38
(1,182)	1:23:A:LEU:HD21	1:52:A:TYR:HE2	3	1.38
(1,182)	1:23:A:LEU:HD22	1:52:A:TYR:HE2	3	1.38
(1,182)	1:23:A:LEU:HD23	1:52:A:TYR:HE2	3	1.38
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	20	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	20	1.37
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	20	1.37
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	2	1.37
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	6	1.37
(1,182)	1:23:A:LEU:HD21	1:52:A:TYR:HE2	18	1.37
(1,182)	1:23:A:LEU:HD22	1:52:A:TYR:HE2	18	1.37
(1,182)	1:23:A:LEU:HD23	1:52:A:TYR:HE2	18	1.37
(1,260)	1:107:B:PRO:HB3	1:127:B:PHE:HE1	4	1.35
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	5	1.35
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	5	1.35
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	5	1.35
(1,498)	1:34:A:ILE:HD11	1:39:A:TYR:HD1	7	1.34
(1,498)	1:34:A:ILE:HD12	1:39:A:TYR:HD1	7	1.34
(1,498)	1:34:A:ILE:HD13	1:39:A:TYR:HD1	7	1.34
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	12	1.33
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	12	1.33
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	12	1.33
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	17	1.33
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	16	1.33
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	16	1.33
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	16	1.33
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	10	1.32
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	10	1.32
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	10	1.32
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	11	1.32
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	11	1.32
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	11	1.32
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	20	1.32
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	20	1.32
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	20	1.32
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	8	1.31
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	8	1.31
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	8	1.31
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	14	1.31
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	14	1.31
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	14	1.31
(1,280)	1:112:B:ALA:HA	1:127:B:PHE:HD1	18	1.31
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	10	1.31
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	15	1.3
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	15	1.3
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	15	1.3
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	1	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	1	1.29
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	1	1.29
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	18	1.27
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	18	1.27
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	18	1.27
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	16	1.26
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	16	1.26
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	16	1.26
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	3	1.24
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	11	1.23
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	11	1.23
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	11	1.23
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	12	1.23
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	12	1.23
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	12	1.23
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	7	1.23
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	3	1.21
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	3	1.21
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	3	1.21
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	2	1.21
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	11	1.21
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	12	1.21
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	12	1.21
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	12	1.21
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	15	1.21
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	15	1.21
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	15	1.21
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	13	1.2
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	13	1.2
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	13	1.2
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	2	1.18
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	2	1.18
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	2	1.18
(1,501)	1:34:A:ILE:HG21	1:39:A:TYR:HD1	14	1.18
(1,501)	1:34:A:ILE:HG22	1:39:A:TYR:HD1	14	1.18
(1,501)	1:34:A:ILE:HG23	1:39:A:TYR:HD1	14	1.18
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	13	1.18
(1,257)	1:41:A:PRO:HB3	1:61:A:PHE:HE1	1	1.17
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	10	1.17
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	10	1.17
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	10	1.17
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	15	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	15	1.16
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	15	1.16
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	5	1.16
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	13	1.15
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	13	1.15
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	13	1.15
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	16	1.15
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	16	1.15
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	16	1.15
(1,276)	1:46:A:ALA:HA	1:61:A:PHE:HD1	11	1.15
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	9	1.14
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	9	1.14
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	9	1.14
(1,258)	1:41:A:PRO:HG2	1:61:A:PHE:HD1	14	1.14
(1,177)	1:23:A:LEU:HG	1:52:A:TYR:HD2	14	1.14
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	19	1.13
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	19	1.13
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	19	1.13
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	19	1.12
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	19	1.12
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	19	1.12
(1,498)	1:34:A:ILE:HD11	1:39:A:TYR:HD1	14	1.12
(1,498)	1:34:A:ILE:HD12	1:39:A:TYR:HD1	14	1.12
(1,498)	1:34:A:ILE:HD13	1:39:A:TYR:HD1	14	1.12
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	9	1.11
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	9	1.11
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	9	1.11
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	1	1.1
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	1	1.1
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	1	1.1
(1,656)	1:57:A:LEU:HA	1:61:A:PHE:HD1	10	1.1
(1,177)	1:23:A:LEU:HG	1:52:A:TYR:HD2	20	1.1
(1,212)	1:34:A:ILE:HD11	1:61:A:PHE:HE2	4	1.09
(1,212)	1:34:A:ILE:HD12	1:61:A:PHE:HE2	4	1.09
(1,212)	1:34:A:ILE:HD13	1:61:A:PHE:HE2	4	1.09
(1,191)	1:89:B:LEU:HD21	1:118:B:TYR:HE2	2	1.09
(1,191)	1:89:B:LEU:HD22	1:118:B:TYR:HE2	2	1.09
(1,191)	1:89:B:LEU:HD23	1:118:B:TYR:HE2	2	1.09
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	6	1.07
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	6	1.07
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	6	1.07
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	20	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	20	1.07
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	20	1.07
(1,180)	1:23:A:LEU:HD11	1:52:A:TYR:HD2	13	1.07
(1,180)	1:23:A:LEU:HD12	1:52:A:TYR:HD2	13	1.07
(1,180)	1:23:A:LEU:HD13	1:52:A:TYR:HD2	13	1.07
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	3	1.05
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	3	1.05
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	3	1.05
(1,186)	1:89:B:LEU:HG	1:118:B:TYR:HD2	14	1.05
(1,177)	1:23:A:LEU:HG	1:52:A:TYR:HD2	2	1.05
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	7	1.04
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	7	1.04
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	7	1.04
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	19	1.04
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	19	1.04
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	19	1.04
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	11	1.04
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	11	1.04
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	11	1.04
(1,191)	1:89:B:LEU:HD21	1:118:B:TYR:HE2	6	1.04
(1,191)	1:89:B:LEU:HD22	1:118:B:TYR:HE2	6	1.04
(1,191)	1:89:B:LEU:HD23	1:118:B:TYR:HE2	6	1.04
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	5	1.03
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	5	1.03
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	5	1.03
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	16	1.03
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	16	1.03
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	16	1.03
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	19	1.03
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	19	1.03
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	19	1.03
(1,191)	1:89:B:LEU:HD21	1:118:B:TYR:HE2	4	1.03
(1,191)	1:89:B:LEU:HD22	1:118:B:TYR:HE2	4	1.03
(1,191)	1:89:B:LEU:HD23	1:118:B:TYR:HE2	4	1.03
(1,257)	1:41:A:PRO:HB3	1:61:A:PHE:HE1	14	1.01
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	4	1.01
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	4	1.01
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	4	1.01
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	9	1.0
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	9	1.0
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	9	1.0
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	3	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	3	1.0
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	3	1.0
(1,212)	1:34:A:ILE:HD11	1:61:A:PHE:HE2	2	1.0
(1,212)	1:34:A:ILE:HD12	1:61:A:PHE:HE2	2	1.0
(1,212)	1:34:A:ILE:HD13	1:61:A:PHE:HE2	2	1.0
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	9	0.99
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	9	0.99
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	9	0.99
(1,258)	1:41:A:PRO:HG2	1:61:A:PHE:HD1	1	0.99
(1,180)	1:23:A:LEU:HD11	1:52:A:TYR:HD2	16	0.99
(1,180)	1:23:A:LEU:HD12	1:52:A:TYR:HD2	16	0.99
(1,180)	1:23:A:LEU:HD13	1:52:A:TYR:HD2	16	0.99
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	16	0.97
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	16	0.97
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	16	0.97
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	13	0.97
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	13	0.97
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	13	0.97
(1,752)	1:123:B:LEU:HA	1:127:B:PHE:HD1	1	0.97
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	17	0.95
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	17	0.95
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	17	0.95
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	4	0.95
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	4	0.95
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	4	0.95
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	8	0.95
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	8	0.95
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	8	0.95
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	12	0.94
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	12	0.94
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	12	0.94
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	9	0.94
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	9	0.94
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	9	0.94
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	17	0.94
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	17	0.94
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	17	0.94
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	7	0.93
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	7	0.93
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	7	0.93
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	11	0.92
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	11	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	11	0.92
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	6	0.91
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	6	0.91
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	6	0.91
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	18	0.9
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	18	0.9
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	18	0.9
(1,297)	1:49:A:ILE:HG21	1:61:A:PHE:HE1	1	0.9
(1,297)	1:49:A:ILE:HG22	1:61:A:PHE:HE1	1	0.9
(1,297)	1:49:A:ILE:HG23	1:61:A:PHE:HE1	1	0.9
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	14	0.9
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	14	0.9
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	14	0.9
(1,212)	1:34:A:ILE:HD11	1:61:A:PHE:HE2	20	0.9
(1,212)	1:34:A:ILE:HD12	1:61:A:PHE:HE2	20	0.9
(1,212)	1:34:A:ILE:HD13	1:61:A:PHE:HE2	20	0.9
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	6	0.9
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	6	0.9
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	6	0.9
(1,191)	1:89:B:LEU:HD21	1:118:B:TYR:HE2	13	0.89
(1,191)	1:89:B:LEU:HD22	1:118:B:TYR:HE2	13	0.89
(1,191)	1:89:B:LEU:HD23	1:118:B:TYR:HE2	13	0.89
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	15	0.88
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	15	0.88
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	15	0.88
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	16	0.88
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	16	0.88
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	16	0.88
(1,660)	1:57:A:LEU:HD21	1:61:A:PHE:HD1	6	0.87
(1,660)	1:57:A:LEU:HD22	1:61:A:PHE:HD1	6	0.87
(1,660)	1:57:A:LEU:HD23	1:61:A:PHE:HD1	6	0.87
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	10	0.87
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	10	0.87
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	10	0.87
(1,260)	1:107:B:PRO:HB3	1:127:B:PHE:HE1	14	0.87
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	18	0.87
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	18	0.87
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	18	0.87
(1,212)	1:34:A:ILE:HD11	1:61:A:PHE:HE2	3	0.86
(1,212)	1:34:A:ILE:HD12	1:61:A:PHE:HE2	3	0.86
(1,212)	1:34:A:ILE:HD13	1:61:A:PHE:HE2	3	0.86
(1,212)	1:34:A:ILE:HD11	1:61:A:PHE:HE2	17	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:34:A:ILE:HD12	1:61:A:PHE:HE2	17	0.86
(1,212)	1:34:A:ILE:HD13	1:61:A:PHE:HE2	17	0.86
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	20	0.85
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	20	0.85
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	20	0.85
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	13	0.85
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	13	0.85
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	13	0.85
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	7	0.85
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	7	0.85
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	7	0.85
(1,261)	1:107:B:PRO:HG2	1:127:B:PHE:HD1	1	0.84
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	1	0.83
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	1	0.83
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	1	0.83
(1,258)	1:41:A:PRO:HG2	1:61:A:PHE:HD1	19	0.82
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	2	0.81
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	2	0.81
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	2	0.81
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	9	0.81
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	9	0.81
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	9	0.81
(1,186)	1:89:B:LEU:HG	1:118:B:TYR:HD2	3	0.81
(1,177)	1:23:A:LEU:HG	1:52:A:TYR:HD2	3	0.81
(1,177)	1:23:A:LEU:HG	1:52:A:TYR:HD2	12	0.81
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	20	0.8
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	20	0.8
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	20	0.8
(1,299)	1:115:B:ILE:HG21	1:127:B:PHE:HE1	14	0.8
(1,299)	1:115:B:ILE:HG22	1:127:B:PHE:HE1	14	0.8
(1,299)	1:115:B:ILE:HG23	1:127:B:PHE:HE1	14	0.8
(1,261)	1:107:B:PRO:HG2	1:127:B:PHE:HD1	4	0.8
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	3	0.8
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	3	0.8
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	3	0.8
(1,2104)	1:43:A:LEU:HD11	1:127:B:PHE:HD1	3	0.78
(1,2104)	1:43:A:LEU:HD12	1:127:B:PHE:HD1	3	0.78
(1,2104)	1:43:A:LEU:HD13	1:127:B:PHE:HD1	3	0.78
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	6	0.78
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	6	0.78
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	6	0.78
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	11	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	11	0.78
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	11	0.78
(1,212)	1:34:A:ILE:HD11	1:61:A:PHE:HE2	5	0.78
(1,212)	1:34:A:ILE:HD12	1:61:A:PHE:HE2	5	0.78
(1,212)	1:34:A:ILE:HD13	1:61:A:PHE:HE2	5	0.78
(1,189)	1:89:B:LEU:HD11	1:118:B:TYR:HD2	3	0.76
(1,189)	1:89:B:LEU:HD12	1:118:B:TYR:HD2	3	0.76
(1,189)	1:89:B:LEU:HD13	1:118:B:TYR:HD2	3	0.76
(1,212)	1:34:A:ILE:HD11	1:61:A:PHE:HE2	7	0.75
(1,212)	1:34:A:ILE:HD12	1:61:A:PHE:HE2	7	0.75
(1,212)	1:34:A:ILE:HD13	1:61:A:PHE:HE2	7	0.75
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	5	0.73
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	5	0.73
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	5	0.73
(1,182)	1:23:A:LEU:HD21	1:52:A:TYR:HE2	12	0.73
(1,182)	1:23:A:LEU:HD22	1:52:A:TYR:HE2	12	0.73
(1,182)	1:23:A:LEU:HD23	1:52:A:TYR:HE2	12	0.73
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	6	0.72
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	6	0.72
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	6	0.72
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	6	0.71
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	6	0.71
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	6	0.71
(1,180)	1:23:A:LEU:HD11	1:52:A:TYR:HD2	2	0.71
(1,180)	1:23:A:LEU:HD12	1:52:A:TYR:HD2	2	0.71
(1,180)	1:23:A:LEU:HD13	1:52:A:TYR:HD2	2	0.71
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	7	0.7
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	7	0.7
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	7	0.7
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	6	0.7
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	6	0.7
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	6	0.7
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	19	0.7
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	19	0.7
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	19	0.7
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	16	0.69
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	16	0.69
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	16	0.69
(1,182)	1:23:A:LEU:HD21	1:52:A:TYR:HE2	6	0.69
(1,182)	1:23:A:LEU:HD22	1:52:A:TYR:HE2	6	0.69
(1,182)	1:23:A:LEU:HD23	1:52:A:TYR:HE2	6	0.69
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	11	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	11	0.67
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	11	0.67
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	1	0.67
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	1	0.67
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	1	0.67
(1,180)	1:23:A:LEU:HD11	1:52:A:TYR:HD2	20	0.67
(1,180)	1:23:A:LEU:HD12	1:52:A:TYR:HD2	20	0.67
(1,180)	1:23:A:LEU:HD13	1:52:A:TYR:HD2	20	0.67
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD21	14	0.66
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD22	14	0.66
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD23	14	0.66
(1,299)	1:115:B:ILE:HG21	1:127:B:PHE:HE1	15	0.66
(1,299)	1:115:B:ILE:HG22	1:127:B:PHE:HE1	15	0.66
(1,299)	1:115:B:ILE:HG23	1:127:B:PHE:HE1	15	0.66
(1,191)	1:89:B:LEU:HD21	1:118:B:TYR:HE2	18	0.66
(1,191)	1:89:B:LEU:HD22	1:118:B:TYR:HE2	18	0.66
(1,191)	1:89:B:LEU:HD23	1:118:B:TYR:HE2	18	0.66
(1,186)	1:89:B:LEU:HG	1:118:B:TYR:HD2	7	0.66
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	19	0.65
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	19	0.65
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	19	0.65
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	16	0.65
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	16	0.65
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	16	0.65
(1,260)	1:107:B:PRO:HB3	1:127:B:PHE:HE1	10	0.65
(1,186)	1:89:B:LEU:HG	1:118:B:TYR:HD2	16	0.65
(1,177)	1:23:A:LEU:HG	1:52:A:TYR:HD2	18	0.65
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD21	2	0.64
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD22	2	0.64
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD23	2	0.64
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	16	0.64
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	16	0.64
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	16	0.64
(1,212)	1:34:A:ILE:HD11	1:61:A:PHE:HE2	10	0.63
(1,212)	1:34:A:ILE:HD12	1:61:A:PHE:HE2	10	0.63
(1,212)	1:34:A:ILE:HD13	1:61:A:PHE:HE2	10	0.63
(1,1252)	1:38:A:LYS:HA	1:39:A:TYR:HD2	7	0.61
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	8	0.61
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	8	0.61
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	8	0.61
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	1	0.61
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	1	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	1	0.61
(1,186)	1:89:B:LEU:HG	1:118:B:TYR:HD2	6	0.61
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	10	0.6
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	10	0.6
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	10	0.6
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	17	0.6
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	17	0.6
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	17	0.6
(1,212)	1:34:A:ILE:HD11	1:61:A:PHE:HE2	15	0.6
(1,212)	1:34:A:ILE:HD12	1:61:A:PHE:HE2	15	0.6
(1,212)	1:34:A:ILE:HD13	1:61:A:PHE:HE2	15	0.6
(1,186)	1:89:B:LEU:HG	1:118:B:TYR:HD2	2	0.6
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	14	0.59
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	14	0.59
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	14	0.59
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	17	0.59
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	17	0.59
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	17	0.59
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	2	0.59
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	2	0.59
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	2	0.59
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	9	0.59
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	9	0.59
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	9	0.59
(1,2105)	1:43:A:LEU:HD21	1:127:B:PHE:HD1	5	0.58
(1,2105)	1:43:A:LEU:HD22	1:127:B:PHE:HD1	5	0.58
(1,2105)	1:43:A:LEU:HD23	1:127:B:PHE:HD1	5	0.58
(1,212)	1:34:A:ILE:HD11	1:61:A:PHE:HE2	9	0.58
(1,212)	1:34:A:ILE:HD12	1:61:A:PHE:HE2	9	0.58
(1,212)	1:34:A:ILE:HD13	1:61:A:PHE:HE2	9	0.58
(1,182)	1:23:A:LEU:HD21	1:52:A:TYR:HE2	16	0.58
(1,182)	1:23:A:LEU:HD22	1:52:A:TYR:HE2	16	0.58
(1,182)	1:23:A:LEU:HD23	1:52:A:TYR:HE2	16	0.58
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	4	0.56
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	4	0.56
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	4	0.56
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	18	0.56
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	18	0.56
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	18	0.56
(1,1256)	1:38:A:LYS:HD2	1:39:A:TYR:HE2	7	0.54
(1,501)	1:34:A:ILE:HG21	1:39:A:TYR:HD1	7	0.54
(1,501)	1:34:A:ILE:HG22	1:39:A:TYR:HD1	7	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:34:A:ILE:HG23	1:39:A:TYR:HD1	7	0.54
(1,260)	1:107:B:PRO:HB3	1:127:B:PHE:HE1	8	0.54
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	4	0.54
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	4	0.54
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	4	0.54
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	14	0.54
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	14	0.54
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	14	0.54
(1,189)	1:89:B:LEU:HD11	1:118:B:TYR:HD2	14	0.54
(1,189)	1:89:B:LEU:HD12	1:118:B:TYR:HD2	14	0.54
(1,189)	1:89:B:LEU:HD13	1:118:B:TYR:HD2	14	0.54
(1,180)	1:23:A:LEU:HD11	1:52:A:TYR:HD2	14	0.54
(1,180)	1:23:A:LEU:HD12	1:52:A:TYR:HD2	14	0.54
(1,180)	1:23:A:LEU:HD13	1:52:A:TYR:HD2	14	0.54
(1,2111)	1:48:A:LYS:HG3	1:129:B:TRP:HE1	2	0.53
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	4	0.53
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	4	0.53
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	4	0.53
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	10	0.53
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	10	0.53
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	10	0.53
(1,177)	1:23:A:LEU:HG	1:52:A:TYR:HD2	7	0.53
(1,2107)	1:43:A:LEU:HD11	1:127:B:PHE:HE1	1	0.52
(1,2107)	1:43:A:LEU:HD12	1:127:B:PHE:HE1	1	0.52
(1,2107)	1:43:A:LEU:HD13	1:127:B:PHE:HE1	1	0.52
(1,2107)	1:43:A:LEU:HD21	1:127:B:PHE:HE1	1	0.52
(1,2107)	1:43:A:LEU:HD22	1:127:B:PHE:HE1	1	0.52
(1,2107)	1:43:A:LEU:HD23	1:127:B:PHE:HE1	1	0.52
(1,261)	1:107:B:PRO:HG2	1:127:B:PHE:HD1	10	0.52
(1,258)	1:41:A:PRO:HG2	1:61:A:PHE:HD1	16	0.52
(1,2157)	1:63:A:TRP:HE1	1:114:B:LYS:HG3	15	0.51
(1,1258)	1:38:A:LYS:HE2	1:39:A:TYR:HD2	7	0.51
(1,299)	1:115:B:ILE:HG21	1:127:B:PHE:HE1	10	0.51
(1,299)	1:115:B:ILE:HG22	1:127:B:PHE:HE1	10	0.51
(1,299)	1:115:B:ILE:HG23	1:127:B:PHE:HE1	10	0.51
(1,214)	1:34:A:ILE:HG21	1:61:A:PHE:HD2	12	0.51
(1,214)	1:34:A:ILE:HG22	1:61:A:PHE:HD2	12	0.51
(1,214)	1:34:A:ILE:HG23	1:61:A:PHE:HD2	12	0.51
(1,2106)	1:43:A:LEU:HD11	1:127:B:PHE:HD1	1	0.5
(1,2106)	1:43:A:LEU:HD12	1:127:B:PHE:HD1	1	0.5
(1,2106)	1:43:A:LEU:HD13	1:127:B:PHE:HD1	1	0.5
(1,2106)	1:43:A:LEU:HD21	1:127:B:PHE:HD1	1	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2106)	1:43:A:LEU:HD22	1:127:B:PHE:HD1	1	0.5
(1,2106)	1:43:A:LEU:HD23	1:127:B:PHE:HD1	1	0.5
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	18	0.5
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	18	0.5
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	18	0.5
(1,212)	1:34:A:ILE:HD11	1:61:A:PHE:HE2	13	0.5
(1,212)	1:34:A:ILE:HD12	1:61:A:PHE:HE2	13	0.5
(1,212)	1:34:A:ILE:HD13	1:61:A:PHE:HE2	13	0.5
(1,1541)	1:125:B:ASP:HB3	1:126:B:ILE:HG21	4	0.49
(1,1541)	1:125:B:ASP:HB3	1:126:B:ILE:HG22	4	0.49
(1,1541)	1:125:B:ASP:HB3	1:126:B:ILE:HG23	4	0.49
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	2	0.49
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	2	0.49
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	2	0.49
(1,260)	1:107:B:PRO:HB3	1:127:B:PHE:HE1	7	0.49
(1,180)	1:23:A:LEU:HD11	1:52:A:TYR:HD2	3	0.49
(1,180)	1:23:A:LEU:HD12	1:52:A:TYR:HD2	3	0.49
(1,180)	1:23:A:LEU:HD13	1:52:A:TYR:HD2	3	0.49
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	8	0.48
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	8	0.48
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	8	0.48
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD21	7	0.47
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD22	7	0.47
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD23	7	0.47
(1,2157)	1:63:A:TRP:HE1	1:114:B:LYS:HG3	2	0.47
(1,1372)	1:77:B:GLU:HG3	1:78:B:LYS:HB3	7	0.47
(1,1140)	1:11:A:GLU:HG3	1:12:A:LYS:HB3	14	0.47
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	11	0.47
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	11	0.47
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	11	0.47
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	20	0.47
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	20	0.47
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	20	0.47
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	4	0.47
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	4	0.47
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	4	0.47
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD11	3	0.46
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD12	3	0.46
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD13	3	0.46
(1,1629)	1:14:A:LYS:HA	1:14:A:LYS:HD2	17	0.46
(1,1499)	1:109:B:LEU:HD11	1:110:B:GLN:HA	7	0.46
(1,1499)	1:109:B:LEU:HD12	1:110:B:GLN:HA	7	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1499)	1:109:B:LEU:HD13	1:110:B:GLN:HA	7	0.46
(1,1499)	1:109:B:LEU:HD21	1:110:B:GLN:HA	7	0.46
(1,1499)	1:109:B:LEU:HD22	1:110:B:GLN:HA	7	0.46
(1,1499)	1:109:B:LEU:HD23	1:110:B:GLN:HA	7	0.46
(1,1378)	1:78:B:LYS:HD2	1:79:B:LYS:H	2	0.46
(1,1267)	1:43:A:LEU:HD11	1:44:A:GLN:HA	7	0.46
(1,1267)	1:43:A:LEU:HD12	1:44:A:GLN:HA	7	0.46
(1,1267)	1:43:A:LEU:HD13	1:44:A:GLN:HA	7	0.46
(1,1267)	1:43:A:LEU:HD21	1:44:A:GLN:HA	7	0.46
(1,1267)	1:43:A:LEU:HD22	1:44:A:GLN:HA	7	0.46
(1,1267)	1:43:A:LEU:HD23	1:44:A:GLN:HA	7	0.46
(1,189)	1:89:B:LEU:HD11	1:118:B:TYR:HD2	7	0.46
(1,189)	1:89:B:LEU:HD12	1:118:B:TYR:HD2	7	0.46
(1,189)	1:89:B:LEU:HD13	1:118:B:TYR:HD2	7	0.46
(1,180)	1:23:A:LEU:HD11	1:52:A:TYR:HD2	7	0.46
(1,180)	1:23:A:LEU:HD12	1:52:A:TYR:HD2	7	0.46
(1,180)	1:23:A:LEU:HD13	1:52:A:TYR:HD2	7	0.46
(1,180)	1:23:A:LEU:HD11	1:52:A:TYR:HD2	12	0.46
(1,180)	1:23:A:LEU:HD12	1:52:A:TYR:HD2	12	0.46
(1,180)	1:23:A:LEU:HD13	1:52:A:TYR:HD2	12	0.46
(1,1453)	1:97:B:ILE:HG21	1:98:B:ASN:HD21	12	0.45
(1,1453)	1:97:B:ILE:HG22	1:98:B:ASN:HD21	12	0.45
(1,1453)	1:97:B:ILE:HG23	1:98:B:ASN:HD21	12	0.45
(1,1140)	1:11:A:GLU:HG3	1:12:A:LYS:HB3	7	0.45
(1,846)	1:50:A:ALA:HA	1:53:A:LEU:HD11	4	0.45
(1,846)	1:50:A:ALA:HA	1:53:A:LEU:HD12	4	0.45
(1,846)	1:50:A:ALA:HA	1:53:A:LEU:HD13	4	0.45
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	3	0.45
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	3	0.45
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	3	0.45
(1,261)	1:107:B:PRO:HG2	1:127:B:PHE:HD1	14	0.45
(1,257)	1:41:A:PRO:HB3	1:61:A:PHE:HE1	20	0.45
(1,1335)	1:73:B:LYS:H	1:74:B:LEU:HD21	11	0.44
(1,1335)	1:73:B:LYS:H	1:74:B:LEU:HD22	11	0.44
(1,1335)	1:73:B:LYS:H	1:74:B:LEU:HD23	11	0.44
(1,1309)	1:59:A:ASP:HB3	1:60:A:ILE:HG21	14	0.44
(1,1309)	1:59:A:ASP:HB3	1:60:A:ILE:HG22	14	0.44
(1,1309)	1:59:A:ASP:HB3	1:60:A:ILE:HG23	14	0.44
(1,1228)	1:35:A:GLU:H	1:36:A:LYS:HD2	16	0.44
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG21	4	0.44
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG22	4	0.44
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG23	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD11	9	0.43
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD12	9	0.43
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD13	9	0.43
(1,1897)	1:80:B:LYS:HA	1:80:B:LYS:HD2	17	0.43
(1,1629)	1:14:A:LYS:HA	1:14:A:LYS:HD2	11	0.43
(1,1267)	1:43:A:LEU:HD11	1:44:A:GLN:HA	3	0.43
(1,1267)	1:43:A:LEU:HD12	1:44:A:GLN:HA	3	0.43
(1,1267)	1:43:A:LEU:HD13	1:44:A:GLN:HA	3	0.43
(1,1267)	1:43:A:LEU:HD21	1:44:A:GLN:HA	3	0.43
(1,1267)	1:43:A:LEU:HD22	1:44:A:GLN:HA	3	0.43
(1,1267)	1:43:A:LEU:HD23	1:44:A:GLN:HA	3	0.43
(1,1267)	1:43:A:LEU:HD11	1:44:A:GLN:HA	20	0.43
(1,1267)	1:43:A:LEU:HD12	1:44:A:GLN:HA	20	0.43
(1,1267)	1:43:A:LEU:HD13	1:44:A:GLN:HA	20	0.43
(1,1267)	1:43:A:LEU:HD21	1:44:A:GLN:HA	20	0.43
(1,1267)	1:43:A:LEU:HD22	1:44:A:GLN:HA	20	0.43
(1,1267)	1:43:A:LEU:HD23	1:44:A:GLN:HA	20	0.43
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	18	0.43
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	18	0.43
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	18	0.43
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	5	0.43
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	5	0.43
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	5	0.43
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD11	19	0.42
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD12	19	0.42
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD13	19	0.42
(1,1499)	1:109:B:LEU:HD11	1:110:B:GLN:HA	4	0.42
(1,1499)	1:109:B:LEU:HD12	1:110:B:GLN:HA	4	0.42
(1,1499)	1:109:B:LEU:HD13	1:110:B:GLN:HA	4	0.42
(1,1499)	1:109:B:LEU:HD21	1:110:B:GLN:HA	4	0.42
(1,1499)	1:109:B:LEU:HD22	1:110:B:GLN:HA	4	0.42
(1,1499)	1:109:B:LEU:HD23	1:110:B:GLN:HA	4	0.42
(1,1267)	1:43:A:LEU:HD11	1:44:A:GLN:HA	11	0.42
(1,1267)	1:43:A:LEU:HD12	1:44:A:GLN:HA	11	0.42
(1,1267)	1:43:A:LEU:HD13	1:44:A:GLN:HA	11	0.42
(1,1267)	1:43:A:LEU:HD21	1:44:A:GLN:HA	11	0.42
(1,1267)	1:43:A:LEU:HD22	1:44:A:GLN:HA	11	0.42
(1,1267)	1:43:A:LEU:HD23	1:44:A:GLN:HA	11	0.42
(1,1167)	1:15:A:ILE:HG13	1:16:A:SER:H	7	0.42
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD11	4	0.42
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD12	4	0.42
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD13	4	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	12	0.42
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	12	0.42
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	12	0.42
(1,1499)	1:109:B:LEU:HD11	1:110:B:GLN:HA	1	0.41
(1,1499)	1:109:B:LEU:HD12	1:110:B:GLN:HA	1	0.41
(1,1499)	1:109:B:LEU:HD13	1:110:B:GLN:HA	1	0.41
(1,1499)	1:109:B:LEU:HD21	1:110:B:GLN:HA	1	0.41
(1,1499)	1:109:B:LEU:HD22	1:110:B:GLN:HA	1	0.41
(1,1499)	1:109:B:LEU:HD23	1:110:B:GLN:HA	1	0.41
(1,1499)	1:109:B:LEU:HD11	1:110:B:GLN:HA	8	0.41
(1,1499)	1:109:B:LEU:HD12	1:110:B:GLN:HA	8	0.41
(1,1499)	1:109:B:LEU:HD13	1:110:B:GLN:HA	8	0.41
(1,1499)	1:109:B:LEU:HD21	1:110:B:GLN:HA	8	0.41
(1,1499)	1:109:B:LEU:HD22	1:110:B:GLN:HA	8	0.41
(1,1499)	1:109:B:LEU:HD23	1:110:B:GLN:HA	8	0.41
(1,1399)	1:81:B:ILE:HG13	1:82:B:SER:H	1	0.41
(1,1399)	1:81:B:ILE:HG13	1:82:B:SER:H	12	0.41
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	13	0.41
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	13	0.41
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	13	0.41
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	20	0.41
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	20	0.41
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	20	0.41
(1,1919)	1:83:B:GLN:H	1:83:B:GLN:HE21	7	0.4
(1,1897)	1:80:B:LYS:HA	1:80:B:LYS:HD2	11	0.4
(1,1499)	1:109:B:LEU:HD11	1:110:B:GLN:HA	11	0.4
(1,1499)	1:109:B:LEU:HD12	1:110:B:GLN:HA	11	0.4
(1,1499)	1:109:B:LEU:HD13	1:110:B:GLN:HA	11	0.4
(1,1499)	1:109:B:LEU:HD21	1:110:B:GLN:HA	11	0.4
(1,1499)	1:109:B:LEU:HD22	1:110:B:GLN:HA	11	0.4
(1,1499)	1:109:B:LEU:HD23	1:110:B:GLN:HA	11	0.4
(1,1267)	1:43:A:LEU:HD11	1:44:A:GLN:HA	4	0.4
(1,1267)	1:43:A:LEU:HD12	1:44:A:GLN:HA	4	0.4
(1,1267)	1:43:A:LEU:HD13	1:44:A:GLN:HA	4	0.4
(1,1267)	1:43:A:LEU:HD21	1:44:A:GLN:HA	4	0.4
(1,1267)	1:43:A:LEU:HD22	1:44:A:GLN:HA	4	0.4
(1,1267)	1:43:A:LEU:HD23	1:44:A:GLN:HA	4	0.4
(1,1167)	1:15:A:ILE:HG13	1:16:A:SER:H	12	0.4
(1,1156)	1:13:A:LYS:HB2	1:14:A:LYS:HG2	11	0.4
(1,1140)	1:11:A:GLU:HG3	1:12:A:LYS:HB3	13	0.4
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG21	2	0.4
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG22	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG23	2	0.4
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	7	0.4
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	7	0.4
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	7	0.4
(1,2109)	1:47:A:LEU:HD11	1:129:B:TRP:HZ3	14	0.39
(1,2109)	1:47:A:LEU:HD12	1:129:B:TRP:HZ3	14	0.39
(1,2109)	1:47:A:LEU:HD13	1:129:B:TRP:HZ3	14	0.39
(1,2109)	1:47:A:LEU:HD11	1:129:B:TRP:HZ3	19	0.39
(1,2109)	1:47:A:LEU:HD12	1:129:B:TRP:HZ3	19	0.39
(1,2109)	1:47:A:LEU:HD13	1:129:B:TRP:HZ3	19	0.39
(1,1998)	1:102:B:LYS:HA	1:102:B:LYS:HE2	11	0.39
(1,1791)	1:54:A:ASN:HA	1:54:A:ASN:HD22	14	0.39
(1,1789)	1:54:A:ASN:H	1:54:A:ASN:HD22	14	0.39
(1,1730)	1:36:A:LYS:HA	1:36:A:LYS:HE2	18	0.39
(1,1499)	1:109:B:LEU:HD11	1:110:B:GLN:HA	10	0.39
(1,1499)	1:109:B:LEU:HD12	1:110:B:GLN:HA	10	0.39
(1,1499)	1:109:B:LEU:HD13	1:110:B:GLN:HA	10	0.39
(1,1499)	1:109:B:LEU:HD21	1:110:B:GLN:HA	10	0.39
(1,1499)	1:109:B:LEU:HD22	1:110:B:GLN:HA	10	0.39
(1,1499)	1:109:B:LEU:HD23	1:110:B:GLN:HA	10	0.39
(1,1372)	1:77:B:GLU:HG3	1:78:B:LYS:HB3	6	0.39
(1,1267)	1:43:A:LEU:HD11	1:44:A:GLN:HA	14	0.39
(1,1267)	1:43:A:LEU:HD12	1:44:A:GLN:HA	14	0.39
(1,1267)	1:43:A:LEU:HD13	1:44:A:GLN:HA	14	0.39
(1,1267)	1:43:A:LEU:HD21	1:44:A:GLN:HA	14	0.39
(1,1267)	1:43:A:LEU:HD22	1:44:A:GLN:HA	14	0.39
(1,1267)	1:43:A:LEU:HD23	1:44:A:GLN:HA	14	0.39
(1,1258)	1:38:A:LYS:HE2	1:39:A:TYR:HD2	14	0.39
(1,1228)	1:35:A:GLU:H	1:36:A:LYS:HD2	20	0.39
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG21	5	0.39
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG22	5	0.39
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG23	5	0.39
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG21	6	0.39
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG22	6	0.39
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG23	6	0.39
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	2	0.39
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	2	0.39
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	2	0.39
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	6	0.39
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	6	0.39
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	6	0.39
(1,261)	1:107:B:PRO:HG2	1:127:B:PHE:HD1	20	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2104)	1:43:A:LEU:HD11	1:127:B:PHE:HD1	2	0.38
(1,2104)	1:43:A:LEU:HD12	1:127:B:PHE:HD1	2	0.38
(1,2104)	1:43:A:LEU:HD13	1:127:B:PHE:HD1	2	0.38
(1,1844)	1:74:B:LEU:H	1:74:B:LEU:HD11	11	0.38
(1,1844)	1:74:B:LEU:H	1:74:B:LEU:HD12	11	0.38
(1,1844)	1:74:B:LEU:H	1:74:B:LEU:HD13	11	0.38
(1,1399)	1:81:B:ILE:HG13	1:82:B:SER:H	4	0.38
(1,1399)	1:81:B:ILE:HG13	1:82:B:SER:H	13	0.38
(1,1267)	1:43:A:LEU:HD11	1:44:A:GLN:HA	8	0.38
(1,1267)	1:43:A:LEU:HD12	1:44:A:GLN:HA	8	0.38
(1,1267)	1:43:A:LEU:HD13	1:44:A:GLN:HA	8	0.38
(1,1267)	1:43:A:LEU:HD21	1:44:A:GLN:HA	8	0.38
(1,1267)	1:43:A:LEU:HD22	1:44:A:GLN:HA	8	0.38
(1,1267)	1:43:A:LEU:HD23	1:44:A:GLN:HA	8	0.38
(1,1267)	1:43:A:LEU:HD11	1:44:A:GLN:HA	17	0.38
(1,1267)	1:43:A:LEU:HD12	1:44:A:GLN:HA	17	0.38
(1,1267)	1:43:A:LEU:HD13	1:44:A:GLN:HA	17	0.38
(1,1267)	1:43:A:LEU:HD21	1:44:A:GLN:HA	17	0.38
(1,1267)	1:43:A:LEU:HD22	1:44:A:GLN:HA	17	0.38
(1,1267)	1:43:A:LEU:HD23	1:44:A:GLN:HA	17	0.38
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	8	0.38
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	8	0.38
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	8	0.38
(1,1167)	1:15:A:ILE:HG13	1:16:A:SER:H	3	0.38
(1,1167)	1:15:A:ILE:HG13	1:16:A:SER:H	9	0.38
(1,1103)	1:7:A:LYS:H	1:8:A:LEU:HD21	11	0.38
(1,1103)	1:7:A:LYS:H	1:8:A:LEU:HD22	11	0.38
(1,1103)	1:7:A:LYS:H	1:8:A:LEU:HD23	11	0.38
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG21	15	0.38
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG22	15	0.38
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG23	15	0.38
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	14	0.38
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	14	0.38
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	14	0.38
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	17	0.38
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	17	0.38
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	17	0.38
(1,191)	1:89:B:LEU:HD21	1:118:B:TYR:HE2	3	0.38
(1,191)	1:89:B:LEU:HD22	1:118:B:TYR:HE2	3	0.38
(1,191)	1:89:B:LEU:HD23	1:118:B:TYR:HE2	3	0.38
(1,186)	1:89:B:LEU:HG	1:118:B:TYR:HD2	13	0.38
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD11	14	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD12	14	0.37
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD13	14	0.37
(1,2111)	1:48:A:LYS:HG3	1:129:B:TRP:HE1	15	0.37
(1,1543)	1:126:B:ILE:HD11	1:127:B:PHE:HD1	1	0.37
(1,1543)	1:126:B:ILE:HD12	1:127:B:PHE:HD1	1	0.37
(1,1543)	1:126:B:ILE:HD13	1:127:B:PHE:HD1	1	0.37
(1,1499)	1:109:B:LEU:HD11	1:110:B:GLN:HA	3	0.37
(1,1499)	1:109:B:LEU:HD12	1:110:B:GLN:HA	3	0.37
(1,1499)	1:109:B:LEU:HD13	1:110:B:GLN:HA	3	0.37
(1,1499)	1:109:B:LEU:HD21	1:110:B:GLN:HA	3	0.37
(1,1499)	1:109:B:LEU:HD22	1:110:B:GLN:HA	3	0.37
(1,1499)	1:109:B:LEU:HD23	1:110:B:GLN:HA	3	0.37
(1,1499)	1:109:B:LEU:HD11	1:110:B:GLN:HA	17	0.37
(1,1499)	1:109:B:LEU:HD12	1:110:B:GLN:HA	17	0.37
(1,1499)	1:109:B:LEU:HD13	1:110:B:GLN:HA	17	0.37
(1,1499)	1:109:B:LEU:HD21	1:110:B:GLN:HA	17	0.37
(1,1499)	1:109:B:LEU:HD22	1:110:B:GLN:HA	17	0.37
(1,1499)	1:109:B:LEU:HD23	1:110:B:GLN:HA	17	0.37
(1,1399)	1:81:B:ILE:HG13	1:82:B:SER:H	18	0.37
(1,1167)	1:15:A:ILE:HG13	1:16:A:SER:H	6	0.37
(1,1167)	1:15:A:ILE:HG13	1:16:A:SER:H	13	0.37
(1,1146)	1:12:A:LYS:HD2	1:13:A:LYS:H	13	0.37
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG21	2	0.37
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG22	2	0.37
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG23	2	0.37
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	8	0.37
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	8	0.37
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	8	0.37
(1,385)	1:20:A:LEU:HD21	1:28:A:ARG:HB2	8	0.37
(1,385)	1:20:A:LEU:HD22	1:28:A:ARG:HB2	8	0.37
(1,385)	1:20:A:LEU:HD23	1:28:A:ARG:HB2	8	0.37
(1,2109)	1:47:A:LEU:HD11	1:129:B:TRP:HZ3	16	0.36
(1,2109)	1:47:A:LEU:HD12	1:129:B:TRP:HZ3	16	0.36
(1,2109)	1:47:A:LEU:HD13	1:129:B:TRP:HZ3	16	0.36
(1,1693)	1:29:A:GLN:H	1:29:A:GLN:HE22	1	0.36
(1,1627)	1:14:A:LYS:H	1:14:A:LYS:HD2	11	0.36
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG21	3	0.36
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG22	3	0.36
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG23	3	0.36
(1,297)	1:49:A:ILE:HG21	1:61:A:PHE:HE1	19	0.36
(1,297)	1:49:A:ILE:HG22	1:61:A:PHE:HE1	19	0.36
(1,297)	1:49:A:ILE:HG23	1:61:A:PHE:HE1	19	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,260)	1:107:B:PRO:HB3	1:127:B:PHE:HE1	1	0.36
(1,186)	1:89:B:LEU:HG	1:118:B:TYR:HD2	4	0.36
(1,2109)	1:47:A:LEU:HD11	1:129:B:TRP:HZ3	1	0.35
(1,2109)	1:47:A:LEU:HD12	1:129:B:TRP:HZ3	1	0.35
(1,2109)	1:47:A:LEU:HD13	1:129:B:TRP:HZ3	1	0.35
(1,2109)	1:47:A:LEU:HD11	1:129:B:TRP:HZ3	3	0.35
(1,2109)	1:47:A:LEU:HD12	1:129:B:TRP:HZ3	3	0.35
(1,2109)	1:47:A:LEU:HD13	1:129:B:TRP:HZ3	3	0.35
(1,1460)	1:101:B:GLU:H	1:102:B:LYS:HD2	16	0.35
(1,1460)	1:101:B:GLU:H	1:102:B:LYS:HD2	20	0.35
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	17	0.35
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	17	0.35
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	17	0.35
(1,1167)	1:15:A:ILE:HG13	1:16:A:SER:H	16	0.35
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG21	14	0.35
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG22	14	0.35
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG23	14	0.35
(1,385)	1:20:A:LEU:HD21	1:28:A:ARG:HB2	10	0.35
(1,385)	1:20:A:LEU:HD22	1:28:A:ARG:HB2	10	0.35
(1,385)	1:20:A:LEU:HD23	1:28:A:ARG:HB2	10	0.35
(1,212)	1:34:A:ILE:HD11	1:61:A:PHE:HE2	6	0.35
(1,212)	1:34:A:ILE:HD12	1:61:A:PHE:HE2	6	0.35
(1,212)	1:34:A:ILE:HD13	1:61:A:PHE:HE2	6	0.35
(1,189)	1:89:B:LEU:HD11	1:118:B:TYR:HD2	2	0.35
(1,189)	1:89:B:LEU:HD12	1:118:B:TYR:HD2	2	0.35
(1,189)	1:89:B:LEU:HD13	1:118:B:TYR:HD2	2	0.35
(1,2105)	1:43:A:LEU:HD21	1:127:B:PHE:HD1	14	0.34
(1,2105)	1:43:A:LEU:HD22	1:127:B:PHE:HD1	14	0.34
(1,2105)	1:43:A:LEU:HD23	1:127:B:PHE:HD1	14	0.34
(1,1499)	1:109:B:LEU:HD11	1:110:B:GLN:HA	19	0.34
(1,1499)	1:109:B:LEU:HD12	1:110:B:GLN:HA	19	0.34
(1,1499)	1:109:B:LEU:HD13	1:110:B:GLN:HA	19	0.34
(1,1499)	1:109:B:LEU:HD21	1:110:B:GLN:HA	19	0.34
(1,1499)	1:109:B:LEU:HD22	1:110:B:GLN:HA	19	0.34
(1,1499)	1:109:B:LEU:HD23	1:110:B:GLN:HA	19	0.34
(1,1399)	1:81:B:ILE:HG13	1:82:B:SER:H	2	0.34
(1,1399)	1:81:B:ILE:HG13	1:82:B:SER:H	3	0.34
(1,1399)	1:81:B:ILE:HG13	1:82:B:SER:H	7	0.34
(1,1399)	1:81:B:ILE:HG13	1:82:B:SER:H	11	0.34
(1,1372)	1:77:B:GLU:HG3	1:78:B:LYS:HB3	12	0.34
(1,1372)	1:77:B:GLU:HG3	1:78:B:LYS:HB3	16	0.34
(1,1167)	1:15:A:ILE:HG13	1:16:A:SER:H	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG21	1	0.34
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG22	1	0.34
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG23	1	0.34
(1,667)	1:72:B:LEU:HD11	1:76:B:ARG:HD2	3	0.34
(1,667)	1:72:B:LEU:HD12	1:76:B:ARG:HD2	3	0.34
(1,667)	1:72:B:LEU:HD13	1:76:B:ARG:HD2	3	0.34
(1,170)	1:71:B:ASN:HA	1:101:B:GLU:HA	4	0.34
(1,170)	1:71:B:ASN:HA	1:101:B:GLU:HA	7	0.34
(1,2142)	1:43:A:LEU:HD11	1:106:B:ASN:H	19	0.33
(1,2142)	1:43:A:LEU:HD12	1:106:B:ASN:H	19	0.33
(1,2142)	1:43:A:LEU:HD13	1:106:B:ASN:H	19	0.33
(1,2142)	1:43:A:LEU:HD21	1:106:B:ASN:H	19	0.33
(1,2142)	1:43:A:LEU:HD22	1:106:B:ASN:H	19	0.33
(1,2142)	1:43:A:LEU:HD23	1:106:B:ASN:H	19	0.33
(1,1880)	1:78:B:LYS:HB3	1:78:B:LYS:HE2	9	0.33
(1,1399)	1:81:B:ILE:HG13	1:82:B:SER:H	16	0.33
(1,1313)	1:62:A:GLN:HG2	1:63:A:TRP:H	11	0.33
(1,1267)	1:43:A:LEU:HD11	1:44:A:GLN:HA	5	0.33
(1,1267)	1:43:A:LEU:HD12	1:44:A:GLN:HA	5	0.33
(1,1267)	1:43:A:LEU:HD13	1:44:A:GLN:HA	5	0.33
(1,1267)	1:43:A:LEU:HD21	1:44:A:GLN:HA	5	0.33
(1,1267)	1:43:A:LEU:HD22	1:44:A:GLN:HA	5	0.33
(1,1267)	1:43:A:LEU:HD23	1:44:A:GLN:HA	5	0.33
(1,1267)	1:43:A:LEU:HD11	1:44:A:GLN:HA	10	0.33
(1,1267)	1:43:A:LEU:HD12	1:44:A:GLN:HA	10	0.33
(1,1267)	1:43:A:LEU:HD13	1:44:A:GLN:HA	10	0.33
(1,1267)	1:43:A:LEU:HD21	1:44:A:GLN:HA	10	0.33
(1,1267)	1:43:A:LEU:HD22	1:44:A:GLN:HA	10	0.33
(1,1267)	1:43:A:LEU:HD23	1:44:A:GLN:HA	10	0.33
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	10	0.33
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	10	0.33
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	10	0.33
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG21	18	0.33
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG22	18	0.33
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG23	18	0.33
(1,1029)	1:72:B:LEU:HA	1:74:B:LEU:HD21	11	0.33
(1,1029)	1:72:B:LEU:HA	1:74:B:LEU:HD22	11	0.33
(1,1029)	1:72:B:LEU:HA	1:74:B:LEU:HD23	11	0.33
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	18	0.33
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	18	0.33
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	18	0.33
(1,621)	1:31:A:ILE:HG21	1:35:A:GLU:HG2	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,621)	1:31:A:ILE:HG22	1:35:A:GLU:HG2	10	0.33
(1,621)	1:31:A:ILE:HG23	1:35:A:GLU:HG2	10	0.33
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	19	0.33
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	19	0.33
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	19	0.33
(1,211)	1:8:A:LEU:HD21	1:35:A:GLU:HB2	11	0.33
(1,211)	1:8:A:LEU:HD22	1:35:A:GLU:HB2	11	0.33
(1,211)	1:8:A:LEU:HD23	1:35:A:GLU:HB2	11	0.33
(1,165)	1:5:A:ASN:HA	1:35:A:GLU:HA	16	0.33
(1,1730)	1:36:A:LYS:HA	1:36:A:LYS:HE2	1	0.32
(1,1499)	1:109:B:LEU:HD11	1:110:B:GLN:HA	20	0.32
(1,1499)	1:109:B:LEU:HD12	1:110:B:GLN:HA	20	0.32
(1,1499)	1:109:B:LEU:HD13	1:110:B:GLN:HA	20	0.32
(1,1499)	1:109:B:LEU:HD21	1:110:B:GLN:HA	20	0.32
(1,1499)	1:109:B:LEU:HD22	1:110:B:GLN:HA	20	0.32
(1,1499)	1:109:B:LEU:HD23	1:110:B:GLN:HA	20	0.32
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	2	0.32
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	2	0.32
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	2	0.32
(1,1399)	1:81:B:ILE:HG13	1:82:B:SER:H	15	0.32
(1,1388)	1:79:B:LYS:HB2	1:80:B:LYS:HG2	11	0.32
(1,1381)	1:78:B:LYS:HD3	1:79:B:LYS:HA	3	0.32
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	3	0.32
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	3	0.32
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	3	0.32
(1,1167)	1:15:A:ILE:HG13	1:16:A:SER:H	15	0.32
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG21	1	0.32
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG22	1	0.32
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG23	1	0.32
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG21	15	0.32
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG22	15	0.32
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG23	15	0.32
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	17	0.32
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	17	0.32
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	17	0.32
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	8	0.32
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	8	0.32
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	8	0.32
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	12	0.32
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	12	0.32
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	12	0.32
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	15	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	15	0.32
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	15	0.32
(1,182)	1:23:A:LEU:HD21	1:52:A:TYR:HE2	8	0.32
(1,182)	1:23:A:LEU:HD22	1:52:A:TYR:HE2	8	0.32
(1,182)	1:23:A:LEU:HD23	1:52:A:TYR:HE2	8	0.32
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	15	0.32
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	15	0.32
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	15	0.32
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD11	1	0.31
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD12	1	0.31
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD13	1	0.31
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD11	7	0.31
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD12	7	0.31
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD13	7	0.31
(1,1499)	1:109:B:LEU:HD11	1:110:B:GLN:HA	2	0.31
(1,1499)	1:109:B:LEU:HD12	1:110:B:GLN:HA	2	0.31
(1,1499)	1:109:B:LEU:HD13	1:110:B:GLN:HA	2	0.31
(1,1499)	1:109:B:LEU:HD21	1:110:B:GLN:HA	2	0.31
(1,1499)	1:109:B:LEU:HD22	1:110:B:GLN:HA	2	0.31
(1,1499)	1:109:B:LEU:HD23	1:110:B:GLN:HA	2	0.31
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	20	0.31
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	20	0.31
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	20	0.31
(1,1319)	1:67:B:MET:HB3	1:68:B:ILE:HD11	8	0.31
(1,1319)	1:67:B:MET:HB3	1:68:B:ILE:HD12	8	0.31
(1,1319)	1:67:B:MET:HB3	1:68:B:ILE:HD13	8	0.31
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG21	3	0.31
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG22	3	0.31
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG23	3	0.31
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG21	11	0.31
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG22	11	0.31
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG23	11	0.31
(1,913)	1:95:B:GLN:HB3	1:98:B:ASN:HD22	12	0.31
(1,874)	1:75:B:ILE:HA	1:78:B:LYS:HE3	19	0.31
(1,385)	1:20:A:LEU:HD21	1:28:A:ARG:HB2	18	0.31
(1,385)	1:20:A:LEU:HD22	1:28:A:ARG:HB2	18	0.31
(1,385)	1:20:A:LEU:HD23	1:28:A:ARG:HB2	18	0.31
(1,257)	1:41:A:PRO:HB3	1:61:A:PHE:HE1	13	0.31
(1,212)	1:34:A:ILE:HD11	1:61:A:PHE:HE2	16	0.31
(1,212)	1:34:A:ILE:HD12	1:61:A:PHE:HE2	16	0.31
(1,212)	1:34:A:ILE:HD13	1:61:A:PHE:HE2	16	0.31
(1,189)	1:89:B:LEU:HD11	1:118:B:TYR:HD2	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,189)	1:89:B:LEU:HD12	1:118:B:TYR:HD2	6	0.31
(1,189)	1:89:B:LEU:HD13	1:118:B:TYR:HD2	6	0.31
(1,189)	1:89:B:LEU:HD11	1:118:B:TYR:HD2	16	0.31
(1,189)	1:89:B:LEU:HD12	1:118:B:TYR:HD2	16	0.31
(1,189)	1:89:B:LEU:HD13	1:118:B:TYR:HD2	16	0.31
(1,165)	1:5:A:ASN:HA	1:35:A:GLU:HA	12	0.31
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD11	18	0.3
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD12	18	0.3
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD13	18	0.3
(1,2105)	1:43:A:LEU:HD21	1:127:B:PHE:HD1	17	0.3
(1,2105)	1:43:A:LEU:HD22	1:127:B:PHE:HD1	17	0.3
(1,2105)	1:43:A:LEU:HD23	1:127:B:PHE:HD1	17	0.3
(1,2104)	1:43:A:LEU:HD11	1:127:B:PHE:HD1	19	0.3
(1,2104)	1:43:A:LEU:HD12	1:127:B:PHE:HD1	19	0.3
(1,2104)	1:43:A:LEU:HD13	1:127:B:PHE:HD1	19	0.3
(1,2059)	1:120:B:ASN:HA	1:120:B:ASN:HD22	14	0.3
(1,1961)	1:95:B:GLN:H	1:95:B:GLN:HE22	1	0.3
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	2	0.3
(1,1499)	1:109:B:LEU:HD11	1:110:B:GLN:HA	6	0.3
(1,1499)	1:109:B:LEU:HD12	1:110:B:GLN:HA	6	0.3
(1,1499)	1:109:B:LEU:HD13	1:110:B:GLN:HA	6	0.3
(1,1499)	1:109:B:LEU:HD21	1:110:B:GLN:HA	6	0.3
(1,1499)	1:109:B:LEU:HD22	1:110:B:GLN:HA	6	0.3
(1,1499)	1:109:B:LEU:HD23	1:110:B:GLN:HA	6	0.3
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	8	0.3
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	8	0.3
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	8	0.3
(1,1267)	1:43:A:LEU:HD11	1:44:A:GLN:HA	6	0.3
(1,1267)	1:43:A:LEU:HD12	1:44:A:GLN:HA	6	0.3
(1,1267)	1:43:A:LEU:HD13	1:44:A:GLN:HA	6	0.3
(1,1267)	1:43:A:LEU:HD21	1:44:A:GLN:HA	6	0.3
(1,1267)	1:43:A:LEU:HD22	1:44:A:GLN:HA	6	0.3
(1,1267)	1:43:A:LEU:HD23	1:44:A:GLN:HA	6	0.3
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD11	20	0.3
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD12	20	0.3
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD13	20	0.3
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG21	13	0.3
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG22	13	0.3
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG23	13	0.3
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG21	7	0.3
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG22	7	0.3
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG23	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	6	0.3
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	6	0.3
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	6	0.3
(1,385)	1:20:A:LEU:HD21	1:28:A:ARG:HB2	4	0.3
(1,385)	1:20:A:LEU:HD22	1:28:A:ARG:HB2	4	0.3
(1,385)	1:20:A:LEU:HD23	1:28:A:ARG:HB2	4	0.3
(1,180)	1:23:A:LEU:HD11	1:52:A:TYR:HD2	18	0.3
(1,180)	1:23:A:LEU:HD12	1:52:A:TYR:HD2	18	0.3
(1,180)	1:23:A:LEU:HD13	1:52:A:TYR:HD2	18	0.3
(1,86)	1:9:A:ILE:HG13	1:59:A:ASP:HB2	18	0.3
(1,2109)	1:47:A:LEU:HD11	1:129:B:TRP:HZ3	9	0.29
(1,2109)	1:47:A:LEU:HD12	1:129:B:TRP:HZ3	9	0.29
(1,2109)	1:47:A:LEU:HD13	1:129:B:TRP:HZ3	9	0.29
(1,1895)	1:80:B:LYS:H	1:80:B:LYS:HD2	11	0.29
(1,1791)	1:54:A:ASN:HA	1:54:A:ASN:HD22	16	0.29
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	18	0.29
(1,1499)	1:109:B:LEU:HD11	1:110:B:GLN:HA	5	0.29
(1,1499)	1:109:B:LEU:HD12	1:110:B:GLN:HA	5	0.29
(1,1499)	1:109:B:LEU:HD13	1:110:B:GLN:HA	5	0.29
(1,1499)	1:109:B:LEU:HD21	1:110:B:GLN:HA	5	0.29
(1,1499)	1:109:B:LEU:HD22	1:110:B:GLN:HA	5	0.29
(1,1499)	1:109:B:LEU:HD23	1:110:B:GLN:HA	5	0.29
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	6	0.29
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	6	0.29
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	6	0.29
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	19	0.29
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	19	0.29
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	19	0.29
(1,1300)	1:53:A:LEU:HD21	1:54:A:ASN:HB2	10	0.29
(1,1300)	1:53:A:LEU:HD22	1:54:A:ASN:HB2	10	0.29
(1,1300)	1:53:A:LEU:HD23	1:54:A:ASN:HB2	10	0.29
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	5	0.29
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	4	0.29
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	4	0.29
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	4	0.29
(1,1150)	1:12:A:LYS:HE3	1:13:A:LYS:H	1	0.29
(1,1140)	1:11:A:GLU:HG3	1:12:A:LYS:HB3	12	0.29
(1,1098)	1:6:A:LEU:H	1:7:A:LYS:HE3	16	0.29
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG21	12	0.29
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG22	12	0.29
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG23	12	0.29
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG21	16	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG22	16	0.29
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG23	16	0.29
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	15	0.29
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	15	0.29
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	15	0.29
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	15	0.29
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	15	0.29
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	15	0.29
(1,429)	1:76:B:ARG:HD2	1:83:B:GLN:HE21	7	0.29
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	3	0.29
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	3	0.29
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	3	0.29
(1,299)	1:115:B:ILE:HG21	1:127:B:PHE:HE1	3	0.29
(1,299)	1:115:B:ILE:HG22	1:127:B:PHE:HE1	3	0.29
(1,299)	1:115:B:ILE:HG23	1:127:B:PHE:HE1	3	0.29
(1,123)	1:13:A:LYS:HE2	1:54:A:ASN:HB2	14	0.29
(1,2104)	1:43:A:LEU:HD11	1:127:B:PHE:HD1	11	0.28
(1,2104)	1:43:A:LEU:HD12	1:127:B:PHE:HD1	11	0.28
(1,2104)	1:43:A:LEU:HD13	1:127:B:PHE:HD1	11	0.28
(1,1998)	1:102:B:LYS:HA	1:102:B:LYS:HE2	3	0.28
(1,1961)	1:95:B:GLN:H	1:95:B:GLN:HE22	19	0.28
(1,1900)	1:80:B:LYS:HA	1:80:B:LYS:HE3	11	0.28
(1,1627)	1:14:A:LYS:H	1:14:A:LYS:HD2	17	0.28
(1,1372)	1:77:B:GLU:HG3	1:78:B:LYS:HB3	14	0.28
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	17	0.28
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	17	0.28
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	17	0.28
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	18	0.28
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	18	0.28
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	18	0.28
(1,1167)	1:15:A:ILE:HG13	1:16:A:SER:H	11	0.28
(1,1167)	1:15:A:ILE:HG13	1:16:A:SER:H	14	0.28
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG21	12	0.28
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG22	12	0.28
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG23	12	0.28
(1,971)	1:13:A:LYS:HG3	1:15:A:ILE:HA	2	0.28
(1,874)	1:75:B:ILE:HA	1:78:B:LYS:HE3	2	0.28
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	1	0.28
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	1	0.28
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	1	0.28
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	3	0.28
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	3	0.28
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	5	0.28
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	5	0.28
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	5	0.28
(1,297)	1:49:A:ILE:HG21	1:61:A:PHE:HE1	4	0.28
(1,297)	1:49:A:ILE:HG22	1:61:A:PHE:HE1	4	0.28
(1,297)	1:49:A:ILE:HG23	1:61:A:PHE:HE1	4	0.28
(1,260)	1:107:B:PRO:HB3	1:127:B:PHE:HE1	19	0.28
(1,260)	1:107:B:PRO:HB3	1:127:B:PHE:HE1	20	0.28
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	19	0.28
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	19	0.28
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	19	0.28
(1,170)	1:71:B:ASN:HA	1:101:B:GLU:HA	2	0.28
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD11	16	0.27
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD12	16	0.27
(1,2159)	1:63:A:TRP:HZ3	1:113:B:LEU:HD13	16	0.27
(1,1998)	1:102:B:LYS:HA	1:102:B:LYS:HE2	2	0.27
(1,1998)	1:102:B:LYS:HA	1:102:B:LYS:HE2	14	0.27
(1,1899)	1:80:B:LYS:HA	1:80:B:LYS:HE2	14	0.27
(1,1731)	1:36:A:LYS:HA	1:36:A:LYS:HE3	17	0.27
(1,1576)	1:8:A:LEU:H	1:8:A:LEU:HD11	11	0.27
(1,1576)	1:8:A:LEU:H	1:8:A:LEU:HD12	11	0.27
(1,1576)	1:8:A:LEU:H	1:8:A:LEU:HD13	11	0.27
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD11	19	0.27
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD12	19	0.27
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD13	19	0.27
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	5	0.27
(1,1460)	1:101:B:GLU:H	1:102:B:LYS:HD2	7	0.27
(1,1460)	1:101:B:GLU:H	1:102:B:LYS:HD2	15	0.27
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	11	0.27
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	11	0.27
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	11	0.27
(1,1378)	1:78:B:LYS:HD2	1:79:B:LYS:H	19	0.27
(1,1372)	1:77:B:GLU:HG3	1:78:B:LYS:HB3	1	0.27
(1,1311)	1:60:A:ILE:HD11	1:61:A:PHE:HD1	10	0.27
(1,1311)	1:60:A:ILE:HD12	1:61:A:PHE:HD1	10	0.27
(1,1311)	1:60:A:ILE:HD13	1:61:A:PHE:HD1	10	0.27
(1,1210)	1:29:A:GLN:HG2	1:30:A:THR:HG21	9	0.27
(1,1210)	1:29:A:GLN:HG2	1:30:A:THR:HG22	9	0.27
(1,1210)	1:29:A:GLN:HG2	1:30:A:THR:HG23	9	0.27
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	7	0.27
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	7	0.27
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	11	0.27
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	11	0.27
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	11	0.27
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	12	0.27
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	12	0.27
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	12	0.27
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	15	0.27
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	15	0.27
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	15	0.27
(1,1140)	1:11:A:GLU:HG3	1:12:A:LYS:HB3	11	0.27
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD11	8	0.27
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD12	8	0.27
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD13	8	0.27
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG21	7	0.27
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG22	7	0.27
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG23	7	0.27
(1,1042)	1:79:B:LYS:HG3	1:81:B:ILE:HA	5	0.27
(1,1018)	1:68:B:ILE:HG21	1:70:B:ASN:HD21	3	0.27
(1,1018)	1:68:B:ILE:HG22	1:70:B:ASN:HD21	3	0.27
(1,1018)	1:68:B:ILE:HG23	1:70:B:ASN:HD21	3	0.27
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	13	0.27
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	13	0.27
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	13	0.27
(1,870)	1:74:B:LEU:HD11	1:77:B:GLU:HG2	11	0.27
(1,870)	1:74:B:LEU:HD12	1:77:B:GLU:HG2	11	0.27
(1,870)	1:74:B:LEU:HD13	1:77:B:GLU:HG2	11	0.27
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	6	0.27
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	6	0.27
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	6	0.27
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	11	0.27
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	11	0.27
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	11	0.27
(1,466)	1:100:B:ILE:HG21	1:106:B:ASN:HB3	13	0.27
(1,466)	1:100:B:ILE:HG22	1:106:B:ASN:HB3	13	0.27
(1,466)	1:100:B:ILE:HG23	1:106:B:ASN:HB3	13	0.27
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	2	0.27
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	2	0.27
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	2	0.27
(1,261)	1:107:B:PRO:HG2	1:127:B:PHE:HD1	16	0.27
(1,170)	1:71:B:ASN:HA	1:101:B:GLU:HA	16	0.27
(1,2174)	1:44:A:GLN:H	1:68:B:ILE:HD11	14	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2174)	1:44:A:GLN:H	1:68:B:ILE:HD12	14	0.26
(1,2174)	1:44:A:GLN:H	1:68:B:ILE:HD13	14	0.26
(1,2109)	1:47:A:LEU:HD11	1:129:B:TRP:HZ3	18	0.26
(1,2109)	1:47:A:LEU:HD12	1:129:B:TRP:HZ3	18	0.26
(1,2109)	1:47:A:LEU:HD13	1:129:B:TRP:HZ3	18	0.26
(1,1999)	1:102:B:LYS:HA	1:102:B:LYS:HE3	17	0.26
(1,1998)	1:102:B:LYS:HA	1:102:B:LYS:HE2	19	0.26
(1,1872)	1:78:B:LYS:H	1:78:B:LYS:HD2	9	0.26
(1,1531)	1:119:B:LEU:HD11	1:120:B:ASN:HB2	8	0.26
(1,1531)	1:119:B:LEU:HD12	1:120:B:ASN:HB2	8	0.26
(1,1531)	1:119:B:LEU:HD13	1:120:B:ASN:HB2	8	0.26
(1,1472)	1:102:B:LYS:HB3	1:103:B:ASN:HB3	7	0.26
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	16	0.26
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	16	0.26
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	16	0.26
(1,1378)	1:78:B:LYS:HD2	1:79:B:LYS:H	15	0.26
(1,1325)	1:69:B:ILE:HD11	1:70:B:ASN:H	15	0.26
(1,1325)	1:69:B:ILE:HD12	1:70:B:ASN:H	15	0.26
(1,1325)	1:69:B:ILE:HD13	1:70:B:ASN:H	15	0.26
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD11	15	0.26
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD12	15	0.26
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD13	15	0.26
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	6	0.26
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	6	0.26
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	6	0.26
(1,1156)	1:13:A:LYS:HB2	1:14:A:LYS:HG2	17	0.26
(1,1150)	1:12:A:LYS:HE3	1:13:A:LYS:H	16	0.26
(1,1146)	1:12:A:LYS:HD2	1:13:A:LYS:H	16	0.26
(1,1097)	1:6:A:LEU:H	1:7:A:LYS:HE2	1	0.26
(1,1093)	1:3:A:ILE:HD11	1:4:A:ASN:H	15	0.26
(1,1093)	1:3:A:ILE:HD12	1:4:A:ASN:H	15	0.26
(1,1093)	1:3:A:ILE:HD13	1:4:A:ASN:H	15	0.26
(1,1092)	1:2:A:ILE:HG21	1:3:A:ILE:HA	18	0.26
(1,1092)	1:2:A:ILE:HG22	1:3:A:ILE:HA	18	0.26
(1,1092)	1:2:A:ILE:HG23	1:3:A:ILE:HA	18	0.26
(1,1085)	1:1:A:MET:HB2	1:2:A:ILE:HB	18	0.26
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	8	0.26
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	8	0.26
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	8	0.26
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	10	0.26
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	10	0.26
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	19	0.26
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	19	0.26
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	19	0.26
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	3	0.26
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	3	0.26
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	3	0.26
(1,732)	1:109:B:LEU:HD11	1:113:B:LEU:HD21	18	0.26
(1,732)	1:109:B:LEU:HD11	1:113:B:LEU:HD22	18	0.26
(1,732)	1:109:B:LEU:HD11	1:113:B:LEU:HD23	18	0.26
(1,732)	1:109:B:LEU:HD12	1:113:B:LEU:HD21	18	0.26
(1,732)	1:109:B:LEU:HD12	1:113:B:LEU:HD22	18	0.26
(1,732)	1:109:B:LEU:HD12	1:113:B:LEU:HD23	18	0.26
(1,732)	1:109:B:LEU:HD13	1:113:B:LEU:HD21	18	0.26
(1,732)	1:109:B:LEU:HD13	1:113:B:LEU:HD22	18	0.26
(1,732)	1:109:B:LEU:HD13	1:113:B:LEU:HD23	18	0.26
(1,732)	1:109:B:LEU:HD21	1:113:B:LEU:HD21	18	0.26
(1,732)	1:109:B:LEU:HD21	1:113:B:LEU:HD22	18	0.26
(1,732)	1:109:B:LEU:HD21	1:113:B:LEU:HD23	18	0.26
(1,732)	1:109:B:LEU:HD22	1:113:B:LEU:HD21	18	0.26
(1,732)	1:109:B:LEU:HD22	1:113:B:LEU:HD22	18	0.26
(1,732)	1:109:B:LEU:HD22	1:113:B:LEU:HD23	18	0.26
(1,732)	1:109:B:LEU:HD23	1:113:B:LEU:HD21	18	0.26
(1,732)	1:109:B:LEU:HD23	1:113:B:LEU:HD22	18	0.26
(1,732)	1:109:B:LEU:HD23	1:113:B:LEU:HD23	18	0.26
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	20	0.26
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	20	0.26
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	20	0.26
(1,583)	1:7:A:LYS:HG2	1:11:A:GLU:HG2	5	0.26
(1,517)	1:72:B:LEU:HD11	1:77:B:GLU:H	18	0.26
(1,517)	1:72:B:LEU:HD12	1:77:B:GLU:H	18	0.26
(1,517)	1:72:B:LEU:HD13	1:77:B:GLU:H	18	0.26
(1,219)	1:100:B:ILE:HG21	1:127:B:PHE:HD2	13	0.26
(1,219)	1:100:B:ILE:HG22	1:127:B:PHE:HD2	13	0.26
(1,219)	1:100:B:ILE:HG23	1:127:B:PHE:HD2	13	0.26
(1,191)	1:89:B:LEU:HD21	1:118:B:TYR:HE2	9	0.26
(1,191)	1:89:B:LEU:HD22	1:118:B:TYR:HE2	9	0.26
(1,191)	1:89:B:LEU:HD23	1:118:B:TYR:HE2	9	0.26
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	10	0.26
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	10	0.26
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	10	0.26
(1,165)	1:5:A:ASN:HA	1:35:A:GLU:HA	7	0.26
(1,149)	1:15:A:ILE:H	1:53:A:LEU:HD21	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:15:A:ILE:H	1:53:A:LEU:HD22	4	0.26
(1,149)	1:15:A:ILE:H	1:53:A:LEU:HD23	4	0.26
(1,95)	1:75:B:ILE:HG13	1:125:B:ASP:HB2	19	0.26
(1,86)	1:9:A:ILE:HG13	1:59:A:ASP:HB2	6	0.26
(1,3)	1:2:A:ILE:HD11	1:64:A:GLN:HB2	7	0.26
(1,3)	1:2:A:ILE:HD12	1:64:A:GLN:HB2	7	0.26
(1,3)	1:2:A:ILE:HD13	1:64:A:GLN:HB2	7	0.26
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD21	6	0.25
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD22	6	0.25
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD23	6	0.25
(1,2157)	1:63:A:TRP:HE1	1:114:B:LYS:HG3	3	0.25
(1,2156)	1:63:A:TRP:HE1	1:114:B:LYS:HA	2	0.25
(1,2105)	1:43:A:LEU:HD21	1:127:B:PHE:HD1	20	0.25
(1,2105)	1:43:A:LEU:HD22	1:127:B:PHE:HD1	20	0.25
(1,2105)	1:43:A:LEU:HD23	1:127:B:PHE:HD1	20	0.25
(1,1998)	1:102:B:LYS:HA	1:102:B:LYS:HE2	20	0.25
(1,1731)	1:36:A:LYS:HA	1:36:A:LYS:HE3	6	0.25
(1,1730)	1:36:A:LYS:HA	1:36:A:LYS:HE2	9	0.25
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD11	14	0.25
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD12	14	0.25
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD13	14	0.25
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	6	0.25
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	13	0.25
(1,1504)	1:110:B:GLN:HE22	1:111:B:LEU:HD21	9	0.25
(1,1504)	1:110:B:GLN:HE22	1:111:B:LEU:HD22	9	0.25
(1,1504)	1:110:B:GLN:HE22	1:111:B:LEU:HD23	9	0.25
(1,1499)	1:109:B:LEU:HD11	1:110:B:GLN:HA	14	0.25
(1,1499)	1:109:B:LEU:HD12	1:110:B:GLN:HA	14	0.25
(1,1499)	1:109:B:LEU:HD13	1:110:B:GLN:HA	14	0.25
(1,1499)	1:109:B:LEU:HD21	1:110:B:GLN:HA	14	0.25
(1,1499)	1:109:B:LEU:HD22	1:110:B:GLN:HA	14	0.25
(1,1499)	1:109:B:LEU:HD23	1:110:B:GLN:HA	14	0.25
(1,1442)	1:95:B:GLN:HG2	1:96:B:THR:HG21	20	0.25
(1,1442)	1:95:B:GLN:HG2	1:96:B:THR:HG22	20	0.25
(1,1442)	1:95:B:GLN:HG2	1:96:B:THR:HG23	20	0.25
(1,1399)	1:81:B:ILE:HG13	1:82:B:SER:H	14	0.25
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	2	0.25
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	3	0.25
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	14	0.25
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	15	0.25
(1,1242)	1:36:A:LYS:HG2	1:37:A:ASN:H	15	0.25
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	1	0.25
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	1	0.25
(1,1146)	1:12:A:LYS:HD2	1:13:A:LYS:H	6	0.25
(1,1140)	1:11:A:GLU:HG3	1:12:A:LYS:HB3	5	0.25
(1,1134)	1:10:A:ARG:HD2	1:11:A:GLU:HA	3	0.25
(1,1101)	1:6:A:LEU:HD11	1:7:A:LYS:HB3	18	0.25
(1,1101)	1:6:A:LEU:HD12	1:7:A:LYS:HB3	18	0.25
(1,1101)	1:6:A:LEU:HD13	1:7:A:LYS:HB3	18	0.25
(1,1098)	1:6:A:LEU:H	1:7:A:LYS:HE3	15	0.25
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG21	14	0.25
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG22	14	0.25
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG23	14	0.25
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG21	11	0.25
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG22	11	0.25
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG23	11	0.25
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG21	13	0.25
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG22	13	0.25
(1,973)	1:13:A:LYS:HG3	1:15:A:ILE:HG23	13	0.25
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD11	8	0.25
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD12	8	0.25
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD13	8	0.25
(1,689)	1:81:B:ILE:HG13	1:85:B:GLU:HG2	15	0.25
(1,622)	1:34:A:ILE:H	1:38:A:LYS:H	20	0.25
(1,571)	1:6:A:LEU:HD11	1:10:A:ARG:HD2	3	0.25
(1,571)	1:6:A:LEU:HD12	1:10:A:ARG:HD2	3	0.25
(1,571)	1:6:A:LEU:HD13	1:10:A:ARG:HD2	3	0.25
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	4	0.25
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	4	0.25
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	4	0.25
(1,385)	1:20:A:LEU:HD21	1:28:A:ARG:HB2	15	0.25
(1,385)	1:20:A:LEU:HD22	1:28:A:ARG:HB2	15	0.25
(1,385)	1:20:A:LEU:HD23	1:28:A:ARG:HB2	15	0.25
(1,216)	1:74:B:LEU:HD21	1:101:B:GLU:HB2	11	0.25
(1,216)	1:74:B:LEU:HD22	1:101:B:GLU:HB2	11	0.25
(1,216)	1:74:B:LEU:HD23	1:101:B:GLU:HB2	11	0.25
(1,182)	1:23:A:LEU:HD21	1:52:A:TYR:HE2	9	0.25
(1,182)	1:23:A:LEU:HD22	1:52:A:TYR:HE2	9	0.25
(1,182)	1:23:A:LEU:HD23	1:52:A:TYR:HE2	9	0.25
(1,143)	1:2:A:ILE:HB	1:40:A:ASN:HD21	14	0.25
(1,44)	1:3:A:ILE:HG13	1:62:A:GLN:HE22	15	0.25
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD21	1	0.24
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD22	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2161)	1:61:A:PHE:HD1	1:109:B:LEU:HD23	1	0.24
(1,1920)	1:83:B:GLN:HA	1:83:B:GLN:HE22	8	0.24
(1,1731)	1:36:A:LYS:HA	1:36:A:LYS:HE3	5	0.24
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	14	0.24
(1,1500)	1:109:B:LEU:HD11	1:110:B:GLN:HB2	2	0.24
(1,1500)	1:109:B:LEU:HD12	1:110:B:GLN:HB2	2	0.24
(1,1500)	1:109:B:LEU:HD13	1:110:B:GLN:HB2	2	0.24
(1,1500)	1:109:B:LEU:HD21	1:110:B:GLN:HB2	2	0.24
(1,1500)	1:109:B:LEU:HD22	1:110:B:GLN:HB2	2	0.24
(1,1500)	1:109:B:LEU:HD23	1:110:B:GLN:HB2	2	0.24
(1,1442)	1:95:B:GLN:HG2	1:96:B:THR:HG21	9	0.24
(1,1442)	1:95:B:GLN:HG2	1:96:B:THR:HG22	9	0.24
(1,1442)	1:95:B:GLN:HG2	1:96:B:THR:HG23	9	0.24
(1,1372)	1:77:B:GLU:HG3	1:78:B:LYS:HB3	5	0.24
(1,1320)	1:67:B:MET:HG2	1:68:B:ILE:HB	16	0.24
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD11	8	0.24
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD12	8	0.24
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD13	8	0.24
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	8	0.24
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD21	3	0.24
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD22	3	0.24
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD23	3	0.24
(1,1233)	1:35:A:GLU:HG2	1:36:A:LYS:HD2	13	0.24
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	13	0.24
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	13	0.24
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	13	0.24
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD11	2	0.24
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD12	2	0.24
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD13	2	0.24
(1,1018)	1:68:B:ILE:HG21	1:70:B:ASN:HD21	7	0.24
(1,1018)	1:68:B:ILE:HG22	1:70:B:ASN:HD21	7	0.24
(1,1018)	1:68:B:ILE:HG23	1:70:B:ASN:HD21	7	0.24
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	14	0.24
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	14	0.24
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	14	0.24
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	19	0.24
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	19	0.24
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	19	0.24
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	20	0.24
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	20	0.24
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	20	0.24
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	7	0.24
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	7	0.24
(1,385)	1:20:A:LEU:HD21	1:28:A:ARG:HB2	9	0.24
(1,385)	1:20:A:LEU:HD22	1:28:A:ARG:HB2	9	0.24
(1,385)	1:20:A:LEU:HD23	1:28:A:ARG:HB2	9	0.24
(1,260)	1:107:B:PRO:HB3	1:127:B:PHE:HE1	15	0.24
(1,257)	1:41:A:PRO:HB3	1:61:A:PHE:HE1	4	0.24
(1,257)	1:41:A:PRO:HB3	1:61:A:PHE:HE1	19	0.24
(1,186)	1:89:B:LEU:HG	1:118:B:TYR:HD2	20	0.24
(1,165)	1:5:A:ASN:HA	1:35:A:GLU:HA	8	0.24
(1,2100)	1:2:A:ILE:HG21	1:109:B:LEU:HD21	17	0.23
(1,2100)	1:2:A:ILE:HG21	1:109:B:LEU:HD22	17	0.23
(1,2100)	1:2:A:ILE:HG21	1:109:B:LEU:HD23	17	0.23
(1,2100)	1:2:A:ILE:HG22	1:109:B:LEU:HD21	17	0.23
(1,2100)	1:2:A:ILE:HG22	1:109:B:LEU:HD22	17	0.23
(1,2100)	1:2:A:ILE:HG22	1:109:B:LEU:HD23	17	0.23
(1,2100)	1:2:A:ILE:HG23	1:109:B:LEU:HD21	17	0.23
(1,2100)	1:2:A:ILE:HG23	1:109:B:LEU:HD22	17	0.23
(1,2100)	1:2:A:ILE:HG23	1:109:B:LEU:HD23	17	0.23
(1,2029)	1:110:B:GLN:H	1:110:B:GLN:HE21	2	0.23
(1,1999)	1:102:B:LYS:HA	1:102:B:LYS:HE3	6	0.23
(1,1900)	1:80:B:LYS:HA	1:80:B:LYS:HE3	17	0.23
(1,1800)	1:62:A:GLN:H	1:62:A:GLN:HE21	4	0.23
(1,1731)	1:36:A:LYS:HA	1:36:A:LYS:HE3	3	0.23
(1,1651)	1:17:A:GLN:H	1:17:A:GLN:HE21	16	0.23
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD11	5	0.23
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD12	5	0.23
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD13	5	0.23
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	3	0.23
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	15	0.23
(1,1487)	1:104:B:LYS:HD2	1:105:B:TYR:HD2	15	0.23
(1,1460)	1:101:B:GLU:H	1:102:B:LYS:HD2	12	0.23
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	3	0.23
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	3	0.23
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	3	0.23
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	13	0.23
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	13	0.23
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	13	0.23
(1,1388)	1:79:B:LYS:HB2	1:80:B:LYS:HG2	17	0.23
(1,1382)	1:78:B:LYS:HE3	1:79:B:LYS:H	15	0.23
(1,1381)	1:78:B:LYS:HD3	1:79:B:LYS:HA	6	0.23
(1,1372)	1:77:B:GLU:HG3	1:78:B:LYS:HB3	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD11	20	0.23
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD12	20	0.23
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD13	20	0.23
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	7	0.23
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD21	9	0.23
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD22	9	0.23
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD23	9	0.23
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD21	20	0.23
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD22	20	0.23
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD23	20	0.23
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	16	0.23
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	16	0.23
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	16	0.23
(1,1146)	1:12:A:LYS:HD2	1:13:A:LYS:H	5	0.23
(1,1098)	1:6:A:LEU:H	1:7:A:LYS:HE3	8	0.23
(1,1058)	1:93:B:SER:HB2	1:95:B:GLN:HB3	16	0.23
(1,1058)	1:93:B:SER:HB3	1:95:B:GLN:HB3	16	0.23
(1,1015)	1:64:A:GLN:HB3	1:66:A:GLU:H	6	0.23
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD11	6	0.23
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD12	6	0.23
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD13	6	0.23
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	2	0.23
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	2	0.23
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	2	0.23
(1,874)	1:75:B:ILE:HA	1:78:B:LYS:HE3	9	0.23
(1,866)	1:74:B:LEU:H	1:77:B:GLU:HG2	7	0.23
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	9	0.23
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	9	0.23
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	9	0.23
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	12	0.23
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	12	0.23
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	12	0.23
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	16	0.23
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	16	0.23
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	16	0.23
(1,736)	1:110:B:GLN:HB3	1:114:B:LYS:HD2	2	0.23
(1,735)	1:110:B:GLN:HB2	1:114:B:LYS:HD2	17	0.23
(1,713)	1:94:B:ARG:HG3	1:98:B:ASN:HD22	12	0.23
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	17	0.23
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	17	0.23
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	17	0.23
(1,299)	1:115:B:ILE:HG21	1:127:B:PHE:HE1	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:115:B:ILE:HG22	1:127:B:PHE:HE1	5	0.23
(1,299)	1:115:B:ILE:HG23	1:127:B:PHE:HE1	5	0.23
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	2	0.23
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	2	0.23
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	2	0.23
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	10	0.23
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	10	0.23
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	10	0.23
(1,213)	1:34:A:ILE:HD11	1:61:A:PHE:HZ	4	0.23
(1,213)	1:34:A:ILE:HD12	1:61:A:PHE:HZ	4	0.23
(1,213)	1:34:A:ILE:HD13	1:61:A:PHE:HZ	4	0.23
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	1	0.23
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	1	0.23
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	1	0.23
(1,165)	1:5:A:ASN:HA	1:35:A:GLU:HA	4	0.23
(1,165)	1:5:A:ASN:HA	1:35:A:GLU:HA	15	0.23
(1,86)	1:9:A:ILE:HG13	1:59:A:ASP:HB2	19	0.23
(1,86)	1:9:A:ILE:HG13	1:59:A:ASP:HB2	20	0.23
(1,2177)	1:44:A:GLN:HB2	1:68:B:ILE:HG21	7	0.22
(1,2177)	1:44:A:GLN:HB2	1:68:B:ILE:HG22	7	0.22
(1,2177)	1:44:A:GLN:HB2	1:68:B:ILE:HG23	7	0.22
(1,2111)	1:48:A:LYS:HG3	1:129:B:TRP:HE1	3	0.22
(1,2110)	1:48:A:LYS:HA	1:129:B:TRP:HE1	18	0.22
(1,2105)	1:43:A:LEU:HD21	1:127:B:PHE:HD1	10	0.22
(1,2105)	1:43:A:LEU:HD22	1:127:B:PHE:HD1	10	0.22
(1,2105)	1:43:A:LEU:HD23	1:127:B:PHE:HD1	10	0.22
(1,2059)	1:120:B:ASN:HA	1:120:B:ASN:HD22	16	0.22
(1,1998)	1:102:B:LYS:HA	1:102:B:LYS:HE2	13	0.22
(1,1895)	1:80:B:LYS:H	1:80:B:LYS:HD2	17	0.22
(1,1731)	1:36:A:LYS:HA	1:36:A:LYS:HE3	2	0.22
(1,1731)	1:36:A:LYS:HA	1:36:A:LYS:HE3	8	0.22
(1,1601)	1:11:A:GLU:H	1:11:A:GLU:HG2	11	0.22
(1,1545)	1:128:B:GLN:HG2	1:129:B:TRP:H	19	0.22
(1,1492)	1:104:B:LYS:HG3	1:105:B:TYR:H	14	0.22
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	1	0.22
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	1	0.22
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	1	0.22
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	10	0.22
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	10	0.22
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	10	0.22
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	14	0.22
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	14	0.22
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	15	0.22
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	15	0.22
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	15	0.22
(1,1397)	1:80:B:LYS:HG2	1:81:B:ILE:HD11	18	0.22
(1,1397)	1:80:B:LYS:HG2	1:81:B:ILE:HD12	18	0.22
(1,1397)	1:80:B:LYS:HG2	1:81:B:ILE:HD13	18	0.22
(1,1378)	1:78:B:LYS:HD2	1:79:B:LYS:H	16	0.22
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD11	18	0.22
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD12	18	0.22
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD13	18	0.22
(1,1344)	1:73:B:LYS:HG2	1:74:B:LEU:HA	16	0.22
(1,1330)	1:72:B:LEU:H	1:73:B:LYS:HE3	7	0.22
(1,1330)	1:72:B:LEU:H	1:73:B:LYS:HE3	14	0.22
(1,1329)	1:72:B:LEU:H	1:73:B:LYS:HE2	13	0.22
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD11	3	0.22
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD12	3	0.22
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD13	3	0.22
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	9	0.22
(1,1228)	1:35:A:GLU:H	1:36:A:LYS:HD2	12	0.22
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	19	0.22
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	19	0.22
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	19	0.22
(1,1172)	1:18:A:SER:H	1:19:A:GLU:HB3	3	0.22
(1,1165)	1:14:A:LYS:HG2	1:15:A:ILE:HD11	15	0.22
(1,1165)	1:14:A:LYS:HG2	1:15:A:ILE:HD12	15	0.22
(1,1165)	1:14:A:LYS:HG2	1:15:A:ILE:HD13	15	0.22
(1,1150)	1:12:A:LYS:HE3	1:13:A:LYS:H	18	0.22
(1,1134)	1:10:A:ARG:HD2	1:11:A:GLU:HA	12	0.22
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD11	6	0.22
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD12	6	0.22
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD13	6	0.22
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD11	9	0.22
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD12	9	0.22
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD13	9	0.22
(1,1098)	1:6:A:LEU:H	1:7:A:LYS:HE3	4	0.22
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD11	16	0.22
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD12	16	0.22
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD13	16	0.22
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD11	1	0.22
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD12	1	0.22
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD13	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD11	6	0.22
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD12	6	0.22
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD13	6	0.22
(1,989)	1:28:A:ARG:HA	1:30:A:THR:HB	9	0.22
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	5	0.22
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	5	0.22
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	5	0.22
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	10	0.22
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	10	0.22
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	10	0.22
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	11	0.22
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	11	0.22
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	11	0.22
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	16	0.22
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	16	0.22
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	16	0.22
(1,864)	1:72:B:LEU:HD21	1:75:B:ILE:HB	18	0.22
(1,864)	1:72:B:LEU:HD22	1:75:B:ILE:HB	18	0.22
(1,864)	1:72:B:LEU:HD23	1:75:B:ILE:HB	18	0.22
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	2	0.22
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	2	0.22
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	2	0.22
(1,735)	1:110:B:GLN:HB2	1:114:B:LYS:HD2	12	0.22
(1,733)	1:110:B:GLN:HA	1:114:B:LYS:HD2	4	0.22
(1,689)	1:81:B:ILE:HG13	1:85:B:GLU:HG2	2	0.22
(1,689)	1:81:B:ILE:HG13	1:85:B:GLU:HG2	11	0.22
(1,689)	1:81:B:ILE:HG13	1:85:B:GLU:HG2	14	0.22
(1,593)	1:15:A:ILE:HG13	1:19:A:GLU:HG2	11	0.22
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG21	4	0.22
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG22	4	0.22
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG23	4	0.22
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG21	15	0.22
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG22	15	0.22
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG23	15	0.22
(1,469)	1:6:A:LEU:HD11	1:11:A:GLU:H	3	0.22
(1,469)	1:6:A:LEU:HD12	1:11:A:GLU:H	3	0.22
(1,469)	1:6:A:LEU:HD13	1:11:A:GLU:H	3	0.22
(1,469)	1:6:A:LEU:HD11	1:11:A:GLU:H	18	0.22
(1,469)	1:6:A:LEU:HD12	1:11:A:GLU:H	18	0.22
(1,469)	1:6:A:LEU:HD13	1:11:A:GLU:H	18	0.22
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	17	0.22
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	17	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	17	0.22
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	19	0.22
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	19	0.22
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	19	0.22
(1,212)	1:34:A:ILE:HD11	1:61:A:PHE:HE2	11	0.22
(1,212)	1:34:A:ILE:HD12	1:61:A:PHE:HE2	11	0.22
(1,212)	1:34:A:ILE:HD13	1:61:A:PHE:HE2	11	0.22
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	10	0.22
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	10	0.22
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	10	0.22
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	17	0.22
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	17	0.22
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	17	0.22
(1,170)	1:71:B:ASN:HA	1:101:B:GLU:HA	10	0.22
(1,165)	1:5:A:ASN:HA	1:35:A:GLU:HA	10	0.22
(1,89)	1:9:A:ILE:HD11	1:59:A:ASP:HB2	13	0.22
(1,89)	1:9:A:ILE:HD12	1:59:A:ASP:HB2	13	0.22
(1,89)	1:9:A:ILE:HD13	1:59:A:ASP:HB2	13	0.22
(1,86)	1:9:A:ILE:HG13	1:59:A:ASP:HB2	17	0.22
(1,2085)	1:63:A:TRP:HE3	1:117:B:TYR:HD1	2	0.21
(1,2085)	1:63:A:TRP:HE3	1:117:B:TYR:HD2	2	0.21
(1,2029)	1:110:B:GLN:H	1:110:B:GLN:HE21	18	0.21
(1,1998)	1:102:B:LYS:HA	1:102:B:LYS:HE2	18	0.21
(1,1879)	1:78:B:LYS:HB3	1:78:B:LYS:HD2	9	0.21
(1,1879)	1:78:B:LYS:HB3	1:78:B:LYS:HD2	17	0.21
(1,1683)	1:28:A:ARG:H	1:28:A:ARG:HD3	14	0.21
(1,1611)	1:12:A:LYS:HB3	1:12:A:LYS:HD2	17	0.21
(1,1604)	1:12:A:LYS:H	1:12:A:LYS:HD2	1	0.21
(1,1545)	1:128:B:GLN:HG2	1:129:B:TRP:H	14	0.21
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD11	1	0.21
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD12	1	0.21
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD13	1	0.21
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	8	0.21
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	9	0.21
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	10	0.21
(1,1404)	1:84:B:SER:H	1:85:B:GLU:HB3	5	0.21
(1,1330)	1:72:B:LEU:H	1:73:B:LYS:HE3	1	0.21
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD11	18	0.21
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD12	18	0.21
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD13	18	0.21
(1,1313)	1:62:A:GLN:HG2	1:63:A:TRP:H	6	0.21
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD11	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD12	1	0.21
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD13	1	0.21
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	13	0.21
(1,1267)	1:43:A:LEU:HD11	1:44:A:GLN:HA	1	0.21
(1,1267)	1:43:A:LEU:HD12	1:44:A:GLN:HA	1	0.21
(1,1267)	1:43:A:LEU:HD13	1:44:A:GLN:HA	1	0.21
(1,1267)	1:43:A:LEU:HD21	1:44:A:GLN:HA	1	0.21
(1,1267)	1:43:A:LEU:HD22	1:44:A:GLN:HA	1	0.21
(1,1267)	1:43:A:LEU:HD23	1:44:A:GLN:HA	1	0.21
(1,1260)	1:38:A:LYS:HG3	1:39:A:TYR:H	14	0.21
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	2	0.21
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	2	0.21
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	2	0.21
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	20	0.21
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	20	0.21
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	20	0.21
(1,1150)	1:12:A:LYS:HE3	1:13:A:LYS:H	4	0.21
(1,1150)	1:12:A:LYS:HE3	1:13:A:LYS:H	19	0.21
(1,1149)	1:12:A:LYS:HD3	1:13:A:LYS:HA	3	0.21
(1,1146)	1:12:A:LYS:HD2	1:13:A:LYS:H	18	0.21
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD11	16	0.21
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD12	16	0.21
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD13	16	0.21
(1,1098)	1:6:A:LEU:H	1:7:A:LYS:HE3	3	0.21
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD11	18	0.21
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD12	18	0.21
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD13	18	0.21
(1,1042)	1:79:B:LYS:HG3	1:81:B:ILE:HA	14	0.21
(1,1018)	1:68:B:ILE:HG21	1:70:B:ASN:HD21	18	0.21
(1,1018)	1:68:B:ILE:HG22	1:70:B:ASN:HD21	18	0.21
(1,1018)	1:68:B:ILE:HG23	1:70:B:ASN:HD21	18	0.21
(1,1015)	1:64:A:GLN:HB3	1:66:A:GLU:H	20	0.21
(1,971)	1:13:A:LYS:HG3	1:15:A:ILE:HA	3	0.21
(1,947)	1:2:A:ILE:HG21	1:4:A:ASN:HD21	18	0.21
(1,947)	1:2:A:ILE:HG22	1:4:A:ASN:HD21	18	0.21
(1,947)	1:2:A:ILE:HG23	1:4:A:ASN:HD21	18	0.21
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	18	0.21
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	18	0.21
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	18	0.21
(1,874)	1:75:B:ILE:HA	1:78:B:LYS:HE3	15	0.21
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	13	0.21
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	13	0.21
(1,786)	1:10:A:ARG:HA	1:13:A:LYS:HE3	14	0.21
(1,735)	1:110:B:GLN:HB2	1:114:B:LYS:HD2	13	0.21
(1,699)	1:85:B:GLU:HG2	1:89:B:LEU:HD21	7	0.21
(1,699)	1:85:B:GLU:HG2	1:89:B:LEU:HD22	7	0.21
(1,699)	1:85:B:GLU:HG2	1:89:B:LEU:HD23	7	0.21
(1,679)	1:73:B:LYS:HG2	1:77:B:GLU:HG2	1	0.21
(1,583)	1:7:A:LYS:HG2	1:11:A:GLU:HG2	12	0.21
(1,583)	1:7:A:LYS:HG2	1:11:A:GLU:HG2	15	0.21
(1,466)	1:100:B:ILE:HG21	1:106:B:ASN:HB3	4	0.21
(1,466)	1:100:B:ILE:HG22	1:106:B:ASN:HB3	4	0.21
(1,466)	1:100:B:ILE:HG23	1:106:B:ASN:HB3	4	0.21
(1,385)	1:20:A:LEU:HD21	1:28:A:ARG:HB2	6	0.21
(1,385)	1:20:A:LEU:HD22	1:28:A:ARG:HB2	6	0.21
(1,385)	1:20:A:LEU:HD23	1:28:A:ARG:HB2	6	0.21
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD21	15	0.21
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD22	15	0.21
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD23	15	0.21
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD21	15	0.21
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD22	15	0.21
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD23	15	0.21
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD21	15	0.21
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD22	15	0.21
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD23	15	0.21
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	5	0.21
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	5	0.21
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	5	0.21
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD21	16	0.21
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD22	16	0.21
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD23	16	0.21
(1,127)	1:79:B:LYS:HE2	1:120:B:ASN:HB2	14	0.21
(1,126)	1:79:B:LYS:HD3	1:120:B:ASN:HB2	16	0.21
(1,93)	1:75:B:ILE:HG12	1:125:B:ASP:HB2	2	0.21
(1,86)	1:9:A:ILE:HG13	1:59:A:ASP:HB2	5	0.21
(1,2122)	1:43:A:LEU:HD21	1:112:B:ALA:HB1	13	0.2
(1,2122)	1:43:A:LEU:HD21	1:112:B:ALA:HB2	13	0.2
(1,2122)	1:43:A:LEU:HD21	1:112:B:ALA:HB3	13	0.2
(1,2122)	1:43:A:LEU:HD22	1:112:B:ALA:HB1	13	0.2
(1,2122)	1:43:A:LEU:HD22	1:112:B:ALA:HB2	13	0.2
(1,2122)	1:43:A:LEU:HD22	1:112:B:ALA:HB3	13	0.2
(1,2122)	1:43:A:LEU:HD23	1:112:B:ALA:HB1	13	0.2
(1,2122)	1:43:A:LEU:HD23	1:112:B:ALA:HB2	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2122)	1:43:A:LEU:HD23	1:112:B:ALA:HB3	13	0.2
(1,2108)	1:47:A:LEU:HD11	1:129:B:TRP:HE1	18	0.2
(1,2108)	1:47:A:LEU:HD12	1:129:B:TRP:HE1	18	0.2
(1,2108)	1:47:A:LEU:HD13	1:129:B:TRP:HE1	18	0.2
(1,2105)	1:43:A:LEU:HD21	1:127:B:PHE:HD1	1	0.2
(1,2105)	1:43:A:LEU:HD22	1:127:B:PHE:HD1	1	0.2
(1,2105)	1:43:A:LEU:HD23	1:127:B:PHE:HD1	1	0.2
(1,2085)	1:63:A:TRP:HE3	1:117:B:TYR:HD1	3	0.2
(1,2085)	1:63:A:TRP:HE3	1:117:B:TYR:HD2	3	0.2
(1,2057)	1:120:B:ASN:H	1:120:B:ASN:HD22	16	0.2
(1,1899)	1:80:B:LYS:HA	1:80:B:LYS:HE2	11	0.2
(1,1731)	1:36:A:LYS:HA	1:36:A:LYS:HE3	13	0.2
(1,1651)	1:17:A:GLN:H	1:17:A:GLN:HE21	20	0.2
(1,1545)	1:128:B:GLN:HG2	1:129:B:TRP:H	6	0.2
(1,1545)	1:128:B:GLN:HG2	1:129:B:TRP:H	11	0.2
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD11	3	0.2
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD12	3	0.2
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD13	3	0.2
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD11	10	0.2
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD12	10	0.2
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD13	10	0.2
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD11	16	0.2
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD12	16	0.2
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD13	16	0.2
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	11	0.2
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	20	0.2
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	5	0.2
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	5	0.2
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	5	0.2
(1,1372)	1:77:B:GLU:HG3	1:78:B:LYS:HB3	17	0.2
(1,1321)	1:67:B:MET:HG2	1:68:B:ILE:HD11	5	0.2
(1,1321)	1:67:B:MET:HG2	1:68:B:ILE:HD12	5	0.2
(1,1321)	1:67:B:MET:HG2	1:68:B:ILE:HD13	5	0.2
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD11	13	0.2
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD12	13	0.2
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD13	13	0.2
(1,1313)	1:62:A:GLN:HG2	1:63:A:TRP:H	13	0.2
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD11	12	0.2
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD12	12	0.2
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD13	12	0.2
(1,1305)	1:54:A:ASN:HD21	1:55:A:THR:H	6	0.2
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	6	0.2
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	12	0.2
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	17	0.2
(1,1256)	1:38:A:LYS:HD2	1:39:A:TYR:HE2	14	0.2
(1,1172)	1:18:A:SER:H	1:19:A:GLU:HB3	2	0.2
(1,1167)	1:15:A:ILE:HG13	1:16:A:SER:H	4	0.2
(1,1150)	1:12:A:LYS:HE3	1:13:A:LYS:H	6	0.2
(1,1146)	1:12:A:LYS:HD2	1:13:A:LYS:H	4	0.2
(1,1112)	1:7:A:LYS:HG2	1:8:A:LEU:HA	15	0.2
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD11	9	0.2
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD12	9	0.2
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD13	9	0.2
(1,957)	1:5:A:ASN:HB2	1:7:A:LYS:HE3	14	0.2
(1,874)	1:75:B:ILE:HA	1:78:B:LYS:HE3	16	0.2
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	4	0.2
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	4	0.2
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	4	0.2
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	17	0.2
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	17	0.2
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	17	0.2
(1,699)	1:85:B:GLU:HG2	1:89:B:LEU:HD21	1	0.2
(1,699)	1:85:B:GLU:HG2	1:89:B:LEU:HD22	1	0.2
(1,699)	1:85:B:GLU:HG2	1:89:B:LEU:HD23	1	0.2
(1,603)	1:19:A:GLU:HG2	1:23:A:LEU:HD21	1	0.2
(1,603)	1:19:A:GLU:HG2	1:23:A:LEU:HD22	1	0.2
(1,603)	1:19:A:GLU:HG2	1:23:A:LEU:HD23	1	0.2
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	9	0.2
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	9	0.2
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	9	0.2
(1,385)	1:20:A:LEU:HD21	1:28:A:ARG:HB2	11	0.2
(1,385)	1:20:A:LEU:HD22	1:28:A:ARG:HB2	11	0.2
(1,385)	1:20:A:LEU:HD23	1:28:A:ARG:HB2	11	0.2
(1,257)	1:41:A:PRO:HB3	1:61:A:PHE:HE1	16	0.2
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	7	0.2
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	7	0.2
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	7	0.2
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	8	0.2
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	8	0.2
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	8	0.2
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	17	0.2
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	17	0.2
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	18	0.2
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	18	0.2
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	18	0.2
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	19	0.2
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	19	0.2
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	19	0.2
(1,165)	1:5:A:ASN:HA	1:35:A:GLU:HA	2	0.2
(1,95)	1:75:B:ILE:HG13	1:125:B:ASP:HB2	13	0.2
(1,86)	1:9:A:ILE:HG13	1:59:A:ASP:HB2	10	0.2
(1,2158)	1:63:A:TRP:HE1	1:113:B:LEU:HD11	18	0.19
(1,2158)	1:63:A:TRP:HE1	1:113:B:LEU:HD12	18	0.19
(1,2158)	1:63:A:TRP:HE1	1:113:B:LEU:HD13	18	0.19
(1,2156)	1:63:A:TRP:HE1	1:114:B:LYS:HA	16	0.19
(1,2111)	1:48:A:LYS:HG3	1:129:B:TRP:HE1	1	0.19
(1,2110)	1:48:A:LYS:HA	1:129:B:TRP:HE1	2	0.19
(1,2100)	1:2:A:ILE:HG21	1:109:B:LEU:HD21	6	0.19
(1,2100)	1:2:A:ILE:HG21	1:109:B:LEU:HD22	6	0.19
(1,2100)	1:2:A:ILE:HG21	1:109:B:LEU:HD23	6	0.19
(1,2100)	1:2:A:ILE:HG22	1:109:B:LEU:HD21	6	0.19
(1,2100)	1:2:A:ILE:HG22	1:109:B:LEU:HD22	6	0.19
(1,2100)	1:2:A:ILE:HG22	1:109:B:LEU:HD23	6	0.19
(1,2100)	1:2:A:ILE:HG23	1:109:B:LEU:HD21	6	0.19
(1,2100)	1:2:A:ILE:HG23	1:109:B:LEU:HD22	6	0.19
(1,2100)	1:2:A:ILE:HG23	1:109:B:LEU:HD23	6	0.19
(1,1998)	1:102:B:LYS:HA	1:102:B:LYS:HE2	9	0.19
(1,1968)	1:95:B:GLN:HB3	1:95:B:GLN:HE21	8	0.19
(1,1872)	1:78:B:LYS:H	1:78:B:LYS:HD2	8	0.19
(1,1872)	1:78:B:LYS:H	1:78:B:LYS:HD2	17	0.19
(1,1730)	1:36:A:LYS:HA	1:36:A:LYS:HE2	6	0.19
(1,1652)	1:17:A:GLN:HA	1:17:A:GLN:HE22	19	0.19
(1,1604)	1:12:A:LYS:H	1:12:A:LYS:HD2	17	0.19
(1,1554)	1:3:A:ILE:H	1:3:A:ILE:HD11	15	0.19
(1,1554)	1:3:A:ILE:H	1:3:A:ILE:HD12	15	0.19
(1,1554)	1:3:A:ILE:H	1:3:A:ILE:HD13	15	0.19
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	7	0.19
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	16	0.19
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	17	0.19
(1,1388)	1:79:B:LYS:HB2	1:80:B:LYS:HG2	10	0.19
(1,1381)	1:78:B:LYS:HD3	1:79:B:LYS:HA	12	0.19
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD11	14	0.19
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD12	14	0.19
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD13	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD11	17	0.19
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD12	17	0.19
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD13	17	0.19
(1,1330)	1:72:B:LEU:H	1:73:B:LYS:HE3	6	0.19
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	16	0.19
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	18	0.19
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	19	0.19
(1,1255)	1:38:A:LYS:HD2	1:39:A:TYR:HD2	11	0.19
(1,1254)	1:38:A:LYS:HD2	1:39:A:TYR:H	16	0.19
(1,1252)	1:38:A:LYS:HA	1:39:A:TYR:HD2	14	0.19
(1,1248)	1:37:A:ASN:HD21	1:38:A:LYS:HD3	11	0.19
(1,1221)	1:31:A:ILE:HG21	1:32:A:ASN:HD21	12	0.19
(1,1221)	1:31:A:ILE:HG22	1:32:A:ASN:HD21	12	0.19
(1,1221)	1:31:A:ILE:HG23	1:32:A:ASN:HD21	12	0.19
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD11	7	0.19
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD12	7	0.19
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD13	7	0.19
(1,1098)	1:6:A:LEU:H	1:7:A:LYS:HE3	10	0.19
(1,1098)	1:6:A:LEU:H	1:7:A:LYS:HE3	12	0.19
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD11	4	0.19
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD12	4	0.19
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD13	4	0.19
(1,1049)	1:86:B:LEU:HD21	1:88:B:ALA:H	3	0.19
(1,1049)	1:86:B:LEU:HD22	1:88:B:ALA:H	3	0.19
(1,1049)	1:86:B:LEU:HD23	1:88:B:ALA:H	3	0.19
(1,978)	1:20:A:LEU:HD21	1:22:A:ALA:H	18	0.19
(1,978)	1:20:A:LEU:HD22	1:22:A:ALA:H	18	0.19
(1,978)	1:20:A:LEU:HD23	1:22:A:ALA:H	18	0.19
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	1	0.19
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	1	0.19
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	1	0.19
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	4	0.19
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	4	0.19
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	4	0.19
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	12	0.19
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	12	0.19
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	12	0.19
(1,786)	1:10:A:ARG:HA	1:13:A:LYS:HE3	8	0.19
(1,780)	1:9:A:ILE:HA	1:12:A:LYS:HE3	18	0.19
(1,640)	1:44:A:GLN:HB3	1:48:A:LYS:HD2	2	0.19
(1,603)	1:19:A:GLU:HG2	1:23:A:LEU:HD21	5	0.19
(1,603)	1:19:A:GLU:HG2	1:23:A:LEU:HD22	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,603)	1:19:A:GLU:HG2	1:23:A:LEU:HD23	5	0.19
(1,589)	1:10:A:ARG:HD3	1:14:A:LYS:HA	20	0.19
(1,583)	1:7:A:LYS:HG2	1:11:A:GLU:HG2	19	0.19
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG21	3	0.19
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG22	3	0.19
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG23	3	0.19
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG21	18	0.19
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG22	18	0.19
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG23	18	0.19
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG21	20	0.19
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG22	20	0.19
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG23	20	0.19
(1,466)	1:100:B:ILE:HG21	1:106:B:ASN:HB3	19	0.19
(1,466)	1:100:B:ILE:HG22	1:106:B:ASN:HB3	19	0.19
(1,466)	1:100:B:ILE:HG23	1:106:B:ASN:HB3	19	0.19
(1,460)	1:34:A:ILE:HG21	1:40:A:ASN:HB3	13	0.19
(1,460)	1:34:A:ILE:HG22	1:40:A:ASN:HB3	13	0.19
(1,460)	1:34:A:ILE:HG23	1:40:A:ASN:HB3	13	0.19
(1,460)	1:34:A:ILE:HG21	1:40:A:ASN:HB3	20	0.19
(1,460)	1:34:A:ILE:HG22	1:40:A:ASN:HB3	20	0.19
(1,460)	1:34:A:ILE:HG23	1:40:A:ASN:HB3	20	0.19
(1,172)	1:71:B:ASN:HA	1:101:B:GLU:HB3	4	0.19
(1,167)	1:5:A:ASN:HA	1:35:A:GLU:HB3	9	0.19
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD21	14	0.19
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD22	14	0.19
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD23	14	0.19
(1,95)	1:75:B:ILE:HG13	1:125:B:ASP:HB2	7	0.19
(1,95)	1:75:B:ILE:HG13	1:125:B:ASP:HB2	10	0.19
(1,2156)	1:63:A:TRP:HE1	1:114:B:LYS:HA	3	0.18
(1,2156)	1:63:A:TRP:HE1	1:114:B:LYS:HA	14	0.18
(1,2110)	1:48:A:LYS:HA	1:129:B:TRP:HE1	16	0.18
(1,2097)	1:2:A:ILE:HD11	1:109:B:LEU:HD21	3	0.18
(1,2097)	1:2:A:ILE:HD11	1:109:B:LEU:HD22	3	0.18
(1,2097)	1:2:A:ILE:HD11	1:109:B:LEU:HD23	3	0.18
(1,2097)	1:2:A:ILE:HD12	1:109:B:LEU:HD21	3	0.18
(1,2097)	1:2:A:ILE:HD12	1:109:B:LEU:HD22	3	0.18
(1,2097)	1:2:A:ILE:HD12	1:109:B:LEU:HD23	3	0.18
(1,2097)	1:2:A:ILE:HD13	1:109:B:LEU:HD21	3	0.18
(1,2097)	1:2:A:ILE:HD13	1:109:B:LEU:HD22	3	0.18
(1,2097)	1:2:A:ILE:HD13	1:109:B:LEU:HD23	3	0.18
(1,2087)	1:2:A:ILE:HD11	1:110:B:GLN:H	11	0.18
(1,2087)	1:2:A:ILE:HD12	1:110:B:GLN:H	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2087)	1:2:A:ILE:HD13	1:110:B:GLN:H	11	0.18
(1,1998)	1:102:B:LYS:HA	1:102:B:LYS:HE2	8	0.18
(1,1998)	1:102:B:LYS:HA	1:102:B:LYS:HE2	17	0.18
(1,1904)	1:80:B:LYS:HB2	1:80:B:LYS:HE2	1	0.18
(1,1869)	1:77:B:GLU:H	1:77:B:GLU:HG2	2	0.18
(1,1869)	1:77:B:GLU:H	1:77:B:GLU:HG2	11	0.18
(1,1801)	1:62:A:GLN:H	1:62:A:GLN:HG2	19	0.18
(1,1632)	1:14:A:LYS:HA	1:14:A:LYS:HE3	17	0.18
(1,1631)	1:14:A:LYS:HA	1:14:A:LYS:HE2	20	0.18
(1,1611)	1:12:A:LYS:HB3	1:12:A:LYS:HD2	9	0.18
(1,1604)	1:12:A:LYS:H	1:12:A:LYS:HD2	9	0.18
(1,1545)	1:128:B:GLN:HG2	1:129:B:TRP:H	8	0.18
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	19	0.18
(1,1504)	1:110:B:GLN:HE22	1:111:B:LEU:HD21	20	0.18
(1,1504)	1:110:B:GLN:HE22	1:111:B:LEU:HD22	20	0.18
(1,1504)	1:110:B:GLN:HE22	1:111:B:LEU:HD23	20	0.18
(1,1487)	1:104:B:LYS:HD2	1:105:B:TYR:HD2	14	0.18
(1,1381)	1:78:B:LYS:HD3	1:79:B:LYS:HA	4	0.18
(1,1344)	1:73:B:LYS:HG2	1:74:B:LEU:HA	1	0.18
(1,1333)	1:72:B:LEU:HD11	1:73:B:LYS:HB3	18	0.18
(1,1333)	1:72:B:LEU:HD12	1:73:B:LYS:HB3	18	0.18
(1,1333)	1:72:B:LEU:HD13	1:73:B:LYS:HB3	18	0.18
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD11	17	0.18
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD12	17	0.18
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD13	17	0.18
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD11	20	0.18
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD12	20	0.18
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD13	20	0.18
(1,1244)	1:36:A:LYS:HG3	1:37:A:ASN:HD21	9	0.18
(1,1210)	1:29:A:GLN:HG2	1:30:A:THR:HG21	19	0.18
(1,1210)	1:29:A:GLN:HG2	1:30:A:THR:HG22	19	0.18
(1,1210)	1:29:A:GLN:HG2	1:30:A:THR:HG23	19	0.18
(1,1209)	1:29:A:GLN:HG2	1:30:A:THR:H	9	0.18
(1,1206)	1:28:A:ARG:HG2	1:29:A:GLN:HB3	10	0.18
(1,1172)	1:18:A:SER:H	1:19:A:GLU:HB3	10	0.18
(1,1150)	1:12:A:LYS:HE3	1:13:A:LYS:H	13	0.18
(1,1146)	1:12:A:LYS:HD2	1:13:A:LYS:H	19	0.18
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD11	5	0.18
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD12	5	0.18
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD13	5	0.18
(1,1018)	1:68:B:ILE:HG21	1:70:B:ASN:HD21	10	0.18
(1,1018)	1:68:B:ILE:HG22	1:70:B:ASN:HD21	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:68:B:ILE:HG23	1:70:B:ASN:HD21	10	0.18
(1,1015)	1:64:A:GLN:HB3	1:66:A:GLU:H	18	0.18
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD11	8	0.18
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD12	8	0.18
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD13	8	0.18
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD11	8	0.18
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD12	8	0.18
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD13	8	0.18
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD11	8	0.18
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD12	8	0.18
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD13	8	0.18
(1,999)	1:53:A:LEU:HD11	1:55:A:THR:H	4	0.18
(1,999)	1:53:A:LEU:HD12	1:55:A:THR:H	4	0.18
(1,999)	1:53:A:LEU:HD13	1:55:A:THR:H	4	0.18
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD11	12	0.18
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD12	12	0.18
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD13	12	0.18
(1,891)	1:83:B:GLN:HE21	1:86:B:LEU:HD21	20	0.18
(1,891)	1:83:B:GLN:HE21	1:86:B:LEU:HD22	20	0.18
(1,891)	1:83:B:GLN:HE21	1:86:B:LEU:HD23	20	0.18
(1,874)	1:75:B:ILE:HA	1:78:B:LYS:HE3	17	0.18
(1,780)	1:9:A:ILE:HA	1:12:A:LYS:HE3	6	0.18
(1,699)	1:85:B:GLU:HG2	1:89:B:LEU:HD21	16	0.18
(1,699)	1:85:B:GLU:HG2	1:89:B:LEU:HD22	16	0.18
(1,699)	1:85:B:GLU:HG2	1:89:B:LEU:HD23	16	0.18
(1,689)	1:81:B:ILE:HG13	1:85:B:GLU:HG2	13	0.18
(1,658)	1:57:A:LEU:HD11	1:61:A:PHE:HD1	15	0.18
(1,658)	1:57:A:LEU:HD12	1:61:A:PHE:HD1	15	0.18
(1,658)	1:57:A:LEU:HD13	1:61:A:PHE:HD1	15	0.18
(1,646)	1:44:A:GLN:HG3	1:48:A:LYS:HE3	20	0.18
(1,593)	1:15:A:ILE:HG13	1:19:A:GLU:HG2	16	0.18
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG21	15	0.18
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG22	15	0.18
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG23	15	0.18
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG21	17	0.18
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG22	17	0.18
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG23	17	0.18
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG21	20	0.18
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG22	20	0.18
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG23	20	0.18
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	11	0.18
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	11	0.18
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD21	2	0.18
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD22	2	0.18
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD23	2	0.18
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD21	2	0.18
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD22	2	0.18
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD23	2	0.18
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD21	2	0.18
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD22	2	0.18
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD23	2	0.18
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG21	3	0.18
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG22	3	0.18
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG23	3	0.18
(1,260)	1:107:B:PRO:HB3	1:127:B:PHE:HE1	5	0.18
(1,258)	1:41:A:PRO:HG2	1:61:A:PHE:HD1	4	0.18
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	20	0.18
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	20	0.18
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	20	0.18
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	5	0.18
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	5	0.18
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	5	0.18
(1,189)	1:89:B:LEU:HD11	1:118:B:TYR:HD2	13	0.18
(1,189)	1:89:B:LEU:HD12	1:118:B:TYR:HD2	13	0.18
(1,189)	1:89:B:LEU:HD13	1:118:B:TYR:HD2	13	0.18
(1,177)	1:23:A:LEU:HG	1:52:A:TYR:HD2	8	0.18
(1,170)	1:71:B:ASN:HA	1:101:B:GLU:HA	18	0.18
(1,165)	1:5:A:ASN:HA	1:35:A:GLU:HA	20	0.18
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD21	20	0.18
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD22	20	0.18
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD23	20	0.18
(1,127)	1:79:B:LYS:HE2	1:120:B:ASN:HB2	16	0.18
(1,108)	1:75:B:ILE:HG21	1:121:B:THR:HG21	4	0.18
(1,108)	1:75:B:ILE:HG21	1:121:B:THR:HG22	4	0.18
(1,108)	1:75:B:ILE:HG21	1:121:B:THR:HG23	4	0.18
(1,108)	1:75:B:ILE:HG22	1:121:B:THR:HG21	4	0.18
(1,108)	1:75:B:ILE:HG22	1:121:B:THR:HG22	4	0.18
(1,108)	1:75:B:ILE:HG22	1:121:B:THR:HG23	4	0.18
(1,108)	1:75:B:ILE:HG23	1:121:B:THR:HG21	4	0.18
(1,108)	1:75:B:ILE:HG23	1:121:B:THR:HG22	4	0.18
(1,108)	1:75:B:ILE:HG23	1:121:B:THR:HG23	4	0.18
(1,95)	1:75:B:ILE:HG13	1:125:B:ASP:HB2	17	0.18
(1,44)	1:3:A:ILE:HG13	1:62:A:GLN:HE22	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:2:A:ILE:HD11	1:64:A:GLN:HB2	3	0.18
(1,3)	1:2:A:ILE:HD12	1:64:A:GLN:HB2	3	0.18
(1,3)	1:2:A:ILE:HD13	1:64:A:GLN:HB2	3	0.18
(1,2)	1:2:A:ILE:HD11	1:64:A:GLN:H	1	0.18
(1,2)	1:2:A:ILE:HD12	1:64:A:GLN:H	1	0.18
(1,2)	1:2:A:ILE:HD13	1:64:A:GLN:H	1	0.18
(1,2156)	1:63:A:TRP:HE1	1:114:B:LYS:HA	9	0.17
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD11	14	0.17
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD12	14	0.17
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD13	14	0.17
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD21	14	0.17
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD22	14	0.17
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD23	14	0.17
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD11	14	0.17
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD12	14	0.17
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD13	14	0.17
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD21	14	0.17
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD22	14	0.17
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD23	14	0.17
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD11	14	0.17
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD12	14	0.17
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD13	14	0.17
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD21	14	0.17
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD22	14	0.17
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD23	14	0.17
(1,2111)	1:48:A:LYS:HG3	1:129:B:TRP:HE1	19	0.17
(1,2087)	1:2:A:ILE:HD11	1:110:B:GLN:H	14	0.17
(1,2087)	1:2:A:ILE:HD12	1:110:B:GLN:H	14	0.17
(1,2087)	1:2:A:ILE:HD13	1:110:B:GLN:H	14	0.17
(1,2086)	1:129:B:TRP:HE3	1:51:A:TYR:HD1	14	0.17
(1,2086)	1:129:B:TRP:HE3	1:51:A:TYR:HD2	14	0.17
(1,1872)	1:78:B:LYS:H	1:78:B:LYS:HD2	11	0.17
(1,1651)	1:17:A:GLN:H	1:17:A:GLN:HE21	12	0.17
(1,1651)	1:17:A:GLN:H	1:17:A:GLN:HE21	17	0.17
(1,1632)	1:14:A:LYS:HA	1:14:A:LYS:HE3	11	0.17
(1,1631)	1:14:A:LYS:HA	1:14:A:LYS:HE2	9	0.17
(1,1601)	1:11:A:GLU:H	1:11:A:GLU:HG2	1	0.17
(1,1569)	1:7:A:LYS:H	1:7:A:LYS:HD3	13	0.17
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD11	11	0.17
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD12	11	0.17
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD13	11	0.17
(1,1530)	1:119:B:LEU:HD11	1:120:B:ASN:H	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1530)	1:119:B:LEU:HD12	1:120:B:ASN:H	8	0.17
(1,1530)	1:119:B:LEU:HD13	1:120:B:ASN:H	8	0.17
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	1	0.17
(1,1465)	1:101:B:GLU:HG2	1:102:B:LYS:HD2	6	0.17
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	4	0.17
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	4	0.17
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	4	0.17
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD21	12	0.17
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD22	12	0.17
(1,1417)	1:88:B:ALA:H	1:89:B:LEU:HD23	12	0.17
(1,1382)	1:78:B:LYS:HE3	1:79:B:LYS:H	19	0.17
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD11	13	0.17
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD12	13	0.17
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD13	13	0.17
(1,1321)	1:67:B:MET:HG2	1:68:B:ILE:HD11	18	0.17
(1,1321)	1:67:B:MET:HG2	1:68:B:ILE:HD12	18	0.17
(1,1321)	1:67:B:MET:HG2	1:68:B:ILE:HD13	18	0.17
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD11	9	0.17
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD12	9	0.17
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD13	9	0.17
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD11	16	0.17
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD12	16	0.17
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD13	16	0.17
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD11	18	0.17
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD12	18	0.17
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD13	18	0.17
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD11	18	0.17
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD12	18	0.17
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD13	18	0.17
(1,1087)	1:1:A:MET:HB3	1:2:A:ILE:HD11	5	0.17
(1,1087)	1:1:A:MET:HB3	1:2:A:ILE:HD12	5	0.17
(1,1087)	1:1:A:MET:HB3	1:2:A:ILE:HD13	5	0.17
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD11	7	0.17
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD12	7	0.17
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD13	7	0.17
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD11	7	0.17
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD12	7	0.17
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD13	7	0.17
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD11	7	0.17
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD12	7	0.17
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD13	7	0.17
(1,1042)	1:79:B:LYS:HG3	1:81:B:ILE:HA	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1042)	1:79:B:LYS:HG3	1:81:B:ILE:HA	11	0.17
(1,1018)	1:68:B:ILE:HG21	1:70:B:ASN:HD21	8	0.17
(1,1018)	1:68:B:ILE:HG22	1:70:B:ASN:HD21	8	0.17
(1,1018)	1:68:B:ILE:HG23	1:70:B:ASN:HD21	8	0.17
(1,978)	1:20:A:LEU:HD21	1:22:A:ALA:H	8	0.17
(1,978)	1:20:A:LEU:HD22	1:22:A:ALA:H	8	0.17
(1,978)	1:20:A:LEU:HD23	1:22:A:ALA:H	8	0.17
(1,969)	1:13:A:LYS:HD3	1:15:A:ILE:HG13	16	0.17
(1,959)	1:7:A:LYS:H	1:9:A:ILE:HD11	4	0.17
(1,959)	1:7:A:LYS:H	1:9:A:ILE:HD12	4	0.17
(1,959)	1:7:A:LYS:H	1:9:A:ILE:HD13	4	0.17
(1,947)	1:2:A:ILE:HG21	1:4:A:ASN:HD21	6	0.17
(1,947)	1:2:A:ILE:HG22	1:4:A:ASN:HD21	6	0.17
(1,947)	1:2:A:ILE:HG23	1:4:A:ASN:HD21	6	0.17
(1,913)	1:95:B:GLN:HB3	1:98:B:ASN:HD22	10	0.17
(1,898)	1:86:B:LEU:HA	1:89:B:LEU:HD21	4	0.17
(1,898)	1:86:B:LEU:HA	1:89:B:LEU:HD22	4	0.17
(1,898)	1:86:B:LEU:HA	1:89:B:LEU:HD23	4	0.17
(1,780)	1:9:A:ILE:HA	1:12:A:LYS:HE3	4	0.17
(1,733)	1:110:B:GLN:HA	1:114:B:LYS:HD2	17	0.17
(1,718)	1:100:B:ILE:H	1:104:B:LYS:H	11	0.17
(1,583)	1:7:A:LYS:HG2	1:11:A:GLU:HG2	6	0.17
(1,583)	1:7:A:LYS:HG2	1:11:A:GLU:HG2	14	0.17
(1,557)	1:116:B:ALA:HA	1:121:B:THR:HG21	9	0.17
(1,557)	1:116:B:ALA:HA	1:121:B:THR:HG22	9	0.17
(1,557)	1:116:B:ALA:HA	1:121:B:THR:HG23	9	0.17
(1,517)	1:72:B:LEU:HD11	1:77:B:GLU:H	3	0.17
(1,517)	1:72:B:LEU:HD12	1:77:B:GLU:H	3	0.17
(1,517)	1:72:B:LEU:HD13	1:77:B:GLU:H	3	0.17
(1,509)	1:50:A:ALA:HA	1:55:A:THR:HG21	9	0.17
(1,509)	1:50:A:ALA:HA	1:55:A:THR:HG22	9	0.17
(1,509)	1:50:A:ALA:HA	1:55:A:THR:HG23	9	0.17
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	10	0.17
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	10	0.17
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	10	0.17
(1,385)	1:20:A:LEU:HD21	1:28:A:ARG:HB2	3	0.17
(1,385)	1:20:A:LEU:HD22	1:28:A:ARG:HB2	3	0.17
(1,385)	1:20:A:LEU:HD23	1:28:A:ARG:HB2	3	0.17
(1,330)	1:86:B:LEU:HD21	1:97:B:ILE:HG12	20	0.17
(1,330)	1:86:B:LEU:HD22	1:97:B:ILE:HG12	20	0.17
(1,330)	1:86:B:LEU:HD23	1:97:B:ILE:HG12	20	0.17
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD21	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD22	7	0.17
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD23	7	0.17
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD21	7	0.17
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD22	7	0.17
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD23	7	0.17
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD21	7	0.17
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD22	7	0.17
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD23	7	0.17
(1,304)	1:17:A:GLN:HA	1:28:A:ARG:HD2	14	0.17
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG21	11	0.17
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG22	11	0.17
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG23	11	0.17
(1,207)	1:73:B:LYS:HE2	1:101:B:GLU:HG2	4	0.17
(1,170)	1:71:B:ASN:HA	1:101:B:GLU:HA	19	0.17
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD21	4	0.17
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD22	4	0.17
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD23	4	0.17
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD21	7	0.17
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD22	7	0.17
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD23	7	0.17
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD21	12	0.17
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD22	12	0.17
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD23	12	0.17
(1,120)	1:76:B:ARG:HG3	1:119:B:LEU:HD21	4	0.17
(1,120)	1:76:B:ARG:HG3	1:119:B:LEU:HD22	4	0.17
(1,120)	1:76:B:ARG:HG3	1:119:B:LEU:HD23	4	0.17
(1,98)	1:75:B:ILE:HD11	1:125:B:ASP:HB2	12	0.17
(1,98)	1:75:B:ILE:HD12	1:125:B:ASP:HB2	12	0.17
(1,98)	1:75:B:ILE:HD13	1:125:B:ASP:HB2	12	0.17
(1,95)	1:75:B:ILE:HG13	1:125:B:ASP:HB2	9	0.17
(1,2157)	1:63:A:TRP:HE1	1:114:B:LYS:HG3	9	0.16
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD11	8	0.16
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD12	8	0.16
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD13	8	0.16
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD21	8	0.16
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD22	8	0.16
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD23	8	0.16
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD11	8	0.16
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD12	8	0.16
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD13	8	0.16
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD21	8	0.16
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD22	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD23	8	0.16
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD11	8	0.16
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD12	8	0.16
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD13	8	0.16
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD21	8	0.16
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD22	8	0.16
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD23	8	0.16
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD11	20	0.16
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD12	20	0.16
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD13	20	0.16
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD21	20	0.16
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD22	20	0.16
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD23	20	0.16
(1,2103)	1:44:A:GLN:HG2	1:130:B:GLN:H	4	0.16
(1,2100)	1:2:A:ILE:HG21	1:109:B:LEU:HD21	20	0.16
(1,2100)	1:2:A:ILE:HG21	1:109:B:LEU:HD22	20	0.16
(1,2100)	1:2:A:ILE:HG21	1:109:B:LEU:HD23	20	0.16
(1,2100)	1:2:A:ILE:HG22	1:109:B:LEU:HD21	20	0.16
(1,2100)	1:2:A:ILE:HG22	1:109:B:LEU:HD22	20	0.16
(1,2100)	1:2:A:ILE:HG22	1:109:B:LEU:HD23	20	0.16
(1,2100)	1:2:A:ILE:HG23	1:109:B:LEU:HD21	20	0.16
(1,2100)	1:2:A:ILE:HG23	1:109:B:LEU:HD22	20	0.16
(1,2100)	1:2:A:ILE:HG23	1:109:B:LEU:HD23	20	0.16
(1,2090)	1:2:A:ILE:HD11	1:110:B:GLN:HE22	4	0.16
(1,2090)	1:2:A:ILE:HD12	1:110:B:GLN:HE22	4	0.16
(1,2090)	1:2:A:ILE:HD13	1:110:B:GLN:HE22	4	0.16
(1,2086)	1:129:B:TRP:HE3	1:51:A:TYR:HD1	19	0.16
(1,2086)	1:129:B:TRP:HE3	1:51:A:TYR:HD2	19	0.16
(1,2083)	1:63:A:TRP:HZ2	1:110:B:GLN:HA	5	0.16
(1,2029)	1:110:B:GLN:H	1:110:B:GLN:HE21	13	0.16
(1,1999)	1:102:B:LYS:HA	1:102:B:LYS:HE3	13	0.16
(1,1998)	1:102:B:LYS:HA	1:102:B:LYS:HE2	6	0.16
(1,1961)	1:95:B:GLN:H	1:95:B:GLN:HE22	12	0.16
(1,1899)	1:80:B:LYS:HA	1:80:B:LYS:HE2	7	0.16
(1,1899)	1:80:B:LYS:HA	1:80:B:LYS:HE2	16	0.16
(1,1761)	1:44:A:GLN:H	1:44:A:GLN:HE21	18	0.16
(1,1730)	1:36:A:LYS:HA	1:36:A:LYS:HE2	11	0.16
(1,1730)	1:36:A:LYS:HA	1:36:A:LYS:HE2	20	0.16
(1,1698)	1:29:A:GLN:HB2	1:29:A:GLN:HE21	1	0.16
(1,1651)	1:17:A:GLN:H	1:17:A:GLN:HE21	19	0.16
(1,1631)	1:14:A:LYS:HA	1:14:A:LYS:HE2	2	0.16
(1,1604)	1:12:A:LYS:H	1:12:A:LYS:HD2	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1575)	1:8:A:LEU:H	1:8:A:LEU:HG	11	0.16
(1,1569)	1:7:A:LYS:H	1:7:A:LYS:HD3	7	0.16
(1,1569)	1:7:A:LYS:H	1:7:A:LYS:HD3	20	0.16
(1,1545)	1:128:B:GLN:HG2	1:129:B:TRP:H	13	0.16
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD11	6	0.16
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD12	6	0.16
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD13	6	0.16
(1,1489)	1:104:B:LYS:HE2	1:105:B:TYR:H	13	0.16
(1,1366)	1:76:B:ARG:HD2	1:77:B:GLU:HA	3	0.16
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD11	7	0.16
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD12	7	0.16
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD13	7	0.16
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD11	10	0.16
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD12	10	0.16
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD13	10	0.16
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD11	15	0.16
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD12	15	0.16
(1,1353)	1:74:B:LEU:HB3	1:75:B:ILE:HD13	15	0.16
(1,1342)	1:73:B:LYS:HE3	1:74:B:LEU:HD21	11	0.16
(1,1342)	1:73:B:LYS:HE3	1:74:B:LEU:HD22	11	0.16
(1,1342)	1:73:B:LYS:HE3	1:74:B:LEU:HD23	11	0.16
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD11	15	0.16
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD12	15	0.16
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD13	15	0.16
(1,1313)	1:62:A:GLN:HG2	1:63:A:TRP:H	20	0.16
(1,1309)	1:59:A:ASP:HB3	1:60:A:ILE:HG21	15	0.16
(1,1309)	1:59:A:ASP:HB3	1:60:A:ILE:HG22	15	0.16
(1,1309)	1:59:A:ASP:HB3	1:60:A:ILE:HG23	15	0.16
(1,1305)	1:54:A:ASN:HD21	1:55:A:THR:H	10	0.16
(1,1305)	1:54:A:ASN:HD21	1:55:A:THR:H	20	0.16
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD21	19	0.16
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD22	19	0.16
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD23	19	0.16
(1,1221)	1:31:A:ILE:HG21	1:32:A:ASN:HD21	11	0.16
(1,1221)	1:31:A:ILE:HG22	1:32:A:ASN:HD21	11	0.16
(1,1221)	1:31:A:ILE:HG23	1:32:A:ASN:HD21	11	0.16
(1,1208)	1:29:A:GLN:HE21	1:30:A:THR:H	13	0.16
(1,1149)	1:12:A:LYS:HD3	1:13:A:LYS:HA	11	0.16
(1,1149)	1:12:A:LYS:HD3	1:13:A:LYS:HA	14	0.16
(1,1139)	1:11:A:GLU:HG2	1:12:A:LYS:H	14	0.16
(1,1134)	1:10:A:ARG:HD2	1:11:A:GLU:HA	10	0.16
(1,1110)	1:7:A:LYS:HE3	1:8:A:LEU:HD21	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1110)	1:7:A:LYS:HE3	1:8:A:LEU:HD22	11	0.16
(1,1110)	1:7:A:LYS:HE3	1:8:A:LEU:HD23	11	0.16
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD11	14	0.16
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD12	14	0.16
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD13	14	0.16
(1,1070)	1:119:B:LEU:HD11	1:121:B:THR:H	4	0.16
(1,1070)	1:119:B:LEU:HD12	1:121:B:THR:H	4	0.16
(1,1070)	1:119:B:LEU:HD13	1:121:B:THR:H	4	0.16
(1,1049)	1:86:B:LEU:HD21	1:88:B:ALA:H	4	0.16
(1,1049)	1:86:B:LEU:HD22	1:88:B:ALA:H	4	0.16
(1,1049)	1:86:B:LEU:HD23	1:88:B:ALA:H	4	0.16
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD11	14	0.16
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD12	14	0.16
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD13	14	0.16
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD11	14	0.16
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD12	14	0.16
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD13	14	0.16
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD11	14	0.16
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD12	14	0.16
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD13	14	0.16
(1,947)	1:2:A:ILE:HG21	1:4:A:ASN:HD21	17	0.16
(1,947)	1:2:A:ILE:HG22	1:4:A:ASN:HD21	17	0.16
(1,947)	1:2:A:ILE:HG23	1:4:A:ASN:HD21	17	0.16
(1,780)	1:9:A:ILE:HA	1:12:A:LYS:HE3	19	0.16
(1,755)	1:123:B:LEU:HD21	1:127:B:PHE:H	1	0.16
(1,755)	1:123:B:LEU:HD22	1:127:B:PHE:H	1	0.16
(1,755)	1:123:B:LEU:HD23	1:127:B:PHE:H	1	0.16
(1,740)	1:110:B:GLN:HG2	1:114:B:LYS:HE2	13	0.16
(1,708)	1:94:B:ARG:HD2	1:98:B:ASN:HD22	17	0.16
(1,689)	1:81:B:ILE:HG13	1:85:B:GLU:HG2	3	0.16
(1,689)	1:81:B:ILE:HG13	1:85:B:GLU:HG2	4	0.16
(1,641)	1:44:A:GLN:HE21	1:48:A:LYS:HB2	2	0.16
(1,603)	1:19:A:GLU:HG2	1:23:A:LEU:HD21	12	0.16
(1,603)	1:19:A:GLU:HG2	1:23:A:LEU:HD22	12	0.16
(1,603)	1:19:A:GLU:HG2	1:23:A:LEU:HD23	12	0.16
(1,585)	1:8:A:LEU:HA	1:12:A:LYS:HB2	9	0.16
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG21	12	0.16
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG22	12	0.16
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG23	12	0.16
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG21	17	0.16
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG22	17	0.16
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG23	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG21	18	0.16
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG22	18	0.16
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG23	18	0.16
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	20	0.16
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	20	0.16
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	20	0.16
(1,385)	1:20:A:LEU:HD21	1:28:A:ARG:HB2	17	0.16
(1,385)	1:20:A:LEU:HD22	1:28:A:ARG:HB2	17	0.16
(1,385)	1:20:A:LEU:HD23	1:28:A:ARG:HB2	17	0.16
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD21	1	0.16
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD22	1	0.16
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD23	1	0.16
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD21	1	0.16
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD22	1	0.16
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD23	1	0.16
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD21	1	0.16
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD22	1	0.16
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD23	1	0.16
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG21	2	0.16
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG22	2	0.16
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG23	2	0.16
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG21	5	0.16
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG22	5	0.16
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG23	5	0.16
(1,261)	1:107:B:PRO:HG2	1:127:B:PHE:HD1	3	0.16
(1,247)	1:25:A:GLU:HG3	1:48:A:LYS:HD3	14	0.16
(1,199)	1:7:A:LYS:HG2	1:35:A:GLU:HB2	13	0.16
(1,189)	1:89:B:LEU:HD11	1:118:B:TYR:HD2	4	0.16
(1,189)	1:89:B:LEU:HD12	1:118:B:TYR:HD2	4	0.16
(1,189)	1:89:B:LEU:HD13	1:118:B:TYR:HD2	4	0.16
(1,172)	1:71:B:ASN:HA	1:101:B:GLU:HB3	9	0.16
(1,156)	1:68:B:ILE:HD11	1:106:B:ASN:HD21	10	0.16
(1,156)	1:68:B:ILE:HD12	1:106:B:ASN:HD21	10	0.16
(1,156)	1:68:B:ILE:HD13	1:106:B:ASN:HD21	10	0.16
(1,104)	1:9:A:ILE:HG21	1:55:A:THR:HG21	4	0.16
(1,104)	1:9:A:ILE:HG21	1:55:A:THR:HG22	4	0.16
(1,104)	1:9:A:ILE:HG21	1:55:A:THR:HG23	4	0.16
(1,104)	1:9:A:ILE:HG22	1:55:A:THR:HG21	4	0.16
(1,104)	1:9:A:ILE:HG22	1:55:A:THR:HG22	4	0.16
(1,104)	1:9:A:ILE:HG22	1:55:A:THR:HG23	4	0.16
(1,104)	1:9:A:ILE:HG23	1:55:A:THR:HG21	4	0.16
(1,104)	1:9:A:ILE:HG23	1:55:A:THR:HG22	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:9:A:ILE:HG23	1:55:A:THR:HG23	4	0.16
(1,98)	1:75:B:ILE:HD11	1:125:B:ASP:HB2	3	0.16
(1,98)	1:75:B:ILE:HD12	1:125:B:ASP:HB2	3	0.16
(1,98)	1:75:B:ILE:HD13	1:125:B:ASP:HB2	3	0.16
(1,81)	1:75:B:ILE:HD11	1:126:B:ILE:HD11	2	0.16
(1,81)	1:75:B:ILE:HD11	1:126:B:ILE:HD12	2	0.16
(1,81)	1:75:B:ILE:HD11	1:126:B:ILE:HD13	2	0.16
(1,81)	1:75:B:ILE:HD12	1:126:B:ILE:HD11	2	0.16
(1,81)	1:75:B:ILE:HD12	1:126:B:ILE:HD12	2	0.16
(1,81)	1:75:B:ILE:HD12	1:126:B:ILE:HD13	2	0.16
(1,81)	1:75:B:ILE:HD13	1:126:B:ILE:HD11	2	0.16
(1,81)	1:75:B:ILE:HD13	1:126:B:ILE:HD12	2	0.16
(1,81)	1:75:B:ILE:HD13	1:126:B:ILE:HD13	2	0.16
(1,3)	1:2:A:ILE:HD11	1:64:A:GLN:HB2	8	0.16
(1,3)	1:2:A:ILE:HD12	1:64:A:GLN:HB2	8	0.16
(1,3)	1:2:A:ILE:HD13	1:64:A:GLN:HB2	8	0.16
(1,2169)	1:43:A:LEU:HD21	1:68:B:ILE:HD11	6	0.15
(1,2169)	1:43:A:LEU:HD21	1:68:B:ILE:HD12	6	0.15
(1,2169)	1:43:A:LEU:HD21	1:68:B:ILE:HD13	6	0.15
(1,2169)	1:43:A:LEU:HD22	1:68:B:ILE:HD11	6	0.15
(1,2169)	1:43:A:LEU:HD22	1:68:B:ILE:HD12	6	0.15
(1,2169)	1:43:A:LEU:HD22	1:68:B:ILE:HD13	6	0.15
(1,2169)	1:43:A:LEU:HD23	1:68:B:ILE:HD11	6	0.15
(1,2169)	1:43:A:LEU:HD23	1:68:B:ILE:HD12	6	0.15
(1,2169)	1:43:A:LEU:HD23	1:68:B:ILE:HD13	6	0.15
(1,2117)	1:43:A:LEU:HD11	1:112:B:ALA:H	13	0.15
(1,2117)	1:43:A:LEU:HD12	1:112:B:ALA:H	13	0.15
(1,2117)	1:43:A:LEU:HD13	1:112:B:ALA:H	13	0.15
(1,2086)	1:129:B:TRP:HE3	1:51:A:TYR:HD1	13	0.15
(1,2086)	1:129:B:TRP:HE3	1:51:A:TYR:HD2	13	0.15
(1,2066)	1:126:B:ILE:H	1:126:B:ILE:HG21	4	0.15
(1,2066)	1:126:B:ILE:H	1:126:B:ILE:HG22	4	0.15
(1,2066)	1:126:B:ILE:H	1:126:B:ILE:HG23	4	0.15
(1,2057)	1:120:B:ASN:H	1:120:B:ASN:HD22	17	0.15
(1,1968)	1:95:B:GLN:HB3	1:95:B:GLN:HE21	7	0.15
(1,1899)	1:80:B:LYS:HA	1:80:B:LYS:HE2	6	0.15
(1,1872)	1:78:B:LYS:H	1:78:B:LYS:HD2	12	0.15
(1,1872)	1:78:B:LYS:H	1:78:B:LYS:HD2	13	0.15
(1,1800)	1:62:A:GLN:H	1:62:A:GLN:HE21	15	0.15
(1,1761)	1:44:A:GLN:H	1:44:A:GLN:HE21	2	0.15
(1,1761)	1:44:A:GLN:H	1:44:A:GLN:HE21	20	0.15
(1,1730)	1:36:A:LYS:HA	1:36:A:LYS:HE2	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1727)	1:36:A:LYS:H	1:36:A:LYS:HE3	16	0.15
(1,1693)	1:29:A:GLN:H	1:29:A:GLN:HE22	7	0.15
(1,1604)	1:12:A:LYS:H	1:12:A:LYS:HD2	3	0.15
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD11	7	0.15
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD12	7	0.15
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD13	7	0.15
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD11	12	0.15
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD12	12	0.15
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD13	12	0.15
(1,1532)	1:119:B:LEU:HD21	1:120:B:ASN:HB2	4	0.15
(1,1532)	1:119:B:LEU:HD22	1:120:B:ASN:HB2	4	0.15
(1,1532)	1:119:B:LEU:HD23	1:120:B:ASN:HB2	4	0.15
(1,1504)	1:110:B:GLN:HE22	1:111:B:LEU:HD21	16	0.15
(1,1504)	1:110:B:GLN:HE22	1:111:B:LEU:HD22	16	0.15
(1,1504)	1:110:B:GLN:HE22	1:111:B:LEU:HD23	16	0.15
(1,1476)	1:102:B:LYS:HG3	1:103:B:ASN:HD21	4	0.15
(1,1453)	1:97:B:ILE:HG21	1:98:B:ASN:HD21	3	0.15
(1,1453)	1:97:B:ILE:HG22	1:98:B:ASN:HD21	3	0.15
(1,1453)	1:97:B:ILE:HG23	1:98:B:ASN:HD21	3	0.15
(1,1453)	1:97:B:ILE:HG21	1:98:B:ASN:HD21	8	0.15
(1,1453)	1:97:B:ILE:HG22	1:98:B:ASN:HD21	8	0.15
(1,1453)	1:97:B:ILE:HG23	1:98:B:ASN:HD21	8	0.15
(1,1443)	1:95:B:GLN:HG3	1:96:B:THR:H	9	0.15
(1,1397)	1:80:B:LYS:HG2	1:81:B:ILE:HD11	4	0.15
(1,1397)	1:80:B:LYS:HG2	1:81:B:ILE:HD12	4	0.15
(1,1397)	1:80:B:LYS:HG2	1:81:B:ILE:HD13	4	0.15
(1,1382)	1:78:B:LYS:HE3	1:79:B:LYS:H	16	0.15
(1,1381)	1:78:B:LYS:HD3	1:79:B:LYS:HA	7	0.15
(1,1372)	1:77:B:GLU:HG3	1:78:B:LYS:HB3	2	0.15
(1,1371)	1:77:B:GLU:HG2	1:78:B:LYS:H	7	0.15
(1,1343)	1:73:B:LYS:HG2	1:74:B:LEU:H	18	0.15
(1,1329)	1:72:B:LEU:H	1:73:B:LYS:HE2	11	0.15
(1,1317)	1:67:B:MET:HB2	1:68:B:ILE:HB	18	0.15
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD11	7	0.15
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD12	7	0.15
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD13	7	0.15
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	10	0.15
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	11	0.15
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	20	0.15
(1,1253)	1:38:A:LYS:HB3	1:39:A:TYR:H	15	0.15
(1,1253)	1:38:A:LYS:HB3	1:39:A:TYR:H	20	0.15
(1,1246)	1:37:A:ASN:HD21	1:38:A:LYS:H	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1228)	1:35:A:GLU:H	1:36:A:LYS:HD2	3	0.15
(1,1228)	1:35:A:GLU:H	1:36:A:LYS:HD2	5	0.15
(1,1221)	1:31:A:ILE:HG21	1:32:A:ASN:HD21	4	0.15
(1,1221)	1:31:A:ILE:HG22	1:32:A:ASN:HD21	4	0.15
(1,1221)	1:31:A:ILE:HG23	1:32:A:ASN:HD21	4	0.15
(1,1150)	1:12:A:LYS:HE3	1:13:A:LYS:H	5	0.15
(1,1147)	1:12:A:LYS:HD2	1:13:A:LYS:HE2	5	0.15
(1,1147)	1:12:A:LYS:HD2	1:13:A:LYS:HE2	18	0.15
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD11	10	0.15
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD12	10	0.15
(1,1121)	1:8:A:LEU:HB3	1:9:A:ILE:HD13	10	0.15
(1,1112)	1:7:A:LYS:HG2	1:8:A:LEU:HA	17	0.15
(1,1098)	1:6:A:LEU:H	1:7:A:LYS:HE3	7	0.15
(1,1098)	1:6:A:LEU:H	1:7:A:LYS:HE3	17	0.15
(1,1055)	1:90:B:LEU:HG	1:92:B:VAL:HG11	5	0.15
(1,1055)	1:90:B:LEU:HG	1:92:B:VAL:HG12	5	0.15
(1,1055)	1:90:B:LEU:HG	1:92:B:VAL:HG13	5	0.15
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD11	4	0.15
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD12	4	0.15
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD13	4	0.15
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD11	20	0.15
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD12	20	0.15
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD13	20	0.15
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD11	20	0.15
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD12	20	0.15
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD13	20	0.15
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD11	20	0.15
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD12	20	0.15
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD13	20	0.15
(1,962)	1:13:A:LYS:H	1:15:A:ILE:HD11	9	0.15
(1,962)	1:13:A:LYS:H	1:15:A:ILE:HD12	9	0.15
(1,962)	1:13:A:LYS:H	1:15:A:ILE:HD13	9	0.15
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD11	4	0.15
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD12	4	0.15
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD13	4	0.15
(1,942)	1:123:B:LEU:HD11	1:126:B:ILE:H	11	0.15
(1,942)	1:123:B:LEU:HD12	1:126:B:ILE:H	11	0.15
(1,942)	1:123:B:LEU:HD13	1:126:B:ILE:H	11	0.15
(1,891)	1:83:B:GLN:HE21	1:86:B:LEU:HD21	7	0.15
(1,891)	1:83:B:GLN:HE21	1:86:B:LEU:HD22	7	0.15
(1,891)	1:83:B:GLN:HE21	1:86:B:LEU:HD23	7	0.15
(1,848)	1:57:A:LEU:HD11	1:60:A:ILE:H	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:57:A:LEU:HD12	1:60:A:ILE:H	7	0.15
(1,848)	1:57:A:LEU:HD13	1:60:A:ILE:H	7	0.15
(1,780)	1:9:A:ILE:HA	1:12:A:LYS:HE3	13	0.15
(1,754)	1:123:B:LEU:HD11	1:127:B:PHE:HD1	5	0.15
(1,754)	1:123:B:LEU:HD12	1:127:B:PHE:HD1	5	0.15
(1,754)	1:123:B:LEU:HD13	1:127:B:PHE:HD1	5	0.15
(1,742)	1:110:B:GLN:HG3	1:114:B:LYS:HE3	6	0.15
(1,737)	1:110:B:GLN:HE21	1:114:B:LYS:HB2	2	0.15
(1,735)	1:110:B:GLN:HB2	1:114:B:LYS:HD2	15	0.15
(1,685)	1:76:B:ARG:HD3	1:80:B:LYS:HA	1	0.15
(1,679)	1:73:B:LYS:HG2	1:77:B:GLU:HG2	9	0.15
(1,639)	1:44:A:GLN:HB2	1:48:A:LYS:HD2	11	0.15
(1,639)	1:44:A:GLN:HB2	1:48:A:LYS:HD2	12	0.15
(1,637)	1:44:A:GLN:HA	1:48:A:LYS:HD2	9	0.15
(1,628)	1:34:A:ILE:HG21	1:38:A:LYS:HG3	11	0.15
(1,628)	1:34:A:ILE:HG22	1:38:A:LYS:HG3	11	0.15
(1,628)	1:34:A:ILE:HG23	1:38:A:LYS:HG3	11	0.15
(1,593)	1:15:A:ILE:HG13	1:19:A:GLU:HG2	14	0.15
(1,385)	1:20:A:LEU:HD21	1:28:A:ARG:HB2	19	0.15
(1,385)	1:20:A:LEU:HD22	1:28:A:ARG:HB2	19	0.15
(1,385)	1:20:A:LEU:HD23	1:28:A:ARG:HB2	19	0.15
(1,363)	1:76:B:ARG:HG2	1:86:B:LEU:HD11	2	0.15
(1,363)	1:76:B:ARG:HG2	1:86:B:LEU:HD12	2	0.15
(1,363)	1:76:B:ARG:HG2	1:86:B:LEU:HD13	2	0.15
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD21	19	0.15
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD22	19	0.15
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD23	19	0.15
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD21	19	0.15
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD22	19	0.15
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD23	19	0.15
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD21	19	0.15
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD22	19	0.15
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD23	19	0.15
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG21	5	0.15
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG22	5	0.15
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG23	5	0.15
(1,260)	1:107:B:PRO:HB3	1:127:B:PHE:HE1	16	0.15
(1,247)	1:25:A:GLU:HG3	1:48:A:LYS:HD3	2	0.15
(1,208)	1:73:B:LYS:HG2	1:101:B:GLU:HB2	6	0.15
(1,158)	1:68:B:ILE:HG21	1:106:B:ASN:HB2	1	0.15
(1,158)	1:68:B:ILE:HG22	1:106:B:ASN:HB2	1	0.15
(1,158)	1:68:B:ILE:HG23	1:106:B:ASN:HB2	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD21	9	0.15
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD22	9	0.15
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD23	9	0.15
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD21	16	0.15
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD22	16	0.15
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD23	16	0.15
(1,108)	1:75:B:ILE:HG21	1:121:B:THR:HG21	14	0.15
(1,108)	1:75:B:ILE:HG21	1:121:B:THR:HG22	14	0.15
(1,108)	1:75:B:ILE:HG21	1:121:B:THR:HG23	14	0.15
(1,108)	1:75:B:ILE:HG22	1:121:B:THR:HG21	14	0.15
(1,108)	1:75:B:ILE:HG22	1:121:B:THR:HG22	14	0.15
(1,108)	1:75:B:ILE:HG22	1:121:B:THR:HG23	14	0.15
(1,108)	1:75:B:ILE:HG23	1:121:B:THR:HG21	14	0.15
(1,108)	1:75:B:ILE:HG23	1:121:B:THR:HG22	14	0.15
(1,108)	1:75:B:ILE:HG23	1:121:B:THR:HG23	14	0.15
(1,86)	1:9:A:ILE:HG13	1:59:A:ASP:HB2	16	0.15
(1,84)	1:9:A:ILE:HG12	1:59:A:ASP:HB2	6	0.15
(1,48)	1:3:A:ILE:HD11	1:62:A:GLN:HG2	7	0.15
(1,48)	1:3:A:ILE:HD12	1:62:A:GLN:HG2	7	0.15
(1,48)	1:3:A:ILE:HD13	1:62:A:GLN:HG2	7	0.15
(1,2156)	1:63:A:TRP:HE1	1:114:B:LYS:HA	1	0.14
(1,2151)	1:46:A:ALA:HB1	1:109:B:LEU:HD21	13	0.14
(1,2151)	1:46:A:ALA:HB1	1:109:B:LEU:HD22	13	0.14
(1,2151)	1:46:A:ALA:HB1	1:109:B:LEU:HD23	13	0.14
(1,2151)	1:46:A:ALA:HB2	1:109:B:LEU:HD21	13	0.14
(1,2151)	1:46:A:ALA:HB2	1:109:B:LEU:HD22	13	0.14
(1,2151)	1:46:A:ALA:HB2	1:109:B:LEU:HD23	13	0.14
(1,2151)	1:46:A:ALA:HB3	1:109:B:LEU:HD21	13	0.14
(1,2151)	1:46:A:ALA:HB3	1:109:B:LEU:HD22	13	0.14
(1,2151)	1:46:A:ALA:HB3	1:109:B:LEU:HD23	13	0.14
(1,2125)	1:43:A:LEU:HD11	1:112:B:ALA:HB1	5	0.14
(1,2125)	1:43:A:LEU:HD11	1:112:B:ALA:HB2	5	0.14
(1,2125)	1:43:A:LEU:HD11	1:112:B:ALA:HB3	5	0.14
(1,2125)	1:43:A:LEU:HD12	1:112:B:ALA:HB1	5	0.14
(1,2125)	1:43:A:LEU:HD12	1:112:B:ALA:HB2	5	0.14
(1,2125)	1:43:A:LEU:HD12	1:112:B:ALA:HB3	5	0.14
(1,2125)	1:43:A:LEU:HD13	1:112:B:ALA:HB1	5	0.14
(1,2125)	1:43:A:LEU:HD13	1:112:B:ALA:HB2	5	0.14
(1,2125)	1:43:A:LEU:HD13	1:112:B:ALA:HB3	5	0.14
(1,2125)	1:43:A:LEU:HD21	1:112:B:ALA:HB1	5	0.14
(1,2125)	1:43:A:LEU:HD21	1:112:B:ALA:HB2	5	0.14
(1,2125)	1:43:A:LEU:HD21	1:112:B:ALA:HB3	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2125)	1:43:A:LEU:HD22	1:112:B:ALA:HB1	5	0.14
(1,2125)	1:43:A:LEU:HD22	1:112:B:ALA:HB2	5	0.14
(1,2125)	1:43:A:LEU:HD22	1:112:B:ALA:HB3	5	0.14
(1,2125)	1:43:A:LEU:HD23	1:112:B:ALA:HB1	5	0.14
(1,2125)	1:43:A:LEU:HD23	1:112:B:ALA:HB2	5	0.14
(1,2125)	1:43:A:LEU:HD23	1:112:B:ALA:HB3	5	0.14
(1,2110)	1:48:A:LYS:HA	1:129:B:TRP:HE1	14	0.14
(1,2093)	1:2:A:ILE:HG21	1:110:B:GLN:HB2	2	0.14
(1,2093)	1:2:A:ILE:HG22	1:110:B:GLN:HB2	2	0.14
(1,2093)	1:2:A:ILE:HG23	1:110:B:GLN:HB2	2	0.14
(1,2087)	1:2:A:ILE:HD11	1:110:B:GLN:H	1	0.14
(1,2087)	1:2:A:ILE:HD12	1:110:B:GLN:H	1	0.14
(1,2087)	1:2:A:ILE:HD13	1:110:B:GLN:H	1	0.14
(1,2068)	1:128:B:GLN:H	1:128:B:GLN:HE21	2	0.14
(1,1995)	1:102:B:LYS:H	1:102:B:LYS:HE3	7	0.14
(1,1995)	1:102:B:LYS:H	1:102:B:LYS:HE3	13	0.14
(1,1904)	1:80:B:LYS:HB2	1:80:B:LYS:HE2	14	0.14
(1,1899)	1:80:B:LYS:HA	1:80:B:LYS:HE2	2	0.14
(1,1872)	1:78:B:LYS:H	1:78:B:LYS:HD2	3	0.14
(1,1730)	1:36:A:LYS:HA	1:36:A:LYS:HE2	14	0.14
(1,1698)	1:29:A:GLN:HB2	1:29:A:GLN:HE21	12	0.14
(1,1652)	1:17:A:GLN:HA	1:17:A:GLN:HE22	14	0.14
(1,1631)	1:14:A:LYS:HA	1:14:A:LYS:HE2	7	0.14
(1,1545)	1:128:B:GLN:HG2	1:129:B:TRP:H	12	0.14
(1,1504)	1:110:B:GLN:HE22	1:111:B:LEU:HD21	18	0.14
(1,1504)	1:110:B:GLN:HE22	1:111:B:LEU:HD22	18	0.14
(1,1504)	1:110:B:GLN:HE22	1:111:B:LEU:HD23	18	0.14
(1,1472)	1:102:B:LYS:HB3	1:103:B:ASN:HB3	16	0.14
(1,1440)	1:95:B:GLN:HE21	1:96:B:THR:H	6	0.14
(1,1397)	1:80:B:LYS:HG2	1:81:B:ILE:HD11	3	0.14
(1,1397)	1:80:B:LYS:HG2	1:81:B:ILE:HD12	3	0.14
(1,1397)	1:80:B:LYS:HG2	1:81:B:ILE:HD13	3	0.14
(1,1330)	1:72:B:LEU:H	1:73:B:LYS:HE3	17	0.14
(1,1330)	1:72:B:LEU:H	1:73:B:LYS:HE3	20	0.14
(1,1329)	1:72:B:LEU:H	1:73:B:LYS:HE2	9	0.14
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD11	10	0.14
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD12	10	0.14
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD13	10	0.14
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD11	18	0.14
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD12	18	0.14
(1,1308)	1:59:A:ASP:HB2	1:60:A:ILE:HD13	18	0.14
(1,1300)	1:53:A:LEU:HD21	1:54:A:ASN:HB2	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1300)	1:53:A:LEU:HD22	1:54:A:ASN:HB2	4	0.14
(1,1300)	1:53:A:LEU:HD23	1:54:A:ASN:HB2	4	0.14
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD21	1	0.14
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD22	1	0.14
(1,1272)	1:44:A:GLN:HE22	1:45:A:LEU:HD23	1	0.14
(1,1260)	1:38:A:LYS:HG3	1:39:A:TYR:H	2	0.14
(1,1255)	1:38:A:LYS:HD2	1:39:A:TYR:HD2	16	0.14
(1,1248)	1:37:A:ASN:HD21	1:38:A:LYS:HD3	16	0.14
(1,1228)	1:35:A:GLU:H	1:36:A:LYS:HD2	17	0.14
(1,1221)	1:31:A:ILE:HG21	1:32:A:ASN:HD21	9	0.14
(1,1221)	1:31:A:ILE:HG22	1:32:A:ASN:HD21	9	0.14
(1,1221)	1:31:A:ILE:HG23	1:32:A:ASN:HD21	9	0.14
(1,1134)	1:10:A:ARG:HD2	1:11:A:GLU:HA	14	0.14
(1,1097)	1:6:A:LEU:H	1:7:A:LYS:HE2	14	0.14
(1,1097)	1:6:A:LEU:H	1:7:A:LYS:HE2	18	0.14
(1,1088)	1:1:A:MET:HG2	1:2:A:ILE:HB	9	0.14
(1,1074)	1:121:B:THR:HG21	1:123:B:LEU:HD21	19	0.14
(1,1074)	1:121:B:THR:HG21	1:123:B:LEU:HD22	19	0.14
(1,1074)	1:121:B:THR:HG21	1:123:B:LEU:HD23	19	0.14
(1,1074)	1:121:B:THR:HG22	1:123:B:LEU:HD21	19	0.14
(1,1074)	1:121:B:THR:HG22	1:123:B:LEU:HD22	19	0.14
(1,1074)	1:121:B:THR:HG22	1:123:B:LEU:HD23	19	0.14
(1,1074)	1:121:B:THR:HG23	1:123:B:LEU:HD21	19	0.14
(1,1074)	1:121:B:THR:HG23	1:123:B:LEU:HD22	19	0.14
(1,1074)	1:121:B:THR:HG23	1:123:B:LEU:HD23	19	0.14
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD11	3	0.14
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD12	3	0.14
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD13	3	0.14
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD11	3	0.14
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD12	3	0.14
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD13	3	0.14
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD11	3	0.14
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD12	3	0.14
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD13	3	0.14
(1,1055)	1:90:B:LEU:HG	1:92:B:VAL:HG11	3	0.14
(1,1055)	1:90:B:LEU:HG	1:92:B:VAL:HG12	3	0.14
(1,1055)	1:90:B:LEU:HG	1:92:B:VAL:HG13	3	0.14
(1,1049)	1:86:B:LEU:HD21	1:88:B:ALA:H	6	0.14
(1,1049)	1:86:B:LEU:HD22	1:88:B:ALA:H	6	0.14
(1,1049)	1:86:B:LEU:HD23	1:88:B:ALA:H	6	0.14
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG21	19	0.14
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG22	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG23	19	0.14
(1,1042)	1:79:B:LYS:HG3	1:81:B:ILE:HA	15	0.14
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD11	10	0.14
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD12	10	0.14
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD13	10	0.14
(1,1012)	1:62:A:GLN:HG3	1:64:A:GLN:H	1	0.14
(1,971)	1:13:A:LYS:HG3	1:15:A:ILE:HA	1	0.14
(1,971)	1:13:A:LYS:HG3	1:15:A:ILE:HA	11	0.14
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD11	7	0.14
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD12	7	0.14
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD13	7	0.14
(1,958)	1:6:A:LEU:HA	1:8:A:LEU:HD21	11	0.14
(1,958)	1:6:A:LEU:HA	1:8:A:LEU:HD22	11	0.14
(1,958)	1:6:A:LEU:HA	1:8:A:LEU:HD23	11	0.14
(1,913)	1:95:B:GLN:HB3	1:98:B:ASN:HD22	1	0.14
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	9	0.14
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	9	0.14
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	9	0.14
(1,864)	1:72:B:LEU:HD21	1:75:B:ILE:HB	3	0.14
(1,864)	1:72:B:LEU:HD22	1:75:B:ILE:HB	3	0.14
(1,864)	1:72:B:LEU:HD23	1:75:B:ILE:HB	3	0.14
(1,848)	1:57:A:LEU:HD11	1:60:A:ILE:H	1	0.14
(1,848)	1:57:A:LEU:HD12	1:60:A:ILE:H	1	0.14
(1,848)	1:57:A:LEU:HD13	1:60:A:ILE:H	1	0.14
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD21	20	0.14
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD22	20	0.14
(1,806)	1:21:A:ALA:H	1:24:A:LEU:HD23	20	0.14
(1,804)	1:20:A:LEU:HA	1:23:A:LEU:HD21	14	0.14
(1,804)	1:20:A:LEU:HA	1:23:A:LEU:HD22	14	0.14
(1,804)	1:20:A:LEU:HA	1:23:A:LEU:HD23	14	0.14
(1,797)	1:17:A:GLN:HE21	1:20:A:LEU:HD21	12	0.14
(1,797)	1:17:A:GLN:HE21	1:20:A:LEU:HD22	12	0.14
(1,797)	1:17:A:GLN:HE21	1:20:A:LEU:HD23	12	0.14
(1,780)	1:9:A:ILE:HA	1:12:A:LYS:HE3	17	0.14
(1,776)	1:8:A:LEU:HD11	1:11:A:GLU:HG2	11	0.14
(1,776)	1:8:A:LEU:HD12	1:11:A:GLU:HG2	11	0.14
(1,776)	1:8:A:LEU:HD13	1:11:A:GLU:HG2	11	0.14
(1,737)	1:110:B:GLN:HE21	1:114:B:LYS:HB2	18	0.14
(1,641)	1:44:A:GLN:HE21	1:48:A:LYS:HB2	5	0.14
(1,637)	1:44:A:GLN:HA	1:48:A:LYS:HD2	11	0.14
(1,583)	1:7:A:LYS:HG2	1:11:A:GLU:HG2	9	0.14
(1,557)	1:116:B:ALA:HA	1:121:B:THR:HG21	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:116:B:ALA:HA	1:121:B:THR:HG22	1	0.14
(1,557)	1:116:B:ALA:HA	1:121:B:THR:HG23	1	0.14
(1,553)	1:107:B:PRO:HG2	1:112:B:ALA:H	8	0.14
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG21	16	0.14
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG22	16	0.14
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG23	16	0.14
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG21	7	0.14
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG22	7	0.14
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG23	7	0.14
(1,455)	1:116:B:ALA:HB1	1:123:B:LEU:HD21	11	0.14
(1,455)	1:116:B:ALA:HB1	1:123:B:LEU:HD22	11	0.14
(1,455)	1:116:B:ALA:HB1	1:123:B:LEU:HD23	11	0.14
(1,455)	1:116:B:ALA:HB2	1:123:B:LEU:HD21	11	0.14
(1,455)	1:116:B:ALA:HB2	1:123:B:LEU:HD22	11	0.14
(1,455)	1:116:B:ALA:HB2	1:123:B:LEU:HD23	11	0.14
(1,455)	1:116:B:ALA:HB3	1:123:B:LEU:HD21	11	0.14
(1,455)	1:116:B:ALA:HB3	1:123:B:LEU:HD22	11	0.14
(1,455)	1:116:B:ALA:HB3	1:123:B:LEU:HD23	11	0.14
(1,425)	1:50:A:ALA:HB1	1:57:A:LEU:HD21	11	0.14
(1,425)	1:50:A:ALA:HB1	1:57:A:LEU:HD22	11	0.14
(1,425)	1:50:A:ALA:HB1	1:57:A:LEU:HD23	11	0.14
(1,425)	1:50:A:ALA:HB2	1:57:A:LEU:HD21	11	0.14
(1,425)	1:50:A:ALA:HB2	1:57:A:LEU:HD22	11	0.14
(1,425)	1:50:A:ALA:HB2	1:57:A:LEU:HD23	11	0.14
(1,425)	1:50:A:ALA:HB3	1:57:A:LEU:HD21	11	0.14
(1,425)	1:50:A:ALA:HB3	1:57:A:LEU:HD22	11	0.14
(1,425)	1:50:A:ALA:HB3	1:57:A:LEU:HD23	11	0.14
(1,385)	1:20:A:LEU:HD21	1:28:A:ARG:HB2	14	0.14
(1,385)	1:20:A:LEU:HD22	1:28:A:ARG:HB2	14	0.14
(1,385)	1:20:A:LEU:HD23	1:28:A:ARG:HB2	14	0.14
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD21	11	0.14
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD22	11	0.14
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD23	11	0.14
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD21	11	0.14
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD22	11	0.14
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD23	11	0.14
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD21	11	0.14
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD22	11	0.14
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD23	11	0.14
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG21	11	0.14
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG22	11	0.14
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG23	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG21	10	0.14
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG22	10	0.14
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG23	10	0.14
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG21	12	0.14
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG22	12	0.14
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG23	12	0.14
(1,198)	1:7:A:LYS:HE2	1:35:A:GLU:HG2	9	0.14
(1,198)	1:7:A:LYS:HE2	1:35:A:GLU:HG2	11	0.14
(1,172)	1:71:B:ASN:HA	1:101:B:GLU:HB3	17	0.14
(1,172)	1:71:B:ASN:HA	1:101:B:GLU:HB3	20	0.14
(1,171)	1:71:B:ASN:HA	1:101:B:GLU:HB2	18	0.14
(1,170)	1:71:B:ASN:HA	1:101:B:GLU:HA	15	0.14
(1,166)	1:5:A:ASN:HA	1:35:A:GLU:HB2	12	0.14
(1,165)	1:5:A:ASN:HA	1:35:A:GLU:HA	13	0.14
(1,165)	1:5:A:ASN:HA	1:35:A:GLU:HA	18	0.14
(1,159)	1:68:B:ILE:HG21	1:106:B:ASN:HD21	6	0.14
(1,159)	1:68:B:ILE:HG22	1:106:B:ASN:HD21	6	0.14
(1,159)	1:68:B:ILE:HG23	1:106:B:ASN:HD21	6	0.14
(1,104)	1:9:A:ILE:HG21	1:55:A:THR:HG21	18	0.14
(1,104)	1:9:A:ILE:HG21	1:55:A:THR:HG22	18	0.14
(1,104)	1:9:A:ILE:HG21	1:55:A:THR:HG23	18	0.14
(1,104)	1:9:A:ILE:HG22	1:55:A:THR:HG21	18	0.14
(1,104)	1:9:A:ILE:HG22	1:55:A:THR:HG22	18	0.14
(1,104)	1:9:A:ILE:HG22	1:55:A:THR:HG23	18	0.14
(1,104)	1:9:A:ILE:HG23	1:55:A:THR:HG21	18	0.14
(1,104)	1:9:A:ILE:HG23	1:55:A:THR:HG22	18	0.14
(1,104)	1:9:A:ILE:HG23	1:55:A:THR:HG23	18	0.14
(1,84)	1:9:A:ILE:HG12	1:59:A:ASP:HB2	9	0.14
(1,66)	1:5:A:ASN:HD22	1:62:A:GLN:HG2	1	0.14
(1,2177)	1:44:A:GLN:HB2	1:68:B:ILE:HG21	5	0.13
(1,2177)	1:44:A:GLN:HB2	1:68:B:ILE:HG22	5	0.13
(1,2177)	1:44:A:GLN:HB2	1:68:B:ILE:HG23	5	0.13
(1,2170)	1:43:A:LEU:HD21	1:68:B:ILE:HG21	10	0.13
(1,2170)	1:43:A:LEU:HD21	1:68:B:ILE:HG22	10	0.13
(1,2170)	1:43:A:LEU:HD21	1:68:B:ILE:HG23	10	0.13
(1,2170)	1:43:A:LEU:HD22	1:68:B:ILE:HG21	10	0.13
(1,2170)	1:43:A:LEU:HD22	1:68:B:ILE:HG22	10	0.13
(1,2170)	1:43:A:LEU:HD22	1:68:B:ILE:HG23	10	0.13
(1,2170)	1:43:A:LEU:HD23	1:68:B:ILE:HG21	10	0.13
(1,2170)	1:43:A:LEU:HD23	1:68:B:ILE:HG22	10	0.13
(1,2170)	1:43:A:LEU:HD23	1:68:B:ILE:HG23	10	0.13
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD11	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD12	20	0.13
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD13	20	0.13
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD21	20	0.13
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD22	20	0.13
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD23	20	0.13
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD11	20	0.13
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD12	20	0.13
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD13	20	0.13
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD21	20	0.13
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD22	20	0.13
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD23	20	0.13
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD11	20	0.13
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD12	20	0.13
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD13	20	0.13
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD21	20	0.13
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD22	20	0.13
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD23	20	0.13
(1,2125)	1:43:A:LEU:HD11	1:112:B:ALA:HB1	6	0.13
(1,2125)	1:43:A:LEU:HD11	1:112:B:ALA:HB2	6	0.13
(1,2125)	1:43:A:LEU:HD11	1:112:B:ALA:HB3	6	0.13
(1,2125)	1:43:A:LEU:HD12	1:112:B:ALA:HB1	6	0.13
(1,2125)	1:43:A:LEU:HD12	1:112:B:ALA:HB2	6	0.13
(1,2125)	1:43:A:LEU:HD12	1:112:B:ALA:HB3	6	0.13
(1,2125)	1:43:A:LEU:HD13	1:112:B:ALA:HB1	6	0.13
(1,2125)	1:43:A:LEU:HD13	1:112:B:ALA:HB2	6	0.13
(1,2125)	1:43:A:LEU:HD13	1:112:B:ALA:HB3	6	0.13
(1,2125)	1:43:A:LEU:HD21	1:112:B:ALA:HB1	6	0.13
(1,2125)	1:43:A:LEU:HD21	1:112:B:ALA:HB2	6	0.13
(1,2125)	1:43:A:LEU:HD21	1:112:B:ALA:HB3	6	0.13
(1,2125)	1:43:A:LEU:HD22	1:112:B:ALA:HB1	6	0.13
(1,2125)	1:43:A:LEU:HD22	1:112:B:ALA:HB2	6	0.13
(1,2125)	1:43:A:LEU:HD22	1:112:B:ALA:HB3	6	0.13
(1,2125)	1:43:A:LEU:HD23	1:112:B:ALA:HB1	6	0.13
(1,2125)	1:43:A:LEU:HD23	1:112:B:ALA:HB2	6	0.13
(1,2125)	1:43:A:LEU:HD23	1:112:B:ALA:HB3	6	0.13
(1,2112)	1:47:A:LEU:HD21	1:123:B:LEU:HD11	20	0.13
(1,2112)	1:47:A:LEU:HD21	1:123:B:LEU:HD12	20	0.13
(1,2112)	1:47:A:LEU:HD21	1:123:B:LEU:HD13	20	0.13
(1,2112)	1:47:A:LEU:HD22	1:123:B:LEU:HD11	20	0.13
(1,2112)	1:47:A:LEU:HD22	1:123:B:LEU:HD12	20	0.13
(1,2112)	1:47:A:LEU:HD22	1:123:B:LEU:HD13	20	0.13
(1,2112)	1:47:A:LEU:HD23	1:123:B:LEU:HD11	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2112)	1:47:A:LEU:HD23	1:123:B:LEU:HD12	20	0.13
(1,2112)	1:47:A:LEU:HD23	1:123:B:LEU:HD13	20	0.13
(1,2111)	1:48:A:LYS:HG3	1:129:B:TRP:HE1	16	0.13
(1,2103)	1:44:A:GLN:HG2	1:130:B:GLN:H	20	0.13
(1,2087)	1:2:A:ILE:HD11	1:110:B:GLN:H	2	0.13
(1,2087)	1:2:A:ILE:HD12	1:110:B:GLN:H	2	0.13
(1,2087)	1:2:A:ILE:HD13	1:110:B:GLN:H	2	0.13
(1,2069)	1:128:B:GLN:H	1:128:B:GLN:HG2	6	0.13
(1,1998)	1:102:B:LYS:HA	1:102:B:LYS:HE2	1	0.13
(1,1998)	1:102:B:LYS:HA	1:102:B:LYS:HE2	5	0.13
(1,1921)	1:83:B:GLN:HB2	1:83:B:GLN:HE21	5	0.13
(1,1921)	1:83:B:GLN:HB2	1:83:B:GLN:HE21	6	0.13
(1,1919)	1:83:B:GLN:H	1:83:B:GLN:HE21	8	0.13
(1,1904)	1:80:B:LYS:HB2	1:80:B:LYS:HE2	2	0.13
(1,1904)	1:80:B:LYS:HB2	1:80:B:LYS:HE2	12	0.13
(1,1899)	1:80:B:LYS:HA	1:80:B:LYS:HE2	20	0.13
(1,1890)	1:79:B:LYS:HA	1:79:B:LYS:HE2	19	0.13
(1,1872)	1:78:B:LYS:H	1:78:B:LYS:HD2	10	0.13
(1,1798)	1:60:A:ILE:H	1:60:A:ILE:HG21	14	0.13
(1,1798)	1:60:A:ILE:H	1:60:A:ILE:HG22	14	0.13
(1,1798)	1:60:A:ILE:H	1:60:A:ILE:HG23	14	0.13
(1,1730)	1:36:A:LYS:HA	1:36:A:LYS:HE2	8	0.13
(1,1693)	1:29:A:GLN:H	1:29:A:GLN:HE22	16	0.13
(1,1636)	1:14:A:LYS:HB2	1:14:A:LYS:HE2	4	0.13
(1,1631)	1:14:A:LYS:HA	1:14:A:LYS:HE2	17	0.13
(1,1537)	1:120:B:ASN:HD21	1:121:B:THR:H	2	0.13
(1,1453)	1:97:B:ILE:HG21	1:98:B:ASN:HD21	2	0.13
(1,1453)	1:97:B:ILE:HG22	1:98:B:ASN:HD21	2	0.13
(1,1453)	1:97:B:ILE:HG23	1:98:B:ASN:HD21	2	0.13
(1,1442)	1:95:B:GLN:HG2	1:96:B:THR:HG21	19	0.13
(1,1442)	1:95:B:GLN:HG2	1:96:B:THR:HG22	19	0.13
(1,1442)	1:95:B:GLN:HG2	1:96:B:THR:HG23	19	0.13
(1,1404)	1:84:B:SER:H	1:85:B:GLU:HB3	20	0.13
(1,1396)	1:80:B:LYS:HD2	1:81:B:ILE:H	8	0.13
(1,1260)	1:38:A:LYS:HG3	1:39:A:TYR:H	4	0.13
(1,1260)	1:38:A:LYS:HG3	1:39:A:TYR:H	7	0.13
(1,1246)	1:37:A:ASN:HD21	1:38:A:LYS:H	20	0.13
(1,1211)	1:29:A:GLN:HG3	1:30:A:THR:H	10	0.13
(1,1210)	1:29:A:GLN:HG2	1:30:A:THR:HG21	7	0.13
(1,1210)	1:29:A:GLN:HG2	1:30:A:THR:HG22	7	0.13
(1,1210)	1:29:A:GLN:HG2	1:30:A:THR:HG23	7	0.13
(1,1156)	1:13:A:LYS:HB2	1:14:A:LYS:HG2	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1156)	1:13:A:LYS:HB2	1:14:A:LYS:HG2	18	0.13
(1,1149)	1:12:A:LYS:HD3	1:13:A:LYS:HA	1	0.13
(1,1147)	1:12:A:LYS:HD2	1:13:A:LYS:HE2	4	0.13
(1,1139)	1:11:A:GLU:HG2	1:12:A:LYS:H	7	0.13
(1,1111)	1:7:A:LYS:HG2	1:8:A:LEU:H	7	0.13
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD11	3	0.13
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD12	3	0.13
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD13	3	0.13
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD11	18	0.13
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD12	18	0.13
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD13	18	0.13
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD11	18	0.13
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD12	18	0.13
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD13	18	0.13
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD11	18	0.13
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD12	18	0.13
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD13	18	0.13
(1,1072)	1:119:B:LEU:HD11	1:121:B:THR:HG21	4	0.13
(1,1072)	1:119:B:LEU:HD11	1:121:B:THR:HG22	4	0.13
(1,1072)	1:119:B:LEU:HD11	1:121:B:THR:HG23	4	0.13
(1,1072)	1:119:B:LEU:HD12	1:121:B:THR:HG21	4	0.13
(1,1072)	1:119:B:LEU:HD12	1:121:B:THR:HG22	4	0.13
(1,1072)	1:119:B:LEU:HD12	1:121:B:THR:HG23	4	0.13
(1,1072)	1:119:B:LEU:HD13	1:121:B:THR:HG21	4	0.13
(1,1072)	1:119:B:LEU:HD13	1:121:B:THR:HG22	4	0.13
(1,1072)	1:119:B:LEU:HD13	1:121:B:THR:HG23	4	0.13
(1,1049)	1:86:B:LEU:HD21	1:88:B:ALA:H	8	0.13
(1,1049)	1:86:B:LEU:HD22	1:88:B:ALA:H	8	0.13
(1,1049)	1:86:B:LEU:HD23	1:88:B:ALA:H	8	0.13
(1,1042)	1:79:B:LYS:HG3	1:81:B:ILE:HA	1	0.13
(1,1042)	1:79:B:LYS:HG3	1:81:B:ILE:HA	2	0.13
(1,1040)	1:79:B:LYS:HD3	1:81:B:ILE:HG13	11	0.13
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD11	7	0.13
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD12	7	0.13
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD13	7	0.13
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD11	14	0.13
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD12	14	0.13
(1,1031)	1:73:B:LYS:HG2	1:75:B:ILE:HD13	14	0.13
(1,1014)	1:64:A:GLN:HB2	1:66:A:GLU:H	6	0.13
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD11	6	0.13
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD12	6	0.13
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD13	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD11	6	0.13
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD12	6	0.13
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD13	6	0.13
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD11	6	0.13
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD12	6	0.13
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD13	6	0.13
(1,981)	1:21:A:ALA:HA	1:23:A:LEU:HG	19	0.13
(1,971)	1:13:A:LYS:HG3	1:15:A:ILE:HA	13	0.13
(1,948)	1:2:A:ILE:HG21	1:4:A:ASN:HD22	13	0.13
(1,948)	1:2:A:ILE:HG22	1:4:A:ASN:HD22	13	0.13
(1,948)	1:2:A:ILE:HG23	1:4:A:ASN:HD22	13	0.13
(1,942)	1:123:B:LEU:HD11	1:126:B:ILE:H	9	0.13
(1,942)	1:123:B:LEU:HD12	1:126:B:ILE:H	9	0.13
(1,942)	1:123:B:LEU:HD13	1:126:B:ILE:H	9	0.13
(1,922)	1:99:B:GLY:H	1:102:B:LYS:HB2	7	0.13
(1,770)	1:6:A:LEU:HD21	1:9:A:ILE:HB	3	0.13
(1,770)	1:6:A:LEU:HD22	1:9:A:ILE:HB	3	0.13
(1,770)	1:6:A:LEU:HD23	1:9:A:ILE:HB	3	0.13
(1,770)	1:6:A:LEU:HD21	1:9:A:ILE:HB	18	0.13
(1,770)	1:6:A:LEU:HD22	1:9:A:ILE:HB	18	0.13
(1,770)	1:6:A:LEU:HD23	1:9:A:ILE:HB	18	0.13
(1,740)	1:110:B:GLN:HG2	1:114:B:LYS:HE2	17	0.13
(1,733)	1:110:B:GLN:HA	1:114:B:LYS:HD2	12	0.13
(1,732)	1:109:B:LEU:HD11	1:113:B:LEU:HD21	8	0.13
(1,732)	1:109:B:LEU:HD11	1:113:B:LEU:HD22	8	0.13
(1,732)	1:109:B:LEU:HD11	1:113:B:LEU:HD23	8	0.13
(1,732)	1:109:B:LEU:HD12	1:113:B:LEU:HD21	8	0.13
(1,732)	1:109:B:LEU:HD12	1:113:B:LEU:HD22	8	0.13
(1,732)	1:109:B:LEU:HD12	1:113:B:LEU:HD23	8	0.13
(1,732)	1:109:B:LEU:HD13	1:113:B:LEU:HD21	8	0.13
(1,732)	1:109:B:LEU:HD13	1:113:B:LEU:HD22	8	0.13
(1,732)	1:109:B:LEU:HD13	1:113:B:LEU:HD23	8	0.13
(1,732)	1:109:B:LEU:HD21	1:113:B:LEU:HD21	8	0.13
(1,732)	1:109:B:LEU:HD21	1:113:B:LEU:HD22	8	0.13
(1,732)	1:109:B:LEU:HD21	1:113:B:LEU:HD23	8	0.13
(1,732)	1:109:B:LEU:HD22	1:113:B:LEU:HD21	8	0.13
(1,732)	1:109:B:LEU:HD22	1:113:B:LEU:HD22	8	0.13
(1,732)	1:109:B:LEU:HD22	1:113:B:LEU:HD23	8	0.13
(1,732)	1:109:B:LEU:HD23	1:113:B:LEU:HD21	8	0.13
(1,732)	1:109:B:LEU:HD23	1:113:B:LEU:HD22	8	0.13
(1,732)	1:109:B:LEU:HD23	1:113:B:LEU:HD23	8	0.13
(1,679)	1:73:B:LYS:HG2	1:77:B:GLU:HG2	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,675)	1:72:B:LEU:HD21	1:76:B:ARG:HD2	5	0.13
(1,675)	1:72:B:LEU:HD22	1:76:B:ARG:HD2	5	0.13
(1,675)	1:72:B:LEU:HD23	1:76:B:ARG:HD2	5	0.13
(1,675)	1:72:B:LEU:HD21	1:76:B:ARG:HD2	6	0.13
(1,675)	1:72:B:LEU:HD22	1:76:B:ARG:HD2	6	0.13
(1,675)	1:72:B:LEU:HD23	1:76:B:ARG:HD2	6	0.13
(1,641)	1:44:A:GLN:HE21	1:48:A:LYS:HB2	10	0.13
(1,636)	1:43:A:LEU:HD11	1:47:A:LEU:HD21	3	0.13
(1,636)	1:43:A:LEU:HD11	1:47:A:LEU:HD22	3	0.13
(1,636)	1:43:A:LEU:HD11	1:47:A:LEU:HD23	3	0.13
(1,636)	1:43:A:LEU:HD12	1:47:A:LEU:HD21	3	0.13
(1,636)	1:43:A:LEU:HD12	1:47:A:LEU:HD22	3	0.13
(1,636)	1:43:A:LEU:HD12	1:47:A:LEU:HD23	3	0.13
(1,636)	1:43:A:LEU:HD13	1:47:A:LEU:HD21	3	0.13
(1,636)	1:43:A:LEU:HD13	1:47:A:LEU:HD22	3	0.13
(1,636)	1:43:A:LEU:HD13	1:47:A:LEU:HD23	3	0.13
(1,636)	1:43:A:LEU:HD21	1:47:A:LEU:HD21	3	0.13
(1,636)	1:43:A:LEU:HD21	1:47:A:LEU:HD22	3	0.13
(1,636)	1:43:A:LEU:HD21	1:47:A:LEU:HD23	3	0.13
(1,636)	1:43:A:LEU:HD22	1:47:A:LEU:HD21	3	0.13
(1,636)	1:43:A:LEU:HD22	1:47:A:LEU:HD22	3	0.13
(1,636)	1:43:A:LEU:HD22	1:47:A:LEU:HD23	3	0.13
(1,636)	1:43:A:LEU:HD23	1:47:A:LEU:HD21	3	0.13
(1,636)	1:43:A:LEU:HD23	1:47:A:LEU:HD22	3	0.13
(1,636)	1:43:A:LEU:HD23	1:47:A:LEU:HD23	3	0.13
(1,593)	1:15:A:ILE:HG13	1:19:A:GLU:HG2	4	0.13
(1,593)	1:15:A:ILE:HG13	1:19:A:GLU:HG2	6	0.13
(1,593)	1:15:A:ILE:HG13	1:19:A:GLU:HG2	15	0.13
(1,583)	1:7:A:LYS:HG2	1:11:A:GLU:HG2	10	0.13
(1,571)	1:6:A:LEU:HD11	1:10:A:ARG:HD2	18	0.13
(1,571)	1:6:A:LEU:HD12	1:10:A:ARG:HD2	18	0.13
(1,571)	1:6:A:LEU:HD13	1:10:A:ARG:HD2	18	0.13
(1,513)	1:50:A:ALA:HB1	1:55:A:THR:HG21	12	0.13
(1,513)	1:50:A:ALA:HB1	1:55:A:THR:HG22	12	0.13
(1,513)	1:50:A:ALA:HB1	1:55:A:THR:HG23	12	0.13
(1,513)	1:50:A:ALA:HB2	1:55:A:THR:HG21	12	0.13
(1,513)	1:50:A:ALA:HB2	1:55:A:THR:HG22	12	0.13
(1,513)	1:50:A:ALA:HB2	1:55:A:THR:HG23	12	0.13
(1,513)	1:50:A:ALA:HB3	1:55:A:THR:HG21	12	0.13
(1,513)	1:50:A:ALA:HB3	1:55:A:THR:HG22	12	0.13
(1,513)	1:50:A:ALA:HB3	1:55:A:THR:HG23	12	0.13
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG21	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG22	3	0.13
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG23	3	0.13
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG21	6	0.13
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG22	6	0.13
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG23	6	0.13
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG21	14	0.13
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG22	14	0.13
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG23	14	0.13
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	12	0.13
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	12	0.13
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	12	0.13
(1,385)	1:20:A:LEU:HD21	1:28:A:ARG:HB2	1	0.13
(1,385)	1:20:A:LEU:HD22	1:28:A:ARG:HB2	1	0.13
(1,385)	1:20:A:LEU:HD23	1:28:A:ARG:HB2	1	0.13
(1,239)	1:90:B:LEU:HD21	1:115:B:ILE:HA	11	0.13
(1,239)	1:90:B:LEU:HD22	1:115:B:ILE:HA	11	0.13
(1,239)	1:90:B:LEU:HD23	1:115:B:ILE:HA	11	0.13
(1,229)	1:24:A:LEU:HD21	1:49:A:ILE:HA	9	0.13
(1,229)	1:24:A:LEU:HD22	1:49:A:ILE:HA	9	0.13
(1,229)	1:24:A:LEU:HD23	1:49:A:ILE:HA	9	0.13
(1,208)	1:73:B:LYS:HG2	1:101:B:GLU:HB2	16	0.13
(1,198)	1:7:A:LYS:HE2	1:35:A:GLU:HG2	20	0.13
(1,190)	1:89:B:LEU:HD11	1:118:B:TYR:HE2	11	0.13
(1,190)	1:89:B:LEU:HD12	1:118:B:TYR:HE2	11	0.13
(1,190)	1:89:B:LEU:HD13	1:118:B:TYR:HE2	11	0.13
(1,186)	1:89:B:LEU:HG	1:118:B:TYR:HD2	8	0.13
(1,165)	1:5:A:ASN:HA	1:35:A:GLU:HA	1	0.13
(1,165)	1:5:A:ASN:HA	1:35:A:GLU:HA	9	0.13
(1,160)	1:81:B:ILE:H	1:119:B:LEU:HD21	8	0.13
(1,160)	1:81:B:ILE:H	1:119:B:LEU:HD22	8	0.13
(1,160)	1:81:B:ILE:H	1:119:B:LEU:HD23	8	0.13
(1,156)	1:68:B:ILE:HD11	1:106:B:ASN:HD21	3	0.13
(1,156)	1:68:B:ILE:HD12	1:106:B:ASN:HD21	3	0.13
(1,156)	1:68:B:ILE:HD13	1:106:B:ASN:HD21	3	0.13
(1,141)	1:2:A:ILE:HG21	1:41:A:PRO:HD2	18	0.13
(1,141)	1:2:A:ILE:HG22	1:41:A:PRO:HD2	18	0.13
(1,141)	1:2:A:ILE:HG23	1:41:A:PRO:HD2	18	0.13
(1,123)	1:13:A:LYS:HE2	1:54:A:ASN:HB2	16	0.13
(1,103)	1:9:A:ILE:HD11	1:55:A:THR:HG21	8	0.13
(1,103)	1:9:A:ILE:HD11	1:55:A:THR:HG22	8	0.13
(1,103)	1:9:A:ILE:HD11	1:55:A:THR:HG23	8	0.13
(1,103)	1:9:A:ILE:HD12	1:55:A:THR:HG21	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,103)	1:9:A:ILE:HD12	1:55:A:THR:HG22	8	0.13
(1,103)	1:9:A:ILE:HD12	1:55:A:THR:HG23	8	0.13
(1,103)	1:9:A:ILE:HD13	1:55:A:THR:HG21	8	0.13
(1,103)	1:9:A:ILE:HD13	1:55:A:THR:HG22	8	0.13
(1,103)	1:9:A:ILE:HD13	1:55:A:THR:HG23	8	0.13
(1,99)	1:75:B:ILE:HD11	1:125:B:ASP:HB3	17	0.13
(1,99)	1:75:B:ILE:HD12	1:125:B:ASP:HB3	17	0.13
(1,99)	1:75:B:ILE:HD13	1:125:B:ASP:HB3	17	0.13
(1,95)	1:75:B:ILE:HG13	1:125:B:ASP:HB2	16	0.13
(1,93)	1:75:B:ILE:HG12	1:125:B:ASP:HB2	4	0.13
(1,84)	1:9:A:ILE:HG12	1:59:A:ASP:HB2	2	0.13
(1,60)	1:69:B:ILE:HD11	1:128:B:GLN:HG2	18	0.13
(1,60)	1:69:B:ILE:HD12	1:128:B:GLN:HG2	18	0.13
(1,60)	1:69:B:ILE:HD13	1:128:B:GLN:HG2	18	0.13
(1,3)	1:2:A:ILE:HD11	1:64:A:GLN:HB2	18	0.13
(1,3)	1:2:A:ILE:HD12	1:64:A:GLN:HB2	18	0.13
(1,3)	1:2:A:ILE:HD13	1:64:A:GLN:HB2	18	0.13
(1,2150)	1:46:A:ALA:HB1	1:109:B:LEU:HD11	11	0.12
(1,2150)	1:46:A:ALA:HB1	1:109:B:LEU:HD12	11	0.12
(1,2150)	1:46:A:ALA:HB1	1:109:B:LEU:HD13	11	0.12
(1,2150)	1:46:A:ALA:HB2	1:109:B:LEU:HD11	11	0.12
(1,2150)	1:46:A:ALA:HB2	1:109:B:LEU:HD12	11	0.12
(1,2150)	1:46:A:ALA:HB2	1:109:B:LEU:HD13	11	0.12
(1,2150)	1:46:A:ALA:HB3	1:109:B:LEU:HD11	11	0.12
(1,2150)	1:46:A:ALA:HB3	1:109:B:LEU:HD12	11	0.12
(1,2150)	1:46:A:ALA:HB3	1:109:B:LEU:HD13	11	0.12
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD11	11	0.12
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD12	11	0.12
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD13	11	0.12
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD21	11	0.12
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD22	11	0.12
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD23	11	0.12
(1,2103)	1:44:A:GLN:HG2	1:130:B:GLN:H	5	0.12
(1,2103)	1:44:A:GLN:HG2	1:130:B:GLN:H	6	0.12
(1,2098)	1:2:A:ILE:HD11	1:109:B:LEU:HD11	18	0.12
(1,2098)	1:2:A:ILE:HD11	1:109:B:LEU:HD12	18	0.12
(1,2098)	1:2:A:ILE:HD11	1:109:B:LEU:HD13	18	0.12
(1,2098)	1:2:A:ILE:HD11	1:109:B:LEU:HD21	18	0.12
(1,2098)	1:2:A:ILE:HD11	1:109:B:LEU:HD22	18	0.12
(1,2098)	1:2:A:ILE:HD11	1:109:B:LEU:HD23	18	0.12
(1,2098)	1:2:A:ILE:HD12	1:109:B:LEU:HD11	18	0.12
(1,2098)	1:2:A:ILE:HD12	1:109:B:LEU:HD12	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2098)	1:2:A:ILE:HD12	1:109:B:LEU:HD13	18	0.12
(1,2098)	1:2:A:ILE:HD12	1:109:B:LEU:HD21	18	0.12
(1,2098)	1:2:A:ILE:HD12	1:109:B:LEU:HD22	18	0.12
(1,2098)	1:2:A:ILE:HD12	1:109:B:LEU:HD23	18	0.12
(1,2098)	1:2:A:ILE:HD13	1:109:B:LEU:HD11	18	0.12
(1,2098)	1:2:A:ILE:HD13	1:109:B:LEU:HD12	18	0.12
(1,2098)	1:2:A:ILE:HD13	1:109:B:LEU:HD13	18	0.12
(1,2098)	1:2:A:ILE:HD13	1:109:B:LEU:HD21	18	0.12
(1,2098)	1:2:A:ILE:HD13	1:109:B:LEU:HD22	18	0.12
(1,2098)	1:2:A:ILE:HD13	1:109:B:LEU:HD23	18	0.12
(1,2087)	1:2:A:ILE:HD11	1:110:B:GLN:H	9	0.12
(1,2087)	1:2:A:ILE:HD12	1:110:B:GLN:H	9	0.12
(1,2087)	1:2:A:ILE:HD13	1:110:B:GLN:H	9	0.12
(1,2085)	1:63:A:TRP:HE3	1:117:B:TYR:HD1	10	0.12
(1,2085)	1:63:A:TRP:HE3	1:117:B:TYR:HD2	10	0.12
(1,2084)	1:129:B:TRP:HZ2	1:44:A:GLN:HA	10	0.12
(1,2038)	1:111:B:LEU:HA	1:111:B:LEU:HD21	11	0.12
(1,2038)	1:111:B:LEU:HA	1:111:B:LEU:HD22	11	0.12
(1,2038)	1:111:B:LEU:HA	1:111:B:LEU:HD23	11	0.12
(1,1998)	1:102:B:LYS:HA	1:102:B:LYS:HE2	15	0.12
(1,1994)	1:102:B:LYS:H	1:102:B:LYS:HD2	13	0.12
(1,1922)	1:83:B:GLN:HB3	1:83:B:GLN:HE21	10	0.12
(1,1919)	1:83:B:GLN:H	1:83:B:GLN:HE21	4	0.12
(1,1919)	1:83:B:GLN:H	1:83:B:GLN:HE21	20	0.12
(1,1899)	1:80:B:LYS:HA	1:80:B:LYS:HE2	9	0.12
(1,1899)	1:80:B:LYS:HA	1:80:B:LYS:HE2	17	0.12
(1,1872)	1:78:B:LYS:H	1:78:B:LYS:HD2	5	0.12
(1,1770)	1:45:A:LEU:HA	1:45:A:LEU:HD21	15	0.12
(1,1770)	1:45:A:LEU:HA	1:45:A:LEU:HD22	15	0.12
(1,1770)	1:45:A:LEU:HA	1:45:A:LEU:HD23	15	0.12
(1,1730)	1:36:A:LYS:HA	1:36:A:LYS:HE2	10	0.12
(1,1730)	1:36:A:LYS:HA	1:36:A:LYS:HE2	19	0.12
(1,1729)	1:36:A:LYS:HA	1:36:A:LYS:HD2	20	0.12
(1,1727)	1:36:A:LYS:H	1:36:A:LYS:HE3	15	0.12
(1,1693)	1:29:A:GLN:H	1:29:A:GLN:HE22	19	0.12
(1,1650)	1:15:A:ILE:HG21	1:15:A:ILE:HD11	1	0.12
(1,1650)	1:15:A:ILE:HG21	1:15:A:ILE:HD12	1	0.12
(1,1650)	1:15:A:ILE:HG21	1:15:A:ILE:HD13	1	0.12
(1,1650)	1:15:A:ILE:HG22	1:15:A:ILE:HD11	1	0.12
(1,1650)	1:15:A:ILE:HG22	1:15:A:ILE:HD12	1	0.12
(1,1650)	1:15:A:ILE:HG22	1:15:A:ILE:HD13	1	0.12
(1,1650)	1:15:A:ILE:HG23	1:15:A:ILE:HD11	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1650)	1:15:A:ILE:HG23	1:15:A:ILE:HD12	1	0.12
(1,1650)	1:15:A:ILE:HG23	1:15:A:ILE:HD13	1	0.12
(1,1636)	1:14:A:LYS:HB2	1:14:A:LYS:HE2	9	0.12
(1,1636)	1:14:A:LYS:HB2	1:14:A:LYS:HE2	16	0.12
(1,1632)	1:14:A:LYS:HA	1:14:A:LYS:HE3	10	0.12
(1,1631)	1:14:A:LYS:HA	1:14:A:LYS:HE2	4	0.12
(1,1552)	1:2:A:ILE:HG21	1:2:A:ILE:HD11	18	0.12
(1,1552)	1:2:A:ILE:HG21	1:2:A:ILE:HD12	18	0.12
(1,1552)	1:2:A:ILE:HG21	1:2:A:ILE:HD13	18	0.12
(1,1552)	1:2:A:ILE:HG22	1:2:A:ILE:HD11	18	0.12
(1,1552)	1:2:A:ILE:HG22	1:2:A:ILE:HD12	18	0.12
(1,1552)	1:2:A:ILE:HG22	1:2:A:ILE:HD13	18	0.12
(1,1552)	1:2:A:ILE:HG23	1:2:A:ILE:HD11	18	0.12
(1,1552)	1:2:A:ILE:HG23	1:2:A:ILE:HD12	18	0.12
(1,1552)	1:2:A:ILE:HG23	1:2:A:ILE:HD13	18	0.12
(1,1545)	1:128:B:GLN:HG2	1:129:B:TRP:H	20	0.12
(1,1531)	1:119:B:LEU:HD11	1:120:B:ASN:HB2	14	0.12
(1,1531)	1:119:B:LEU:HD12	1:120:B:ASN:HB2	14	0.12
(1,1531)	1:119:B:LEU:HD13	1:120:B:ASN:HB2	14	0.12
(1,1492)	1:104:B:LYS:HG3	1:105:B:TYR:H	17	0.12
(1,1465)	1:101:B:GLU:HG2	1:102:B:LYS:HD2	12	0.12
(1,1404)	1:84:B:SER:H	1:85:B:GLU:HB3	8	0.12
(1,1404)	1:84:B:SER:H	1:85:B:GLU:HB3	14	0.12
(1,1396)	1:80:B:LYS:HD2	1:81:B:ILE:H	19	0.12
(1,1396)	1:80:B:LYS:HD2	1:81:B:ILE:H	20	0.12
(1,1366)	1:76:B:ARG:HD2	1:77:B:GLU:HA	12	0.12
(1,1362)	1:76:B:ARG:H	1:77:B:GLU:HG3	20	0.12
(1,1343)	1:73:B:LYS:HG2	1:74:B:LEU:H	7	0.12
(1,1330)	1:72:B:LEU:H	1:73:B:LYS:HE3	16	0.12
(1,1329)	1:72:B:LEU:H	1:73:B:LYS:HE2	5	0.12
(1,1329)	1:72:B:LEU:H	1:73:B:LYS:HE2	10	0.12
(1,1320)	1:67:B:MET:HG2	1:68:B:ILE:HB	6	0.12
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD11	2	0.12
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD12	2	0.12
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD13	2	0.12
(1,1313)	1:62:A:GLN:HG2	1:63:A:TRP:H	4	0.12
(1,1313)	1:62:A:GLN:HG2	1:63:A:TRP:H	19	0.12
(1,1305)	1:54:A:ASN:HD21	1:55:A:THR:H	18	0.12
(1,1286)	1:48:A:LYS:HB2	1:49:A:ILE:HG12	4	0.12
(1,1268)	1:43:A:LEU:HD11	1:44:A:GLN:HB2	10	0.12
(1,1268)	1:43:A:LEU:HD12	1:44:A:GLN:HB2	10	0.12
(1,1268)	1:43:A:LEU:HD13	1:44:A:GLN:HB2	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1268)	1:43:A:LEU:HD21	1:44:A:GLN:HB2	10	0.12
(1,1268)	1:43:A:LEU:HD22	1:44:A:GLN:HB2	10	0.12
(1,1268)	1:43:A:LEU:HD23	1:44:A:GLN:HB2	10	0.12
(1,1221)	1:31:A:ILE:HG21	1:32:A:ASN:HD21	15	0.12
(1,1221)	1:31:A:ILE:HG22	1:32:A:ASN:HD21	15	0.12
(1,1221)	1:31:A:ILE:HG23	1:32:A:ASN:HD21	15	0.12
(1,1211)	1:29:A:GLN:HG3	1:30:A:THR:H	3	0.12
(1,1208)	1:29:A:GLN:HE21	1:30:A:THR:H	2	0.12
(1,1208)	1:29:A:GLN:HE21	1:30:A:THR:H	20	0.12
(1,1206)	1:28:A:ARG:HG2	1:29:A:GLN:HB3	9	0.12
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD21	14	0.12
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD22	14	0.12
(1,1185)	1:22:A:ALA:H	1:23:A:LEU:HD23	14	0.12
(1,1184)	1:22:A:ALA:H	1:23:A:LEU:HG	9	0.12
(1,1149)	1:12:A:LYS:HD3	1:13:A:LYS:HA	8	0.12
(1,1147)	1:12:A:LYS:HD2	1:13:A:LYS:HE2	19	0.12
(1,1098)	1:6:A:LEU:H	1:7:A:LYS:HE3	2	0.12
(1,1098)	1:6:A:LEU:H	1:7:A:LYS:HE3	19	0.12
(1,1097)	1:6:A:LEU:H	1:7:A:LYS:HE2	9	0.12
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD11	12	0.12
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD12	12	0.12
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD13	12	0.12
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD11	19	0.12
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD12	19	0.12
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD13	19	0.12
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD11	2	0.12
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD12	2	0.12
(1,1086)	1:1:A:MET:HB2	1:2:A:ILE:HD13	2	0.12
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD11	12	0.12
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD12	12	0.12
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD13	12	0.12
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD11	12	0.12
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD12	12	0.12
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD13	12	0.12
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD11	12	0.12
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD12	12	0.12
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD13	12	0.12
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD11	19	0.12
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD12	19	0.12
(1,1073)	1:121:B:THR:HG21	1:123:B:LEU:HD13	19	0.12
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD11	19	0.12
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD12	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1073)	1:121:B:THR:HG22	1:123:B:LEU:HD13	19	0.12
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD11	19	0.12
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD12	19	0.12
(1,1073)	1:121:B:THR:HG23	1:123:B:LEU:HD13	19	0.12
(1,1055)	1:90:B:LEU:HG	1:92:B:VAL:HG11	8	0.12
(1,1055)	1:90:B:LEU:HG	1:92:B:VAL:HG12	8	0.12
(1,1055)	1:90:B:LEU:HG	1:92:B:VAL:HG13	8	0.12
(1,1042)	1:79:B:LYS:HG3	1:81:B:ILE:HA	3	0.12
(1,1040)	1:79:B:LYS:HD3	1:81:B:ILE:HG13	12	0.12
(1,1040)	1:79:B:LYS:HD3	1:81:B:ILE:HG13	15	0.12
(1,1018)	1:68:B:ILE:HG21	1:70:B:ASN:HD21	9	0.12
(1,1018)	1:68:B:ILE:HG22	1:70:B:ASN:HD21	9	0.12
(1,1018)	1:68:B:ILE:HG23	1:70:B:ASN:HD21	9	0.12
(1,1018)	1:68:B:ILE:HG21	1:70:B:ASN:HD21	13	0.12
(1,1018)	1:68:B:ILE:HG22	1:70:B:ASN:HD21	13	0.12
(1,1018)	1:68:B:ILE:HG23	1:70:B:ASN:HD21	13	0.12
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD11	3	0.12
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD12	3	0.12
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD13	3	0.12
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD11	3	0.12
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD12	3	0.12
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD13	3	0.12
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD11	3	0.12
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD12	3	0.12
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD13	3	0.12
(1,981)	1:21:A:ALA:HA	1:23:A:LEU:HG	15	0.12
(1,971)	1:13:A:LYS:HG3	1:15:A:ILE:HA	6	0.12
(1,962)	1:13:A:LYS:H	1:15:A:ILE:HD11	4	0.12
(1,962)	1:13:A:LYS:H	1:15:A:ILE:HD12	4	0.12
(1,962)	1:13:A:LYS:H	1:15:A:ILE:HD13	4	0.12
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD11	16	0.12
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD12	16	0.12
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD13	16	0.12
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD11	11	0.12
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD12	11	0.12
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD13	11	0.12
(1,913)	1:95:B:GLN:HB3	1:98:B:ASN:HD22	15	0.12
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	8	0.12
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	8	0.12
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	8	0.12
(1,848)	1:57:A:LEU:HD11	1:60:A:ILE:H	9	0.12
(1,848)	1:57:A:LEU:HD12	1:60:A:ILE:H	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:57:A:LEU:HD13	1:60:A:ILE:H	9	0.12
(1,848)	1:57:A:LEU:HD11	1:60:A:ILE:H	19	0.12
(1,848)	1:57:A:LEU:HD12	1:60:A:ILE:H	19	0.12
(1,848)	1:57:A:LEU:HD13	1:60:A:ILE:H	19	0.12
(1,780)	1:9:A:ILE:HA	1:12:A:LYS:HE3	9	0.12
(1,772)	1:8:A:LEU:H	1:11:A:GLU:HG2	7	0.12
(1,762)	1:5:A:ASN:HB2	1:8:A:LEU:HD21	13	0.12
(1,762)	1:5:A:ASN:HB2	1:8:A:LEU:HD22	13	0.12
(1,762)	1:5:A:ASN:HB2	1:8:A:LEU:HD23	13	0.12
(1,740)	1:110:B:GLN:HG2	1:114:B:LYS:HE2	12	0.12
(1,708)	1:94:B:ARG:HD2	1:98:B:ASN:HD22	7	0.12
(1,699)	1:85:B:GLU:HG2	1:89:B:LEU:HD21	12	0.12
(1,699)	1:85:B:GLU:HG2	1:89:B:LEU:HD22	12	0.12
(1,699)	1:85:B:GLU:HG2	1:89:B:LEU:HD23	12	0.12
(1,689)	1:81:B:ILE:HG13	1:85:B:GLU:HG2	18	0.12
(1,675)	1:72:B:LEU:HD21	1:76:B:ARG:HD2	14	0.12
(1,675)	1:72:B:LEU:HD22	1:76:B:ARG:HD2	14	0.12
(1,675)	1:72:B:LEU:HD23	1:76:B:ARG:HD2	14	0.12
(1,641)	1:44:A:GLN:HE21	1:48:A:LYS:HB2	11	0.12
(1,641)	1:44:A:GLN:HE21	1:48:A:LYS:HB2	12	0.12
(1,639)	1:44:A:GLN:HB2	1:48:A:LYS:HD2	15	0.12
(1,637)	1:44:A:GLN:HA	1:48:A:LYS:HD2	1	0.12
(1,637)	1:44:A:GLN:HA	1:48:A:LYS:HD2	3	0.12
(1,637)	1:44:A:GLN:HA	1:48:A:LYS:HD2	7	0.12
(1,637)	1:44:A:GLN:HA	1:48:A:LYS:HD2	16	0.12
(1,612)	1:28:A:ARG:HD2	1:32:A:ASN:HD22	2	0.12
(1,593)	1:15:A:ILE:HG13	1:19:A:GLU:HG2	1	0.12
(1,587)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	8	0.12
(1,587)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	8	0.12
(1,587)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	8	0.12
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG21	2	0.12
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG22	2	0.12
(1,523)	1:76:B:ARG:HB2	1:81:B:ILE:HG23	2	0.12
(1,458)	1:34:A:ILE:HD11	1:40:A:ASN:HB3	8	0.12
(1,458)	1:34:A:ILE:HD12	1:40:A:ASN:HB3	8	0.12
(1,458)	1:34:A:ILE:HD13	1:40:A:ASN:HB3	8	0.12
(1,425)	1:50:A:ALA:HB1	1:57:A:LEU:HD21	7	0.12
(1,425)	1:50:A:ALA:HB1	1:57:A:LEU:HD22	7	0.12
(1,425)	1:50:A:ALA:HB1	1:57:A:LEU:HD23	7	0.12
(1,425)	1:50:A:ALA:HB2	1:57:A:LEU:HD21	7	0.12
(1,425)	1:50:A:ALA:HB2	1:57:A:LEU:HD22	7	0.12
(1,425)	1:50:A:ALA:HB2	1:57:A:LEU:HD23	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,425)	1:50:A:ALA:HB3	1:57:A:LEU:HD21	7	0.12
(1,425)	1:50:A:ALA:HB3	1:57:A:LEU:HD22	7	0.12
(1,425)	1:50:A:ALA:HB3	1:57:A:LEU:HD23	7	0.12
(1,396)	1:115:B:ILE:H	1:123:B:LEU:HD21	6	0.12
(1,396)	1:115:B:ILE:H	1:123:B:LEU:HD22	6	0.12
(1,396)	1:115:B:ILE:H	1:123:B:LEU:HD23	6	0.12
(1,396)	1:115:B:ILE:H	1:123:B:LEU:HD21	11	0.12
(1,396)	1:115:B:ILE:H	1:123:B:LEU:HD22	11	0.12
(1,396)	1:115:B:ILE:H	1:123:B:LEU:HD23	11	0.12
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	1	0.12
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	1	0.12
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	1	0.12
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	13	0.12
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	13	0.12
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	13	0.12
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	15	0.12
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	15	0.12
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	15	0.12
(1,385)	1:20:A:LEU:HD21	1:28:A:ARG:HB2	20	0.12
(1,385)	1:20:A:LEU:HD22	1:28:A:ARG:HB2	20	0.12
(1,385)	1:20:A:LEU:HD23	1:28:A:ARG:HB2	20	0.12
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD21	9	0.12
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD22	9	0.12
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD23	9	0.12
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD21	9	0.12
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD22	9	0.12
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD23	9	0.12
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD21	9	0.12
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD22	9	0.12
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD23	9	0.12
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD21	5	0.12
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD22	5	0.12
(1,315)	1:46:A:ALA:HB1	1:57:A:LEU:HD23	5	0.12
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD21	5	0.12
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD22	5	0.12
(1,315)	1:46:A:ALA:HB2	1:57:A:LEU:HD23	5	0.12
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD21	5	0.12
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD22	5	0.12
(1,315)	1:46:A:ALA:HB3	1:57:A:LEU:HD23	5	0.12
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG21	6	0.12
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG22	6	0.12
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG23	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG21	8	0.12
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG22	8	0.12
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG23	8	0.12
(1,239)	1:90:B:LEU:HD21	1:115:B:ILE:HA	9	0.12
(1,239)	1:90:B:LEU:HD22	1:115:B:ILE:HA	9	0.12
(1,239)	1:90:B:LEU:HD23	1:115:B:ILE:HA	9	0.12
(1,229)	1:24:A:LEU:HD21	1:49:A:ILE:HA	2	0.12
(1,229)	1:24:A:LEU:HD22	1:49:A:ILE:HA	2	0.12
(1,229)	1:24:A:LEU:HD23	1:49:A:ILE:HA	2	0.12
(1,229)	1:24:A:LEU:HD21	1:49:A:ILE:HA	14	0.12
(1,229)	1:24:A:LEU:HD22	1:49:A:ILE:HA	14	0.12
(1,229)	1:24:A:LEU:HD23	1:49:A:ILE:HA	14	0.12
(1,207)	1:73:B:LYS:HE2	1:101:B:GLU:HG2	8	0.12
(1,207)	1:73:B:LYS:HE2	1:101:B:GLU:HG2	17	0.12
(1,207)	1:73:B:LYS:HE2	1:101:B:GLU:HG2	20	0.12
(1,194)	1:7:A:LYS:HD3	1:35:A:GLU:HB2	20	0.12
(1,191)	1:89:B:LEU:HD21	1:118:B:TYR:HE2	1	0.12
(1,191)	1:89:B:LEU:HD22	1:118:B:TYR:HE2	1	0.12
(1,191)	1:89:B:LEU:HD23	1:118:B:TYR:HE2	1	0.12
(1,181)	1:23:A:LEU:HD11	1:52:A:TYR:HE2	11	0.12
(1,181)	1:23:A:LEU:HD12	1:52:A:TYR:HE2	11	0.12
(1,181)	1:23:A:LEU:HD13	1:52:A:TYR:HE2	11	0.12
(1,165)	1:5:A:ASN:HA	1:35:A:GLU:HA	5	0.12
(1,160)	1:81:B:ILE:H	1:119:B:LEU:HD21	4	0.12
(1,160)	1:81:B:ILE:H	1:119:B:LEU:HD22	4	0.12
(1,160)	1:81:B:ILE:H	1:119:B:LEU:HD23	4	0.12
(1,156)	1:68:B:ILE:HD11	1:106:B:ASN:HD21	12	0.12
(1,156)	1:68:B:ILE:HD12	1:106:B:ASN:HD21	12	0.12
(1,156)	1:68:B:ILE:HD13	1:106:B:ASN:HD21	12	0.12
(1,154)	1:68:B:ILE:HB	1:106:B:ASN:HD21	2	0.12
(1,154)	1:68:B:ILE:HB	1:106:B:ASN:HD21	4	0.12
(1,154)	1:68:B:ILE:HB	1:106:B:ASN:HD21	18	0.12
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD21	6	0.12
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD22	6	0.12
(1,138)	1:79:B:LYS:HE3	1:119:B:LEU:HD23	6	0.12
(1,127)	1:79:B:LYS:HE2	1:120:B:ASN:HB2	1	0.12
(1,112)	1:10:A:ARG:HA	1:53:A:LEU:HD11	10	0.12
(1,112)	1:10:A:ARG:HA	1:53:A:LEU:HD12	10	0.12
(1,112)	1:10:A:ARG:HA	1:53:A:LEU:HD13	10	0.12
(1,107)	1:75:B:ILE:HD11	1:121:B:THR:HG21	12	0.12
(1,107)	1:75:B:ILE:HD11	1:121:B:THR:HG22	12	0.12
(1,107)	1:75:B:ILE:HD11	1:121:B:THR:HG23	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	1:75:B:ILE:HD12	1:121:B:THR:HG21	12	0.12
(1,107)	1:75:B:ILE:HD12	1:121:B:THR:HG22	12	0.12
(1,107)	1:75:B:ILE:HD12	1:121:B:THR:HG23	12	0.12
(1,107)	1:75:B:ILE:HD13	1:121:B:THR:HG21	12	0.12
(1,107)	1:75:B:ILE:HD13	1:121:B:THR:HG22	12	0.12
(1,107)	1:75:B:ILE:HD13	1:121:B:THR:HG23	12	0.12
(1,86)	1:9:A:ILE:HG13	1:59:A:ASP:HB2	9	0.12
(1,19)	1:3:A:ILE:HD11	1:64:A:GLN:HB3	9	0.12
(1,19)	1:3:A:ILE:HD12	1:64:A:GLN:HB3	9	0.12
(1,19)	1:3:A:ILE:HD13	1:64:A:GLN:HB3	9	0.12
(1,5)	1:68:B:ILE:HD11	1:130:B:GLN:H	9	0.12
(1,5)	1:68:B:ILE:HD12	1:130:B:GLN:H	9	0.12
(1,5)	1:68:B:ILE:HD13	1:130:B:GLN:H	9	0.12
(1,5)	1:68:B:ILE:HD11	1:130:B:GLN:H	14	0.12
(1,5)	1:68:B:ILE:HD12	1:130:B:GLN:H	14	0.12
(1,5)	1:68:B:ILE:HD13	1:130:B:GLN:H	14	0.12
(1,5)	1:68:B:ILE:HD11	1:130:B:GLN:H	15	0.12
(1,5)	1:68:B:ILE:HD12	1:130:B:GLN:H	15	0.12
(1,5)	1:68:B:ILE:HD13	1:130:B:GLN:H	15	0.12
(1,4)	1:2:A:ILE:H	1:64:A:GLN:HB2	17	0.12
(1,2)	1:2:A:ILE:HD11	1:64:A:GLN:H	6	0.12
(1,2)	1:2:A:ILE:HD12	1:64:A:GLN:H	6	0.12
(1,2)	1:2:A:ILE:HD13	1:64:A:GLN:H	6	0.12
(1,2)	1:2:A:ILE:HD11	1:64:A:GLN:H	10	0.12
(1,2)	1:2:A:ILE:HD12	1:64:A:GLN:H	10	0.12
(1,2)	1:2:A:ILE:HD13	1:64:A:GLN:H	10	0.12
(1,1)	1:2:A:ILE:H	1:64:A:GLN:HB2	17	0.12
(1,2179)	1:44:A:GLN:HE22	1:68:B:ILE:HD11	9	0.11
(1,2179)	1:44:A:GLN:HE22	1:68:B:ILE:HD12	9	0.11
(1,2179)	1:44:A:GLN:HE22	1:68:B:ILE:HD13	9	0.11
(1,2177)	1:44:A:GLN:HB2	1:68:B:ILE:HG21	11	0.11
(1,2177)	1:44:A:GLN:HB2	1:68:B:ILE:HG22	11	0.11
(1,2177)	1:44:A:GLN:HB2	1:68:B:ILE:HG23	11	0.11
(1,2170)	1:43:A:LEU:HD21	1:68:B:ILE:HG21	8	0.11
(1,2170)	1:43:A:LEU:HD21	1:68:B:ILE:HG22	8	0.11
(1,2170)	1:43:A:LEU:HD21	1:68:B:ILE:HG23	8	0.11
(1,2170)	1:43:A:LEU:HD22	1:68:B:ILE:HG21	8	0.11
(1,2170)	1:43:A:LEU:HD22	1:68:B:ILE:HG22	8	0.11
(1,2170)	1:43:A:LEU:HD22	1:68:B:ILE:HG23	8	0.11
(1,2170)	1:43:A:LEU:HD23	1:68:B:ILE:HG21	8	0.11
(1,2170)	1:43:A:LEU:HD23	1:68:B:ILE:HG22	8	0.11
(1,2170)	1:43:A:LEU:HD23	1:68:B:ILE:HG23	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2165)	1:64:A:GLN:H	1:110:B:GLN:HG2	18	0.11
(1,2156)	1:63:A:TRP:HE1	1:114:B:LYS:HA	15	0.11
(1,2142)	1:43:A:LEU:HD11	1:106:B:ASN:H	13	0.11
(1,2142)	1:43:A:LEU:HD12	1:106:B:ASN:H	13	0.11
(1,2142)	1:43:A:LEU:HD13	1:106:B:ASN:H	13	0.11
(1,2142)	1:43:A:LEU:HD21	1:106:B:ASN:H	13	0.11
(1,2142)	1:43:A:LEU:HD22	1:106:B:ASN:H	13	0.11
(1,2142)	1:43:A:LEU:HD23	1:106:B:ASN:H	13	0.11
(1,2138)	1:43:A:LEU:HD11	1:107:B:PRO:HB2	19	0.11
(1,2138)	1:43:A:LEU:HD12	1:107:B:PRO:HB2	19	0.11
(1,2138)	1:43:A:LEU:HD13	1:107:B:PRO:HB2	19	0.11
(1,2138)	1:43:A:LEU:HD21	1:107:B:PRO:HB2	19	0.11
(1,2138)	1:43:A:LEU:HD22	1:107:B:PRO:HB2	19	0.11
(1,2138)	1:43:A:LEU:HD23	1:107:B:PRO:HB2	19	0.11
(1,2131)	1:41:A:PRO:HG2	1:109:B:LEU:HD21	20	0.11
(1,2131)	1:41:A:PRO:HG2	1:109:B:LEU:HD22	20	0.11
(1,2131)	1:41:A:PRO:HG2	1:109:B:LEU:HD23	20	0.11
(1,2100)	1:2:A:ILE:HG21	1:109:B:LEU:HD21	19	0.11
(1,2100)	1:2:A:ILE:HG21	1:109:B:LEU:HD22	19	0.11
(1,2100)	1:2:A:ILE:HG21	1:109:B:LEU:HD23	19	0.11
(1,2100)	1:2:A:ILE:HG22	1:109:B:LEU:HD21	19	0.11
(1,2100)	1:2:A:ILE:HG22	1:109:B:LEU:HD22	19	0.11
(1,2100)	1:2:A:ILE:HG22	1:109:B:LEU:HD23	19	0.11
(1,2100)	1:2:A:ILE:HG23	1:109:B:LEU:HD21	19	0.11
(1,2100)	1:2:A:ILE:HG23	1:109:B:LEU:HD22	19	0.11
(1,2100)	1:2:A:ILE:HG23	1:109:B:LEU:HD23	19	0.11
(1,2086)	1:129:B:TRP:HE3	1:51:A:TYR:HD1	1	0.11
(1,2086)	1:129:B:TRP:HE3	1:51:A:TYR:HD2	1	0.11
(1,2086)	1:129:B:TRP:HE3	1:51:A:TYR:HD1	11	0.11
(1,2086)	1:129:B:TRP:HE3	1:51:A:TYR:HD2	11	0.11
(1,2060)	1:120:B:ASN:HB3	1:120:B:ASN:HD21	15	0.11
(1,2023)	1:106:B:ASN:H	1:106:B:ASN:HD21	2	0.11
(1,1999)	1:102:B:LYS:HA	1:102:B:LYS:HE3	4	0.11
(1,1998)	1:102:B:LYS:HA	1:102:B:LYS:HE2	16	0.11
(1,1997)	1:102:B:LYS:HA	1:102:B:LYS:HD2	20	0.11
(1,1962)	1:95:B:GLN:H	1:95:B:GLN:HG2	12	0.11
(1,1961)	1:95:B:GLN:H	1:95:B:GLN:HE22	9	0.11
(1,1904)	1:80:B:LYS:HB2	1:80:B:LYS:HE2	3	0.11
(1,1904)	1:80:B:LYS:HB2	1:80:B:LYS:HE2	5	0.11
(1,1904)	1:80:B:LYS:HB2	1:80:B:LYS:HE2	10	0.11
(1,1904)	1:80:B:LYS:HB2	1:80:B:LYS:HE2	19	0.11
(1,1899)	1:80:B:LYS:HA	1:80:B:LYS:HE2	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1880)	1:78:B:LYS:HB3	1:78:B:LYS:HE2	2	0.11
(1,1872)	1:78:B:LYS:H	1:78:B:LYS:HD2	1	0.11
(1,1872)	1:78:B:LYS:H	1:78:B:LYS:HD2	7	0.11
(1,1837)	1:73:B:LYS:H	1:73:B:LYS:HD3	6	0.11
(1,1789)	1:54:A:ASN:H	1:54:A:ASN:HD22	17	0.11
(1,1755)	1:40:A:ASN:H	1:40:A:ASN:HD21	14	0.11
(1,1693)	1:29:A:GLN:H	1:29:A:GLN:HE22	5	0.11
(1,1652)	1:17:A:GLN:HA	1:17:A:GLN:HE22	6	0.11
(1,1651)	1:17:A:GLN:H	1:17:A:GLN:HE21	5	0.11
(1,1631)	1:14:A:LYS:HA	1:14:A:LYS:HE2	12	0.11
(1,1604)	1:12:A:LYS:H	1:12:A:LYS:HD2	11	0.11
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD11	9	0.11
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD12	9	0.11
(1,1540)	1:125:B:ASP:HB2	1:126:B:ILE:HD13	9	0.11
(1,1489)	1:104:B:LYS:HE2	1:105:B:TYR:H	4	0.11
(1,1487)	1:104:B:LYS:HD2	1:105:B:TYR:HD2	16	0.11
(1,1486)	1:104:B:LYS:HD2	1:105:B:TYR:H	13	0.11
(1,1453)	1:97:B:ILE:HG21	1:98:B:ASN:HD21	13	0.11
(1,1453)	1:97:B:ILE:HG22	1:98:B:ASN:HD21	13	0.11
(1,1453)	1:97:B:ILE:HG23	1:98:B:ASN:HD21	13	0.11
(1,1442)	1:95:B:GLN:HG2	1:96:B:THR:HG21	16	0.11
(1,1442)	1:95:B:GLN:HG2	1:96:B:THR:HG22	16	0.11
(1,1442)	1:95:B:GLN:HG2	1:96:B:THR:HG23	16	0.11
(1,1366)	1:76:B:ARG:HD2	1:77:B:GLU:HA	8	0.11
(1,1366)	1:76:B:ARG:HD2	1:77:B:GLU:HA	9	0.11
(1,1362)	1:76:B:ARG:H	1:77:B:GLU:HG3	2	0.11
(1,1330)	1:72:B:LEU:H	1:73:B:LYS:HE3	4	0.11
(1,1319)	1:67:B:MET:HB3	1:68:B:ILE:HD11	20	0.11
(1,1319)	1:67:B:MET:HB3	1:68:B:ILE:HD12	20	0.11
(1,1319)	1:67:B:MET:HB3	1:68:B:ILE:HD13	20	0.11
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD11	1	0.11
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD12	1	0.11
(1,1318)	1:67:B:MET:HB2	1:68:B:ILE:HD13	1	0.11
(1,1255)	1:38:A:LYS:HD2	1:39:A:TYR:HD2	2	0.11
(1,1255)	1:38:A:LYS:HD2	1:39:A:TYR:HD2	19	0.11
(1,1221)	1:31:A:ILE:HG21	1:32:A:ASN:HD21	16	0.11
(1,1221)	1:31:A:ILE:HG22	1:32:A:ASN:HD21	16	0.11
(1,1221)	1:31:A:ILE:HG23	1:32:A:ASN:HD21	16	0.11
(1,1210)	1:29:A:GLN:HG2	1:30:A:THR:HG21	3	0.11
(1,1210)	1:29:A:GLN:HG2	1:30:A:THR:HG22	3	0.11
(1,1210)	1:29:A:GLN:HG2	1:30:A:THR:HG23	3	0.11
(1,1172)	1:18:A:SER:H	1:19:A:GLU:HB3	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1165)	1:14:A:LYS:HG2	1:15:A:ILE:HD11	7	0.11
(1,1165)	1:14:A:LYS:HG2	1:15:A:ILE:HD12	7	0.11
(1,1165)	1:14:A:LYS:HG2	1:15:A:ILE:HD13	7	0.11
(1,1165)	1:14:A:LYS:HG2	1:15:A:ILE:HD11	14	0.11
(1,1165)	1:14:A:LYS:HG2	1:15:A:ILE:HD12	14	0.11
(1,1165)	1:14:A:LYS:HG2	1:15:A:ILE:HD13	14	0.11
(1,1164)	1:14:A:LYS:HD2	1:15:A:ILE:H	2	0.11
(1,1140)	1:11:A:GLU:HG3	1:12:A:LYS:HB3	1	0.11
(1,1134)	1:10:A:ARG:HD2	1:11:A:GLU:HA	9	0.11
(1,1134)	1:10:A:ARG:HD2	1:11:A:GLU:HA	19	0.11
(1,1112)	1:7:A:LYS:HG2	1:8:A:LEU:HA	5	0.11
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD11	17	0.11
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD12	17	0.11
(1,1089)	1:1:A:MET:HG2	1:2:A:ILE:HD13	17	0.11
(1,1055)	1:90:B:LEU:HG	1:92:B:VAL:HG11	16	0.11
(1,1055)	1:90:B:LEU:HG	1:92:B:VAL:HG12	16	0.11
(1,1055)	1:90:B:LEU:HG	1:92:B:VAL:HG13	16	0.11
(1,1042)	1:79:B:LYS:HG3	1:81:B:ILE:HA	4	0.11
(1,1042)	1:79:B:LYS:HG3	1:81:B:ILE:HA	12	0.11
(1,1040)	1:79:B:LYS:HD3	1:81:B:ILE:HG13	14	0.11
(1,1028)	1:71:B:ASN:HB2	1:73:B:LYS:HE3	10	0.11
(1,1021)	1:69:B:ILE:HB	1:71:B:ASN:HD22	15	0.11
(1,1019)	1:68:B:ILE:HG21	1:70:B:ASN:HD22	4	0.11
(1,1019)	1:68:B:ILE:HG22	1:70:B:ASN:HD22	4	0.11
(1,1019)	1:68:B:ILE:HG23	1:70:B:ASN:HD22	4	0.11
(1,1005)	1:58:A:GLU:H	1:60:A:ILE:HD11	6	0.11
(1,1005)	1:58:A:GLU:H	1:60:A:ILE:HD12	6	0.11
(1,1005)	1:58:A:GLU:H	1:60:A:ILE:HD13	6	0.11
(1,1004)	1:57:A:LEU:HD11	1:59:A:ASP:H	5	0.11
(1,1004)	1:57:A:LEU:HD12	1:59:A:ASP:H	5	0.11
(1,1004)	1:57:A:LEU:HD13	1:59:A:ASP:H	5	0.11
(1,1003)	1:55:A:THR:HG21	1:57:A:LEU:HD21	3	0.11
(1,1003)	1:55:A:THR:HG21	1:57:A:LEU:HD22	3	0.11
(1,1003)	1:55:A:THR:HG21	1:57:A:LEU:HD23	3	0.11
(1,1003)	1:55:A:THR:HG22	1:57:A:LEU:HD21	3	0.11
(1,1003)	1:55:A:THR:HG22	1:57:A:LEU:HD22	3	0.11
(1,1003)	1:55:A:THR:HG22	1:57:A:LEU:HD23	3	0.11
(1,1003)	1:55:A:THR:HG23	1:57:A:LEU:HD21	3	0.11
(1,1003)	1:55:A:THR:HG23	1:57:A:LEU:HD22	3	0.11
(1,1003)	1:55:A:THR:HG23	1:57:A:LEU:HD23	3	0.11
(1,1000)	1:53:A:LEU:HD11	1:55:A:THR:HB	17	0.11
(1,1000)	1:53:A:LEU:HD12	1:55:A:THR:HB	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1000)	1:53:A:LEU:HD13	1:55:A:THR:HB	17	0.11
(1,981)	1:21:A:ALA:HA	1:23:A:LEU:HG	6	0.11
(1,971)	1:13:A:LYS:HG3	1:15:A:ILE:HA	12	0.11
(1,971)	1:13:A:LYS:HG3	1:15:A:ILE:HA	16	0.11
(1,965)	1:13:A:LYS:HB2	1:15:A:ILE:HG12	6	0.11
(1,951)	1:3:A:ILE:HG12	1:5:A:ASN:HD22	5	0.11
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD11	18	0.11
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD12	18	0.11
(1,940)	1:116:B:ALA:HA	1:119:B:LEU:HD13	18	0.11
(1,913)	1:95:B:GLN:HB3	1:98:B:ASN:HD22	11	0.11
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD21	7	0.11
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD22	7	0.11
(1,900)	1:87:B:ALA:H	1:90:B:LEU:HD23	7	0.11
(1,877)	1:75:B:ILE:HG21	1:78:B:LYS:HE3	15	0.11
(1,877)	1:75:B:ILE:HG22	1:78:B:LYS:HE3	15	0.11
(1,877)	1:75:B:ILE:HG23	1:78:B:LYS:HE3	15	0.11
(1,848)	1:57:A:LEU:HD11	1:60:A:ILE:H	2	0.11
(1,848)	1:57:A:LEU:HD12	1:60:A:ILE:H	2	0.11
(1,848)	1:57:A:LEU:HD13	1:60:A:ILE:H	2	0.11
(1,786)	1:10:A:ARG:HA	1:13:A:LYS:HE3	4	0.11
(1,783)	1:9:A:ILE:HG21	1:12:A:LYS:HE3	10	0.11
(1,783)	1:9:A:ILE:HG22	1:12:A:LYS:HE3	10	0.11
(1,783)	1:9:A:ILE:HG23	1:12:A:LYS:HE3	10	0.11
(1,780)	1:9:A:ILE:HA	1:12:A:LYS:HE3	16	0.11
(1,769)	1:6:A:LEU:HD11	1:9:A:ILE:H	18	0.11
(1,769)	1:6:A:LEU:HD12	1:9:A:ILE:H	18	0.11
(1,769)	1:6:A:LEU:HD13	1:9:A:ILE:H	18	0.11
(1,685)	1:76:B:ARG:HD3	1:80:B:LYS:HA	6	0.11
(1,679)	1:73:B:LYS:HG2	1:77:B:GLU:HG2	14	0.11
(1,675)	1:72:B:LEU:HD21	1:76:B:ARG:HD2	7	0.11
(1,675)	1:72:B:LEU:HD22	1:76:B:ARG:HD2	7	0.11
(1,675)	1:72:B:LEU:HD23	1:76:B:ARG:HD2	7	0.11
(1,675)	1:72:B:LEU:HD21	1:76:B:ARG:HD2	12	0.11
(1,675)	1:72:B:LEU:HD22	1:76:B:ARG:HD2	12	0.11
(1,675)	1:72:B:LEU:HD23	1:76:B:ARG:HD2	12	0.11
(1,655)	1:55:A:THR:HG21	1:59:A:ASP:HB2	5	0.11
(1,655)	1:55:A:THR:HG22	1:59:A:ASP:HB2	5	0.11
(1,655)	1:55:A:THR:HG23	1:59:A:ASP:HB2	5	0.11
(1,583)	1:7:A:LYS:HG2	1:11:A:GLU:HG2	8	0.11
(1,579)	1:6:A:LEU:HD21	1:10:A:ARG:HD2	7	0.11
(1,579)	1:6:A:LEU:HD22	1:10:A:ARG:HD2	7	0.11
(1,579)	1:6:A:LEU:HD23	1:10:A:ARG:HD2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,569)	1:6:A:LEU:HD11	1:10:A:ARG:HB2	20	0.11
(1,569)	1:6:A:LEU:HD12	1:10:A:ARG:HB2	20	0.11
(1,569)	1:6:A:LEU:HD13	1:10:A:ARG:HB2	20	0.11
(1,524)	1:76:B:ARG:HD2	1:81:B:ILE:HG21	4	0.11
(1,524)	1:76:B:ARG:HD2	1:81:B:ILE:HG22	4	0.11
(1,524)	1:76:B:ARG:HD2	1:81:B:ILE:HG23	4	0.11
(1,441)	1:90:B:LEU:HD11	1:97:B:ILE:HD11	7	0.11
(1,441)	1:90:B:LEU:HD11	1:97:B:ILE:HD12	7	0.11
(1,441)	1:90:B:LEU:HD11	1:97:B:ILE:HD13	7	0.11
(1,441)	1:90:B:LEU:HD12	1:97:B:ILE:HD11	7	0.11
(1,441)	1:90:B:LEU:HD12	1:97:B:ILE:HD12	7	0.11
(1,441)	1:90:B:LEU:HD12	1:97:B:ILE:HD13	7	0.11
(1,441)	1:90:B:LEU:HD13	1:97:B:ILE:HD11	7	0.11
(1,441)	1:90:B:LEU:HD13	1:97:B:ILE:HD12	7	0.11
(1,441)	1:90:B:LEU:HD13	1:97:B:ILE:HD13	7	0.11
(1,399)	1:10:A:ARG:HD2	1:17:A:GLN:HE21	8	0.11
(1,397)	1:10:A:ARG:HB3	1:17:A:GLN:HE21	3	0.11
(1,391)	1:86:B:LEU:HD21	1:94:B:ARG:HB2	18	0.11
(1,391)	1:86:B:LEU:HD22	1:94:B:ARG:HB2	18	0.11
(1,391)	1:86:B:LEU:HD23	1:94:B:ARG:HB2	18	0.11
(1,385)	1:20:A:LEU:HD21	1:28:A:ARG:HB2	13	0.11
(1,385)	1:20:A:LEU:HD22	1:28:A:ARG:HB2	13	0.11
(1,385)	1:20:A:LEU:HD23	1:28:A:ARG:HB2	13	0.11
(1,385)	1:20:A:LEU:HD21	1:28:A:ARG:HB2	16	0.11
(1,385)	1:20:A:LEU:HD22	1:28:A:ARG:HB2	16	0.11
(1,385)	1:20:A:LEU:HD23	1:28:A:ARG:HB2	16	0.11
(1,363)	1:76:B:ARG:HG2	1:86:B:LEU:HD11	8	0.11
(1,363)	1:76:B:ARG:HG2	1:86:B:LEU:HD12	8	0.11
(1,363)	1:76:B:ARG:HG2	1:86:B:LEU:HD13	8	0.11
(1,362)	1:76:B:ARG:HB3	1:86:B:LEU:HD11	20	0.11
(1,362)	1:76:B:ARG:HB3	1:86:B:LEU:HD12	20	0.11
(1,362)	1:76:B:ARG:HB3	1:86:B:LEU:HD13	20	0.11
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD21	6	0.11
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD22	6	0.11
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD23	6	0.11
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD21	6	0.11
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD22	6	0.11
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD23	6	0.11
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD21	6	0.11
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD22	6	0.11
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD23	6	0.11
(1,330)	1:86:B:LEU:HD21	1:97:B:ILE:HG12	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:86:B:LEU:HD22	1:97:B:ILE:HG12	3	0.11
(1,330)	1:86:B:LEU:HD23	1:97:B:ILE:HG12	3	0.11
(1,330)	1:86:B:LEU:HD21	1:97:B:ILE:HG12	19	0.11
(1,330)	1:86:B:LEU:HD22	1:97:B:ILE:HG12	19	0.11
(1,330)	1:86:B:LEU:HD23	1:97:B:ILE:HG12	19	0.11
(1,327)	1:83:B:GLN:HB3	1:94:B:ARG:HA	2	0.11
(1,299)	1:115:B:ILE:HG21	1:127:B:PHE:HE1	12	0.11
(1,299)	1:115:B:ILE:HG22	1:127:B:PHE:HE1	12	0.11
(1,299)	1:115:B:ILE:HG23	1:127:B:PHE:HE1	12	0.11
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG21	9	0.11
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG22	9	0.11
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG23	9	0.11
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG21	8	0.11
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG22	8	0.11
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG23	8	0.11
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG21	17	0.11
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG22	17	0.11
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG23	17	0.11
(1,253)	1:90:B:LEU:H	1:111:B:LEU:HD21	15	0.11
(1,253)	1:90:B:LEU:H	1:111:B:LEU:HD22	15	0.11
(1,253)	1:90:B:LEU:H	1:111:B:LEU:HD23	15	0.11
(1,247)	1:25:A:GLU:HG3	1:48:A:LYS:HD3	1	0.11
(1,239)	1:90:B:LEU:HD21	1:115:B:ILE:HA	3	0.11
(1,239)	1:90:B:LEU:HD22	1:115:B:ILE:HA	3	0.11
(1,239)	1:90:B:LEU:HD23	1:115:B:ILE:HA	3	0.11
(1,233)	1:90:B:LEU:HA	1:115:B:ILE:HG12	12	0.11
(1,229)	1:24:A:LEU:HD21	1:49:A:ILE:HA	8	0.11
(1,229)	1:24:A:LEU:HD22	1:49:A:ILE:HA	8	0.11
(1,229)	1:24:A:LEU:HD23	1:49:A:ILE:HA	8	0.11
(1,213)	1:34:A:ILE:HD11	1:61:A:PHE:HZ	5	0.11
(1,213)	1:34:A:ILE:HD12	1:61:A:PHE:HZ	5	0.11
(1,213)	1:34:A:ILE:HD13	1:61:A:PHE:HZ	5	0.11
(1,212)	1:34:A:ILE:HD11	1:61:A:PHE:HE2	19	0.11
(1,212)	1:34:A:ILE:HD12	1:61:A:PHE:HE2	19	0.11
(1,212)	1:34:A:ILE:HD13	1:61:A:PHE:HE2	19	0.11
(1,199)	1:7:A:LYS:HG2	1:35:A:GLU:HB2	17	0.11
(1,187)	1:89:B:LEU:HD11	1:118:B:TYR:H	10	0.11
(1,187)	1:89:B:LEU:HD12	1:118:B:TYR:H	10	0.11
(1,187)	1:89:B:LEU:HD13	1:118:B:TYR:H	10	0.11
(1,182)	1:23:A:LEU:HD21	1:52:A:TYR:HE2	5	0.11
(1,182)	1:23:A:LEU:HD22	1:52:A:TYR:HE2	5	0.11
(1,182)	1:23:A:LEU:HD23	1:52:A:TYR:HE2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,165)	1:5:A:ASN:HA	1:35:A:GLU:HA	17	0.11
(1,154)	1:68:B:ILE:HB	1:106:B:ASN:HD21	19	0.11
(1,152)	1:15:A:ILE:HG13	1:53:A:LEU:HD21	11	0.11
(1,152)	1:15:A:ILE:HG13	1:53:A:LEU:HD22	11	0.11
(1,152)	1:15:A:ILE:HG13	1:53:A:LEU:HD23	11	0.11
(1,145)	1:2:A:ILE:HD11	1:40:A:ASN:HD21	2	0.11
(1,145)	1:2:A:ILE:HD12	1:40:A:ASN:HD21	2	0.11
(1,145)	1:2:A:ILE:HD13	1:40:A:ASN:HD21	2	0.11
(1,143)	1:2:A:ILE:HB	1:40:A:ASN:HD21	2	0.11
(1,135)	1:79:B:LYS:HD2	1:119:B:LEU:HD21	6	0.11
(1,135)	1:79:B:LYS:HD2	1:119:B:LEU:HD22	6	0.11
(1,135)	1:79:B:LYS:HD2	1:119:B:LEU:HD23	6	0.11
(1,135)	1:79:B:LYS:HD2	1:119:B:LEU:HD21	20	0.11
(1,135)	1:79:B:LYS:HD2	1:119:B:LEU:HD22	20	0.11
(1,135)	1:79:B:LYS:HD2	1:119:B:LEU:HD23	20	0.11
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD21	3	0.11
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD22	3	0.11
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD23	3	0.11
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD21	10	0.11
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD22	10	0.11
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD23	10	0.11
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD21	14	0.11
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD22	14	0.11
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD23	14	0.11
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD21	18	0.11
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD22	18	0.11
(1,132)	1:13:A:LYS:HE3	1:53:A:LEU:HD23	18	0.11
(1,128)	1:79:B:LYS:HE3	1:120:B:ASN:HB2	1	0.11
(1,86)	1:9:A:ILE:HG13	1:59:A:ASP:HB2	7	0.11
(1,76)	1:9:A:ILE:HD11	1:60:A:ILE:HD11	2	0.11
(1,76)	1:9:A:ILE:HD11	1:60:A:ILE:HD12	2	0.11
(1,76)	1:9:A:ILE:HD11	1:60:A:ILE:HD13	2	0.11
(1,76)	1:9:A:ILE:HD12	1:60:A:ILE:HD11	2	0.11
(1,76)	1:9:A:ILE:HD12	1:60:A:ILE:HD12	2	0.11
(1,76)	1:9:A:ILE:HD12	1:60:A:ILE:HD13	2	0.11
(1,76)	1:9:A:ILE:HD13	1:60:A:ILE:HD11	2	0.11
(1,76)	1:9:A:ILE:HD13	1:60:A:ILE:HD12	2	0.11
(1,76)	1:9:A:ILE:HD13	1:60:A:ILE:HD13	2	0.11
(1,2174)	1:44:A:GLN:H	1:68:B:ILE:HD11	11	0.1
(1,2174)	1:44:A:GLN:H	1:68:B:ILE:HD12	11	0.1
(1,2174)	1:44:A:GLN:H	1:68:B:ILE:HD13	11	0.1
(1,2165)	1:64:A:GLN:H	1:110:B:GLN:HG2	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD11	6	0.1
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD12	6	0.1
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD13	6	0.1
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD21	6	0.1
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD22	6	0.1
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD23	6	0.1
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD11	6	0.1
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD12	6	0.1
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD13	6	0.1
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD21	6	0.1
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD22	6	0.1
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD23	6	0.1
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD11	6	0.1
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD12	6	0.1
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD13	6	0.1
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD21	6	0.1
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD22	6	0.1
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD23	6	0.1
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD11	17	0.1
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD12	17	0.1
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD13	17	0.1
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD21	17	0.1
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD22	17	0.1
(1,2152)	1:46:A:ALA:HB1	1:109:B:LEU:HD23	17	0.1
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD11	17	0.1
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD12	17	0.1
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD13	17	0.1
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD21	17	0.1
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD22	17	0.1
(1,2152)	1:46:A:ALA:HB2	1:109:B:LEU:HD23	17	0.1
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD11	17	0.1
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD12	17	0.1
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD13	17	0.1
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD21	17	0.1
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD22	17	0.1
(1,2152)	1:46:A:ALA:HB3	1:109:B:LEU:HD23	17	0.1
(1,2125)	1:43:A:LEU:HD11	1:112:B:ALA:HB1	13	0.1
(1,2125)	1:43:A:LEU:HD11	1:112:B:ALA:HB2	13	0.1
(1,2125)	1:43:A:LEU:HD11	1:112:B:ALA:HB3	13	0.1
(1,2125)	1:43:A:LEU:HD12	1:112:B:ALA:HB1	13	0.1
(1,2125)	1:43:A:LEU:HD12	1:112:B:ALA:HB2	13	0.1
(1,2125)	1:43:A:LEU:HD12	1:112:B:ALA:HB3	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2125)	1:43:A:LEU:HD13	1:112:B:ALA:HB1	13	0.1
(1,2125)	1:43:A:LEU:HD13	1:112:B:ALA:HB2	13	0.1
(1,2125)	1:43:A:LEU:HD13	1:112:B:ALA:HB3	13	0.1
(1,2125)	1:43:A:LEU:HD21	1:112:B:ALA:HB1	13	0.1
(1,2125)	1:43:A:LEU:HD21	1:112:B:ALA:HB2	13	0.1
(1,2125)	1:43:A:LEU:HD21	1:112:B:ALA:HB3	13	0.1
(1,2125)	1:43:A:LEU:HD22	1:112:B:ALA:HB1	13	0.1
(1,2125)	1:43:A:LEU:HD22	1:112:B:ALA:HB2	13	0.1
(1,2125)	1:43:A:LEU:HD22	1:112:B:ALA:HB3	13	0.1
(1,2125)	1:43:A:LEU:HD23	1:112:B:ALA:HB1	13	0.1
(1,2125)	1:43:A:LEU:HD23	1:112:B:ALA:HB2	13	0.1
(1,2125)	1:43:A:LEU:HD23	1:112:B:ALA:HB3	13	0.1
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD11	13	0.1
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD12	13	0.1
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD13	13	0.1
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD21	13	0.1
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD22	13	0.1
(1,2115)	1:40:A:ASN:H	1:109:B:LEU:HD23	13	0.1
(1,2103)	1:44:A:GLN:HG2	1:130:B:GLN:H	13	0.1
(1,2103)	1:44:A:GLN:HG2	1:130:B:GLN:H	17	0.1
(1,2069)	1:128:B:GLN:H	1:128:B:GLN:HG2	14	0.1
(1,2029)	1:110:B:GLN:H	1:110:B:GLN:HE21	20	0.1
(1,1968)	1:95:B:GLN:HB3	1:95:B:GLN:HE21	19	0.1
(1,1922)	1:83:B:GLN:HB3	1:83:B:GLN:HE21	8	0.1
(1,1918)	1:81:B:ILE:HG21	1:81:B:ILE:HD11	7	0.1
(1,1918)	1:81:B:ILE:HG21	1:81:B:ILE:HD12	7	0.1
(1,1918)	1:81:B:ILE:HG21	1:81:B:ILE:HD13	7	0.1
(1,1918)	1:81:B:ILE:HG22	1:81:B:ILE:HD11	7	0.1
(1,1918)	1:81:B:ILE:HG22	1:81:B:ILE:HD12	7	0.1
(1,1918)	1:81:B:ILE:HG22	1:81:B:ILE:HD13	7	0.1
(1,1918)	1:81:B:ILE:HG23	1:81:B:ILE:HD11	7	0.1
(1,1918)	1:81:B:ILE:HG23	1:81:B:ILE:HD12	7	0.1
(1,1918)	1:81:B:ILE:HG23	1:81:B:ILE:HD13	7	0.1
(1,1904)	1:80:B:LYS:HB2	1:80:B:LYS:HE2	9	0.1
(1,1904)	1:80:B:LYS:HB2	1:80:B:LYS:HE2	18	0.1
(1,1899)	1:80:B:LYS:HA	1:80:B:LYS:HE2	5	0.1
(1,1872)	1:78:B:LYS:H	1:78:B:LYS:HD2	14	0.1
(1,1869)	1:77:B:GLU:H	1:77:B:GLU:HG2	20	0.1
(1,1799)	1:60:A:ILE:HG21	1:60:A:ILE:HD11	15	0.1
(1,1799)	1:60:A:ILE:HG21	1:60:A:ILE:HD12	15	0.1
(1,1799)	1:60:A:ILE:HG21	1:60:A:ILE:HD13	15	0.1
(1,1799)	1:60:A:ILE:HG22	1:60:A:ILE:HD11	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1799)	1:60:A:ILE:HG22	1:60:A:ILE:HD12	15	0.1
(1,1799)	1:60:A:ILE:HG22	1:60:A:ILE:HD13	15	0.1
(1,1799)	1:60:A:ILE:HG23	1:60:A:ILE:HD11	15	0.1
(1,1799)	1:60:A:ILE:HG23	1:60:A:ILE:HD12	15	0.1
(1,1799)	1:60:A:ILE:HG23	1:60:A:ILE:HD13	15	0.1
(1,1792)	1:54:A:ASN:HB3	1:54:A:ASN:HD21	19	0.1
(1,1761)	1:44:A:GLN:H	1:44:A:GLN:HE21	12	0.1
(1,1760)	1:43:A:LEU:HA	1:43:A:LEU:HD11	1	0.1
(1,1760)	1:43:A:LEU:HA	1:43:A:LEU:HD12	1	0.1
(1,1760)	1:43:A:LEU:HA	1:43:A:LEU:HD13	1	0.1
(1,1760)	1:43:A:LEU:HA	1:43:A:LEU:HD21	1	0.1
(1,1760)	1:43:A:LEU:HA	1:43:A:LEU:HD22	1	0.1
(1,1760)	1:43:A:LEU:HA	1:43:A:LEU:HD23	1	0.1
(1,1755)	1:40:A:ASN:H	1:40:A:ASN:HD21	6	0.1
(1,1651)	1:17:A:GLN:H	1:17:A:GLN:HE21	4	0.1
(1,1636)	1:14:A:LYS:HB2	1:14:A:LYS:HE2	2	0.1
(1,1632)	1:14:A:LYS:HA	1:14:A:LYS:HE3	14	0.1
(1,1631)	1:14:A:LYS:HA	1:14:A:LYS:HE2	11	0.1
(1,1631)	1:14:A:LYS:HA	1:14:A:LYS:HE2	18	0.1
(1,1604)	1:12:A:LYS:H	1:12:A:LYS:HD2	12	0.1
(1,1518)	1:114:B:LYS:HB2	1:115:B:ILE:HG12	12	0.1
(1,1476)	1:102:B:LYS:HG3	1:103:B:ASN:HD21	3	0.1
(1,1388)	1:79:B:LYS:HB2	1:80:B:LYS:HG2	19	0.1
(1,1381)	1:78:B:LYS:HD3	1:79:B:LYS:HA	18	0.1
(1,1333)	1:72:B:LEU:HD11	1:73:B:LYS:HB3	3	0.1
(1,1333)	1:72:B:LEU:HD12	1:73:B:LYS:HB3	3	0.1
(1,1333)	1:72:B:LEU:HD13	1:73:B:LYS:HB3	3	0.1
(1,1279)	1:45:A:LEU:HD21	1:46:A:ALA:HA	9	0.1
(1,1279)	1:45:A:LEU:HD22	1:46:A:ALA:HA	9	0.1
(1,1279)	1:45:A:LEU:HD23	1:46:A:ALA:HA	9	0.1
(1,1164)	1:14:A:LYS:HD2	1:15:A:ILE:H	4	0.1
(1,1150)	1:12:A:LYS:HE3	1:13:A:LYS:H	15	0.1
(1,1112)	1:7:A:LYS:HG2	1:8:A:LEU:HA	6	0.1
(1,1101)	1:6:A:LEU:HD11	1:7:A:LYS:HB3	3	0.1
(1,1101)	1:6:A:LEU:HD12	1:7:A:LYS:HB3	3	0.1
(1,1101)	1:6:A:LEU:HD13	1:7:A:LYS:HB3	3	0.1
(1,1075)	1:123:B:LEU:HD11	1:125:B:ASP:H	15	0.1
(1,1075)	1:123:B:LEU:HD12	1:125:B:ASP:H	15	0.1
(1,1075)	1:123:B:LEU:HD13	1:125:B:ASP:H	15	0.1
(1,1052)	1:87:B:ALA:HA	1:89:B:LEU:HG	19	0.1
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG21	9	0.1
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG22	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1044)	1:79:B:LYS:HG3	1:81:B:ILE:HG23	9	0.1
(1,1042)	1:79:B:LYS:HG3	1:81:B:ILE:HA	13	0.1
(1,1036)	1:79:B:LYS:HB2	1:81:B:ILE:HG12	14	0.1
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD11	15	0.1
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD12	15	0.1
(1,1002)	1:55:A:THR:HG21	1:57:A:LEU:HD13	15	0.1
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD11	15	0.1
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD12	15	0.1
(1,1002)	1:55:A:THR:HG22	1:57:A:LEU:HD13	15	0.1
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD11	15	0.1
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD12	15	0.1
(1,1002)	1:55:A:THR:HG23	1:57:A:LEU:HD13	15	0.1
(1,965)	1:13:A:LYS:HB2	1:15:A:ILE:HG12	14	0.1
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD11	2	0.1
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD12	2	0.1
(1,960)	1:7:A:LYS:HG2	1:9:A:ILE:HD13	2	0.1
(1,951)	1:3:A:ILE:HG12	1:5:A:ASN:HD22	20	0.1
(1,947)	1:2:A:ILE:HG21	1:4:A:ASN:HD21	3	0.1
(1,947)	1:2:A:ILE:HG22	1:4:A:ASN:HD21	3	0.1
(1,947)	1:2:A:ILE:HG23	1:4:A:ASN:HD21	3	0.1
(1,848)	1:57:A:LEU:HD11	1:60:A:ILE:H	10	0.1
(1,848)	1:57:A:LEU:HD12	1:60:A:ILE:H	10	0.1
(1,848)	1:57:A:LEU:HD13	1:60:A:ILE:H	10	0.1
(1,737)	1:110:B:GLN:HE21	1:114:B:LYS:HB2	4	0.1
(1,689)	1:81:B:ILE:HG13	1:85:B:GLU:HG2	12	0.1
(1,684)	1:75:B:ILE:HG21	1:79:B:LYS:HG2	18	0.1
(1,684)	1:75:B:ILE:HG22	1:79:B:LYS:HG2	18	0.1
(1,684)	1:75:B:ILE:HG23	1:79:B:LYS:HG2	18	0.1
(1,679)	1:73:B:LYS:HG2	1:77:B:GLU:HG2	16	0.1
(1,603)	1:19:A:GLU:HG2	1:23:A:LEU:HD21	19	0.1
(1,603)	1:19:A:GLU:HG2	1:23:A:LEU:HD22	19	0.1
(1,603)	1:19:A:GLU:HG2	1:23:A:LEU:HD23	19	0.1
(1,535)	1:81:B:ILE:HG21	1:86:B:LEU:HA	7	0.1
(1,535)	1:81:B:ILE:HG22	1:86:B:LEU:HA	7	0.1
(1,535)	1:81:B:ILE:HG23	1:86:B:LEU:HA	7	0.1
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG21	9	0.1
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG22	9	0.1
(1,475)	1:10:A:ARG:HB2	1:15:A:ILE:HG23	9	0.1
(1,390)	1:49:A:ILE:H	1:57:A:LEU:HD21	5	0.1
(1,390)	1:49:A:ILE:H	1:57:A:LEU:HD22	5	0.1
(1,390)	1:49:A:ILE:H	1:57:A:LEU:HD23	5	0.1
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD21	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD22	16	0.1
(1,333)	1:112:B:ALA:HB1	1:123:B:LEU:HD23	16	0.1
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD21	16	0.1
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD22	16	0.1
(1,333)	1:112:B:ALA:HB2	1:123:B:LEU:HD23	16	0.1
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD21	16	0.1
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD22	16	0.1
(1,333)	1:112:B:ALA:HB3	1:123:B:LEU:HD23	16	0.1
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG21	14	0.1
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG22	14	0.1
(1,270)	1:97:B:ILE:HG13	1:115:B:ILE:HG23	14	0.1
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG21	7	0.1
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG22	7	0.1
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG23	7	0.1
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG21	9	0.1
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG22	9	0.1
(1,265)	1:31:A:ILE:HG13	1:49:A:ILE:HG23	9	0.1
(1,239)	1:90:B:LEU:HD21	1:115:B:ILE:HA	14	0.1
(1,239)	1:90:B:LEU:HD22	1:115:B:ILE:HA	14	0.1
(1,239)	1:90:B:LEU:HD23	1:115:B:ILE:HA	14	0.1
(1,233)	1:90:B:LEU:HA	1:115:B:ILE:HG12	16	0.1
(1,229)	1:24:A:LEU:HD21	1:49:A:ILE:HA	20	0.1
(1,229)	1:24:A:LEU:HD22	1:49:A:ILE:HA	20	0.1
(1,229)	1:24:A:LEU:HD23	1:49:A:ILE:HA	20	0.1
(1,217)	1:100:B:ILE:HD11	1:127:B:PHE:HE2	15	0.1
(1,217)	1:100:B:ILE:HD12	1:127:B:PHE:HE2	15	0.1
(1,217)	1:100:B:ILE:HD13	1:127:B:PHE:HE2	15	0.1
(1,216)	1:74:B:LEU:HD21	1:101:B:GLU:HB2	20	0.1
(1,216)	1:74:B:LEU:HD22	1:101:B:GLU:HB2	20	0.1
(1,216)	1:74:B:LEU:HD23	1:101:B:GLU:HB2	20	0.1
(1,207)	1:73:B:LYS:HE2	1:101:B:GLU:HG2	10	0.1
(1,193)	1:7:A:LYS:HD2	1:35:A:GLU:HG3	1	0.1
(1,193)	1:7:A:LYS:HD2	1:35:A:GLU:HG3	17	0.1
(1,172)	1:71:B:ASN:HA	1:101:B:GLU:HB3	2	0.1
(1,170)	1:71:B:ASN:HA	1:101:B:GLU:HA	1	0.1
(1,165)	1:5:A:ASN:HA	1:35:A:GLU:HA	6	0.1
(1,148)	1:2:A:ILE:HG21	1:40:A:ASN:HD21	6	0.1
(1,148)	1:2:A:ILE:HG22	1:40:A:ASN:HD21	6	0.1
(1,148)	1:2:A:ILE:HG23	1:40:A:ASN:HD21	6	0.1
(1,129)	1:13:A:LYS:HD2	1:53:A:LEU:HD21	18	0.1
(1,129)	1:13:A:LYS:HD2	1:53:A:LEU:HD22	18	0.1
(1,129)	1:13:A:LYS:HD2	1:53:A:LEU:HD23	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,108)	1:75:B:ILE:HG21	1:121:B:THR:HG21	10	0.1
(1,108)	1:75:B:ILE:HG21	1:121:B:THR:HG22	10	0.1
(1,108)	1:75:B:ILE:HG21	1:121:B:THR:HG23	10	0.1
(1,108)	1:75:B:ILE:HG22	1:121:B:THR:HG21	10	0.1
(1,108)	1:75:B:ILE:HG22	1:121:B:THR:HG22	10	0.1
(1,108)	1:75:B:ILE:HG22	1:121:B:THR:HG23	10	0.1
(1,108)	1:75:B:ILE:HG23	1:121:B:THR:HG21	10	0.1
(1,108)	1:75:B:ILE:HG23	1:121:B:THR:HG22	10	0.1
(1,108)	1:75:B:ILE:HG23	1:121:B:THR:HG23	10	0.1
(1,104)	1:9:A:ILE:HG21	1:55:A:THR:HG21	2	0.1
(1,104)	1:9:A:ILE:HG21	1:55:A:THR:HG22	2	0.1
(1,104)	1:9:A:ILE:HG21	1:55:A:THR:HG23	2	0.1
(1,104)	1:9:A:ILE:HG22	1:55:A:THR:HG21	2	0.1
(1,104)	1:9:A:ILE:HG22	1:55:A:THR:HG22	2	0.1
(1,104)	1:9:A:ILE:HG22	1:55:A:THR:HG23	2	0.1
(1,104)	1:9:A:ILE:HG23	1:55:A:THR:HG21	2	0.1
(1,104)	1:9:A:ILE:HG23	1:55:A:THR:HG22	2	0.1
(1,104)	1:9:A:ILE:HG23	1:55:A:THR:HG23	2	0.1
(1,49)	1:3:A:ILE:HD11	1:62:A:GLN:HG3	2	0.1
(1,49)	1:3:A:ILE:HD12	1:62:A:GLN:HG3	2	0.1
(1,49)	1:3:A:ILE:HD13	1:62:A:GLN:HG3	2	0.1
(1,4)	1:2:A:ILE:H	1:64:A:GLN:HB2	16	0.1
(1,1)	1:2:A:ILE:H	1:64:A:GLN:HB2	16	0.1

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

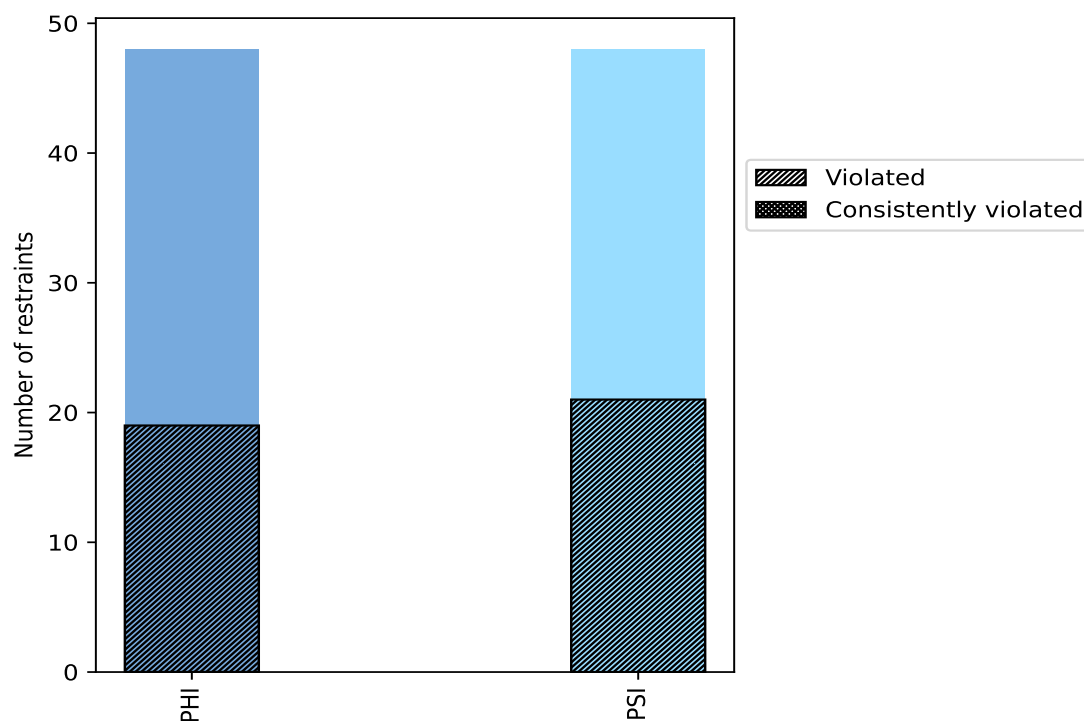
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	48	50.0	19	39.6	19.8	0	0.0	0.0
PSI	48	50.0	21	43.8	21.9	0	0.0	0.0
Total	96	100.0	40	41.7	41.7	0	0.0	0.0

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 [i](#)



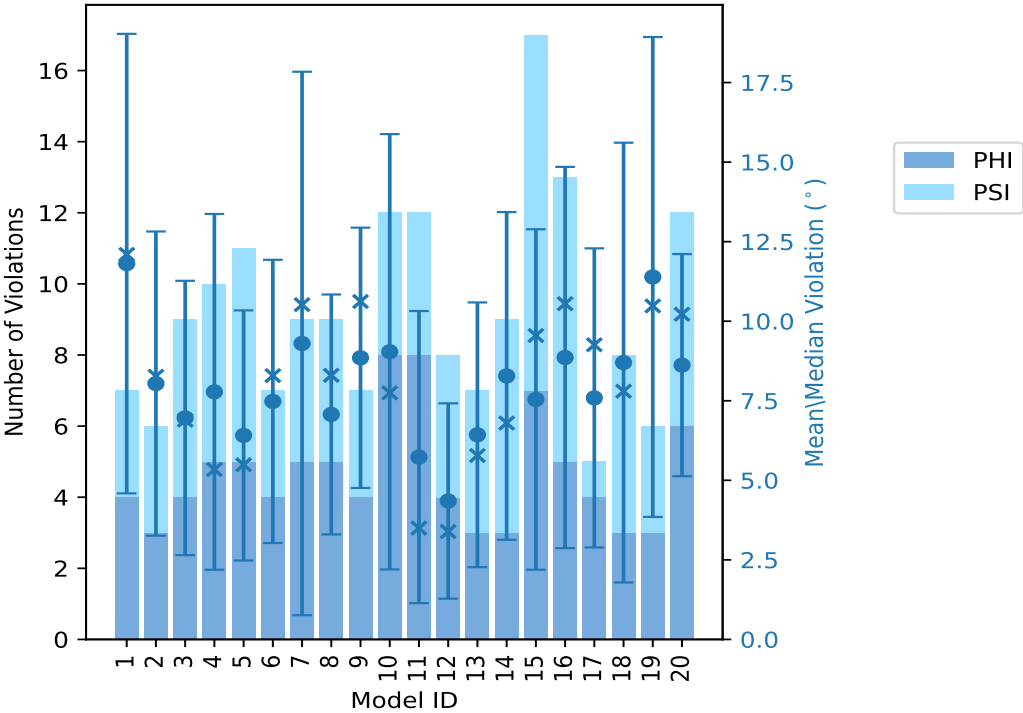
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [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 (°)
	PHI	PSI	Total				
1	4	3	7	11.81	27.17	7.22	12.1
2	3	3	6	8.04	13.05	4.78	8.27
3	4	5	9	6.96	12.33	4.31	6.89
4	5	5	10	7.78	18.37	5.59	5.34
5	5	6	11	6.41	13.83	3.93	5.49
6	4	3	7	7.48	12.94	4.45	8.29
7	5	4	9	9.3	29.76	8.54	10.52
8	5	4	9	7.07	11.83	3.77	8.3
9	4	3	7	8.85	13.01	4.09	10.62
10	8	4	12	9.04	25.41	6.84	7.75
11	8	4	12	5.73	13.94	4.59	3.5
12	4	4	8	4.35	10.89	3.07	3.39
13	3	4	7	6.43	12.92	4.16	5.78
14	3	6	9	8.28	17.11	5.15	6.8
15	7	10	17	7.54	20.74	5.35	9.55
16	5	8	13	8.86	23.55	5.99	10.55
17	4	1	5	7.59	12.87	4.7	9.26
18	3	5	8	8.7	25.04	6.91	7.8
19	3	3	6	11.39	26.28	7.54	10.48
20	6	6	12	8.62	13.49	3.49	10.22

10.2.1 Bar graph : Dihedral 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

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	
PHI	PSI	Total	Count ¹	%
4	7	11	1	5.0
4	3	7	2	10.0
3	2	5	3	15.0
1	2	3	4	20.0
2	3	5	5	25.0
0	1	1	6	30.0
1	1	2	7	35.0
0	0	0	8	40.0
1	0	1	9	45.0
0	0	0	10	50.0
1	0	1	11	55.0

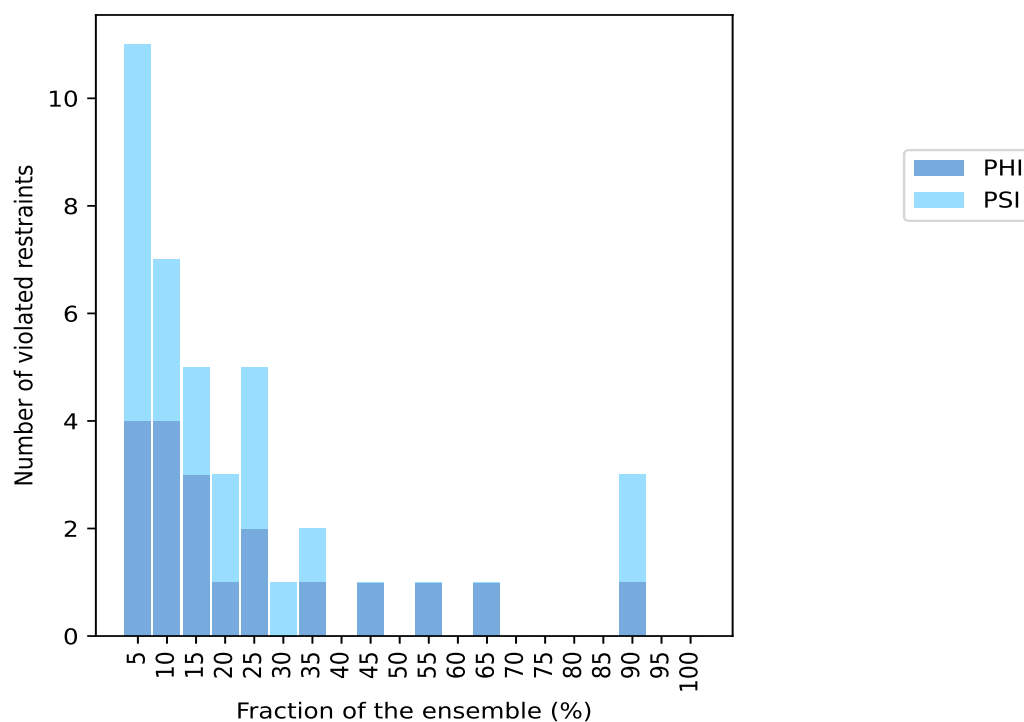
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
1	0	1	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
1	2	3	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)

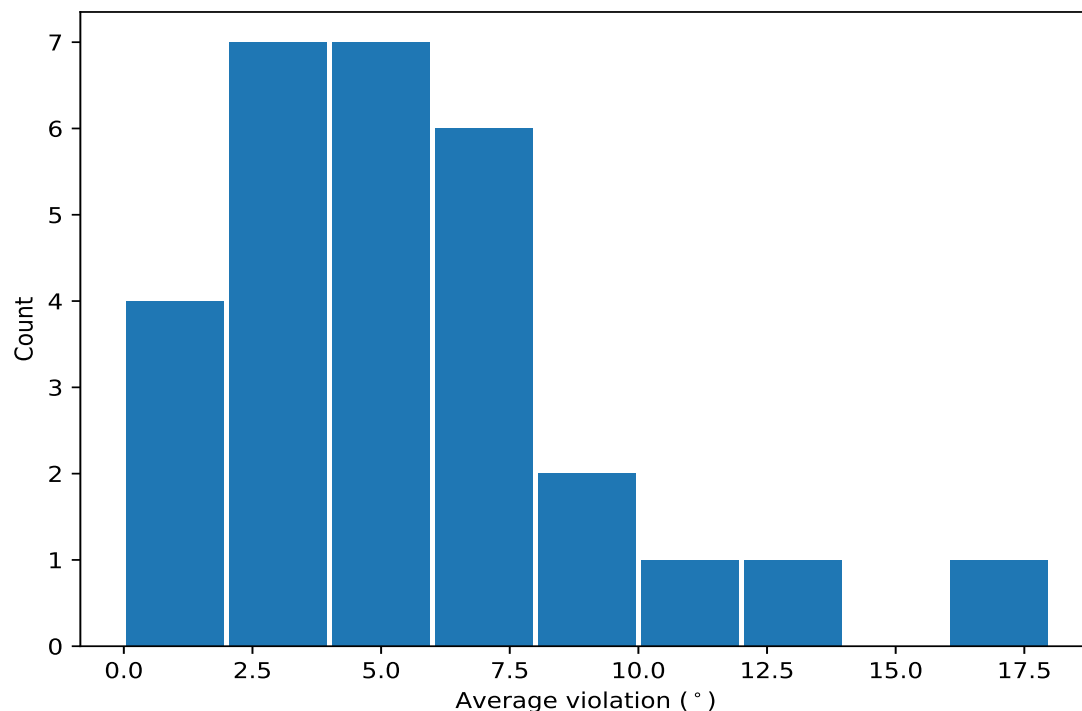


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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

in the ensemble



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
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	18	16.81	7.63	15.3
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	18	12.71	0.7	12.77
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	18	11.7	2.34	12.12
(1,3)	1:6:A:LEU:C	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	13	5.75	3.78	5.78
(1,29)	1:32:A:ASN:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	11	9.94	3.55	11.01
(1,25)	1:28:A:ARG:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	9	3.75	3.0	2.44
(1,28)	1:31:A:ILE:C	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	7	7.38	2.47	8.29
(1,55)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:LYS:N	7	3.69	1.38	3.8
(1,54)	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	1:12:A:LYS:N	6	7.44	3.48	9.36
(1,61)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:GLU:N	5	6.56	3.4	6.8
(1,47)	1:57:A:LEU:C	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	5	4.32	2.71	3.36
(1,60)	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	1:18:A:SER:N	5	4.3	2.51	3.42
(1,13)	1:16:A:SER:C	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	5	3.0	1.39	2.64
(1,59)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:GLN:N	5	1.56	0.54	1.43
(1,90)	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	1:54:A:ASN:N	4	8.32	2.88	8.19
(1,62)	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	1:20:A:LEU:N	4	3.93	2.33	3.56
(1,1)	1:1:A:MET:C	1:2:A:ILE:N	1:2:A:ILE:CA	1:2:A:ILE:C	4	1.77	0.85	1.44
(1,43)	1:51:A:TYR:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	3	6.9	4.18	6.58
(1,41)	1:49:A:ILE:C	1:50:A:ALA:N	1:50:A:ALA:CA	1:50:A:ALA:C	3	6.33	4.69	4.97
(1,23)	1:26:A:VAL:C	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	3	4.28	2.3	3.79

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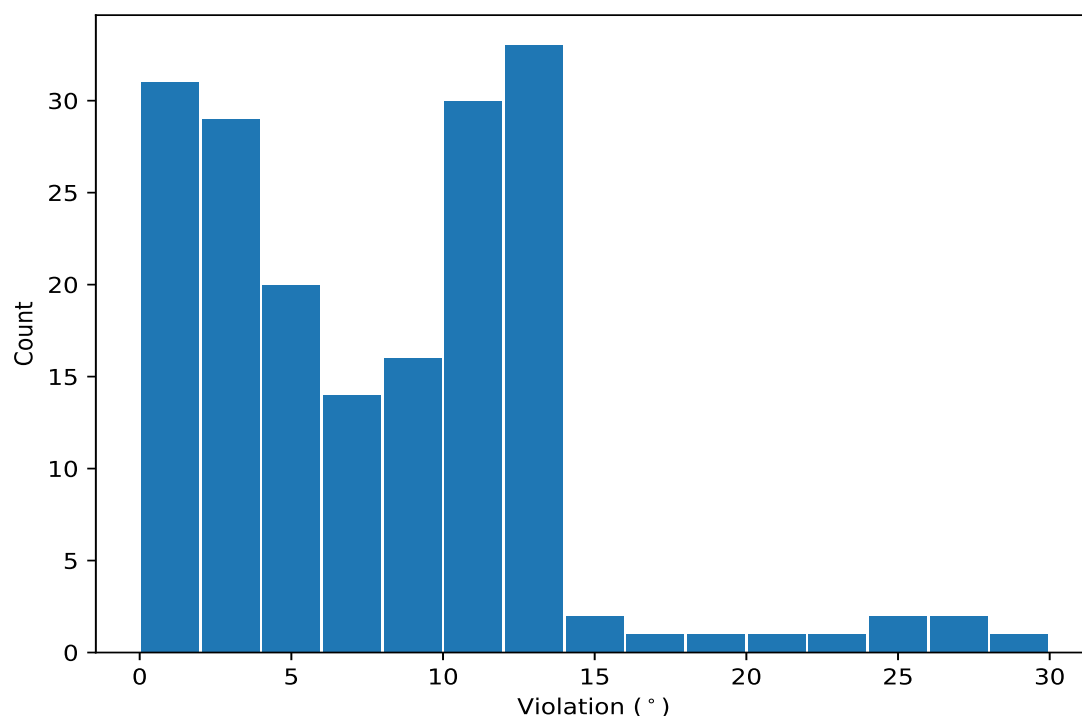
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,50)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:LEU:N	3	3.7	1.15	4.35
(1,95)	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	1:60:A:ILE:N	3	1.91	0.66	2.23
(1,87)	1:50:A:ALA:N	1:50:A:ALA:CA	1:50:A:ALA:C	1:51:A:TYR:N	2	7.13	5.67	7.13
(1,7)	1:10:A:ARG:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	2	4.63	0.09	4.63
(1,34)	1:42:A:SER:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	2	4.36	1.42	4.36
(1,74)	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	1:34:A:ILE:N	2	4.16	2.72	4.16
(1,94)	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	1:59:A:ASP:N	2	3.56	1.94	3.56
(1,8)	1:11:A:GLU:C	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	2	3.0	0.68	3.0
(1,45)	1:54:A:ASN:C	1:55:A:THR:N	1:55:A:THR:CA	1:55:A:THR:C	2	1.46	0.4	1.46

¹ Number of violated models, ²Standard 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 (°)
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	7	29.76
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	1	27.17
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	19	26.28
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	10	25.41
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	18	25.04
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	16	23.55
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	15	20.74
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	4	18.37
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	14	17.11
(1,29)	1:32:A:ASN:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	10	14.14
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	10	14.01
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	11	13.94
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	5	13.83
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	10	13.78
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	14	13.77
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	20	13.49
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	15	13.24
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	7	13.07
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	2	13.05
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	9	13.01
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	4	13.01
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	2	12.94
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	6	12.94
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	13	12.92
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	17	12.87
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	19	12.82
(1,87)	1:50:A:ALA:N	1:50:A:ALA:CA	1:50:A:ALA:C	1:51:A:TYR:N	16	12.8
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	4	12.78
(1,29)	1:32:A:ASN:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	1	12.73
(1,29)	1:32:A:ASN:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	4	12.71
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	19	12.68
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	1	12.65
(1,41)	1:49:A:ILE:C	1:50:A:ALA:N	1:50:A:ALA:CA	1:50:A:ALA:C	16	12.64
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	9	12.39
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	3	12.33
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	2	12.31
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	16	12.24
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	14	12.21
(1,43)	1:51:A:TYR:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	9	12.18
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1	12.1
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	6	12.03
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	11	12.02
(1,29)	1:32:A:ASN:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	15	12.01
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	16	12.0
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	3	11.97
(1,90)	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	1:54:A:ASN:N	10	11.93
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	8	11.83
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	17	11.79
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	8	11.66
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	13	11.62
(1,20)	1:23:A:LEU:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	20	11.49
(1,48)	1:58:A:GLU:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	15	11.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	5	11.09
(1,29)	1:32:A:ASN:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	7	11.05
(1,29)	1:32:A:ASN:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	20	11.01
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	12	10.89
(1,54)	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	1:12:A:LYS:N	3	10.88
(1,29)	1:32:A:ASN:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	18	10.87
(1,28)	1:31:A:ILE:C	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	7	10.85
(1,4)	1:7:A:LYS:C	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:C	11	10.84
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	15	10.79
(1,29)	1:32:A:ASN:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	16	10.78
(1,76)	1:35:A:GLU:N	1:35:A:GLU:CA	1:35:A:GLU:C	1:36:A:LYS:N	20	10.69
(1,61)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:GLU:N	3	10.68
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	9	10.62
(1,3)	1:6:A:LEU:C	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	20	10.6
(1,80)	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	1:44:A:GLN:N	16	10.55
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	7	10.52
(1,3)	1:6:A:LEU:C	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	15	10.5
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	6	10.4
(1,90)	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	1:54:A:ASN:N	14	10.28
(1,25)	1:28:A:ARG:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	20	10.25
(1,71)	1:30:A:THR:N	1:30:A:THR:CA	1:30:A:THR:C	1:31:A:ILE:N	20	10.19
(1,3)	1:6:A:LEU:C	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	5	10.14
(1,93)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:GLU:N	15	9.96
(1,61)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:GLU:N	8	9.84
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	11	9.81
(1,54)	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	1:12:A:LYS:N	15	9.71
(1,54)	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	1:12:A:LYS:N	8	9.69
(1,28)	1:31:A:ILE:C	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	18	9.63
(1,88)	1:51:A:TYR:N	1:51:A:TYR:CA	1:51:A:TYR:C	1:52:A:TYR:N	15	9.55
(1,3)	1:6:A:LEU:C	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	17	9.26
(1,47)	1:57:A:LEU:C	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	5	9.07
(1,54)	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	1:12:A:LYS:N	20	9.04
(1,28)	1:31:A:ILE:C	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1	8.75
(1,3)	1:6:A:LEU:C	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	18	8.72
(1,60)	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	1:18:A:SER:N	8	8.3
(1,28)	1:31:A:ILE:C	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	19	8.29
(1,3)	1:6:A:LEU:C	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	6	8.29
(1,25)	1:28:A:ARG:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	10	8.13
(1,29)	1:32:A:ASN:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	9	7.45
(1,2)	1:5:A:ASN:C	1:6:A:LEU:N	1:6:A:LEU:CA	1:6:A:LEU:C	11	7.44
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	13	7.43
(1,44)	1:52:A:TYR:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	10	7.37
(1,62)	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	1:20:A:LEU:N	1	7.31
(1,23)	1:26:A:VAL:C	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	20	7.3
(1,74)	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	1:34:A:ILE:N	18	6.89
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	3	6.89
(1,61)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:GLU:N	14	6.8
(1,73)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLY:N	5	6.64
(1,43)	1:51:A:TYR:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	12	6.58
(1,55)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:LYS:N	6	6.14
(1,90)	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	1:54:A:ASN:N	16	6.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,60)	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	1:18:A:SER:N	14	6.0
(1,34)	1:42:A:SER:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	12	5.78
(1,3)	1:6:A:LEU:C	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	13	5.78
(1,28)	1:31:A:ILE:C	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	14	5.74
(1,96)	1:60:A:ILE:N	1:60:A:ILE:CA	1:60:A:ILE:C	1:61:A:PHE:N	4	5.7
(1,94)	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	1:59:A:ASP:N	5	5.49
(1,47)	1:57:A:LEU:C	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	10	5.4
(1,41)	1:49:A:ILE:C	1:50:A:ALA:N	1:50:A:ALA:CA	1:50:A:ALA:C	9	4.97
(1,13)	1:16:A:SER:C	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	4	4.97
(1,90)	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	1:54:A:ASN:N	15	4.96
(1,62)	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	1:20:A:LEU:N	7	4.79
(1,7)	1:10:A:ARG:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	8	4.72
(1,50)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:LEU:N	11	4.66
(1,7)	1:10:A:ARG:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	20	4.54
(1,29)	1:32:A:ASN:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	19	4.45
(1,50)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:LEU:N	5	4.35
(1,55)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:LYS:N	5	4.27
(1,28)	1:31:A:ILE:C	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	16	4.27
(1,13)	1:16:A:SER:C	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	2	4.23
(1,55)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:LYS:N	16	4.17
(1,28)	1:31:A:ILE:C	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	15	4.13
(1,55)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:LYS:N	19	3.8
(1,23)	1:26:A:VAL:C	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	4	3.79
(1,54)	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	1:12:A:LYS:N	2	3.78
(1,8)	1:11:A:GLU:C	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	13	3.68
(1,55)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:LYS:N	18	3.52
(1,60)	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	1:18:A:SER:N	12	3.42
(1,61)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:GLU:N	18	3.38
(1,47)	1:57:A:LEU:C	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	12	3.36
(1,25)	1:28:A:ARG:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	3	3.31
(1,1)	1:1:A:MET:C	1:2:A:ILE:N	1:2:A:ILE:CA	1:2:A:ILE:C	8	3.18
(1,3)	1:6:A:LEU:C	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	3	3.16
(1,34)	1:42:A:SER:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	16	2.94
(1,67)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:GLU:N	20	2.78
(1,3)	1:6:A:LEU:C	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	8	2.66
(1,13)	1:16:A:SER:C	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	10	2.64
(1,59)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:GLN:N	15	2.61
(1,55)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:LYS:N	4	2.59
(1,25)	1:28:A:ARG:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	5	2.59
(1,95)	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	1:60:A:ILE:N	10	2.51
(1,25)	1:28:A:ARG:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	4	2.44
(1,62)	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	1:20:A:LEU:N	12	2.33
(1,8)	1:11:A:GLU:C	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	11	2.33
(1,47)	1:57:A:LEU:C	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	15	2.24
(1,95)	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	1:60:A:ILE:N	13	2.23
(1,60)	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	1:18:A:SER:N	3	2.22
(1,25)	1:28:A:ARG:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	17	2.17
(1,29)	1:32:A:ASN:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	11	2.14
(1,61)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:GLU:N	16	2.09
(1,50)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:LEU:N	20	2.08
(1,43)	1:51:A:TYR:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	1	1.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,3)	1:6:A:LEU:C	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	2	1.94
(1,45)	1:54:A:ASN:C	1:55:A:THR:N	1:55:A:THR:CA	1:55:A:THR:C	17	1.85
(1,25)	1:28:A:ARG:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	8	1.79
(1,13)	1:16:A:SER:C	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	15	1.76
(1,23)	1:26:A:VAL:C	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	5	1.74
(1,1)	1:1:A:MET:C	1:2:A:ILE:N	1:2:A:ILE:CA	1:2:A:ILE:C	10	1.7
(1,94)	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	1:59:A:ASP:N	15	1.62
(1,25)	1:28:A:ARG:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	11	1.58
(1,60)	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	1:18:A:SER:N	15	1.55
(1,54)	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	1:12:A:LYS:N	18	1.54
(1,47)	1:57:A:LEU:C	1:58:A:GLU:N	1:58:A:GLU:CA	1:58:A:GLU:C	14	1.52
(1,25)	1:28:A:ARG:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	6	1.47
(1,87)	1:50:A:ALA:N	1:50:A:ALA:CA	1:50:A:ALA:C	1:51:A:TYR:N	11	1.46
(1,59)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:GLN:N	4	1.45
(1,74)	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	1:34:A:ILE:N	15	1.44
(1,59)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:GLN:N	12	1.43
(1,3)	1:6:A:LEU:C	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	10	1.43
(1,13)	1:16:A:SER:C	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	7	1.4
(1,41)	1:49:A:ILE:C	1:50:A:ALA:N	1:50:A:ALA:CA	1:50:A:ALA:C	11	1.39
(1,89)	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	1:53:A:LEU:N	9	1.36
(1,55)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:LYS:N	13	1.36
(1,62)	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	1:20:A:LEU:N	5	1.3
(1,59)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:GLN:N	7	1.21
(1,3)	1:6:A:LEU:C	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	11	1.19
(1,1)	1:1:A:MET:C	1:2:A:ILE:N	1:2:A:ILE:CA	1:2:A:ILE:C	3	1.17
(1,59)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:GLN:N	14	1.12
(1,45)	1:54:A:ASN:C	1:55:A:THR:N	1:55:A:THR:CA	1:55:A:THR:C	6	1.06
(1,3)	1:6:A:LEU:C	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	12	1.04
(1,1)	1:1:A:MET:C	1:2:A:ILE:N	1:2:A:ILE:CA	1:2:A:ILE:C	7	1.04
(1,95)	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	1:60:A:ILE:N	16	1.0