



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 02:29 PM UTC

PDB ID : 2LXC / pdb_00002lxc
BMRB ID : 18671
Title : Solution structure of the complex between the Sgt2 homodimerization domain and the Get5 UBL domain
Authors : Chartron, J.W.; Vandervelde, D.G.; Clemons Jr., W.M.
Deposited on : 2012-08-19

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

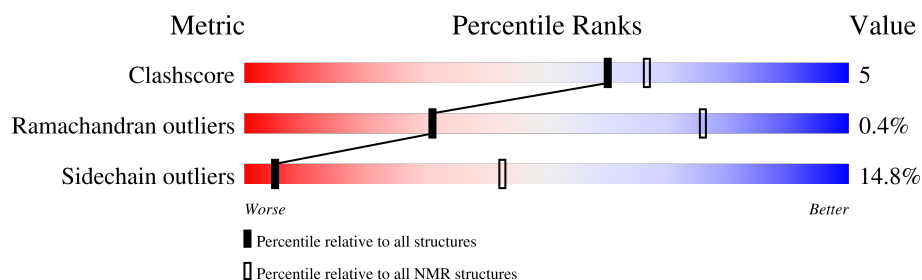
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 60%.

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	81	 75% 20% 5%
2	B	74	 64% 12% 24%
2	C	74	 64% 14% 23%

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:74-A:150, B:4-B:59, C:3-C:59 (190)	0.74	8

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 2 clusters and 3 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3521 atoms, of which 1771 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin-like protein MDY2.

Mol	Chain	Residues	Atoms						Trace
1	A	81	Total	C	H	N	O	S	0
			1337	416	693	107	119	2	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	MET	-	initiating methionine	UNP Q12285
A	152	LEU	-	expression tag	UNP Q12285
A	153	GLU	-	expression tag	UNP Q12285

- Molecule 2 is a protein called Small glutamine-rich tetratricopeptide repeat-containing protein 2.

Mol	Chain	Residues	Atoms						Trace
2	B	74	Total	C	H	N	O	S	0
			1092	344	539	88	119	2	
2	C	74	Total	C	H	N	O	S	0
			1092	344	539	88	119	2	

There are 6 discrepancies between the modelled and reference sequences:

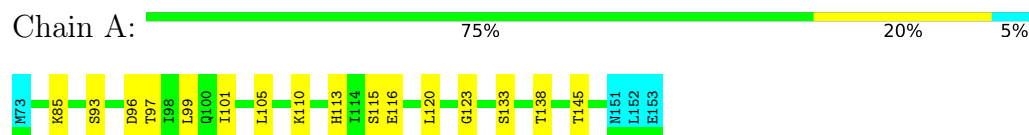
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	expression tag	UNP Q12118
B	0	VAL	-	expression tag	UNP Q12118
B	1	ASP	-	expression tag	UNP Q12118
C	-1	SER	-	expression tag	UNP Q12118
C	0	VAL	-	expression tag	UNP Q12118
C	1	ASP	-	expression tag	UNP Q12118

4 Residue-property plots

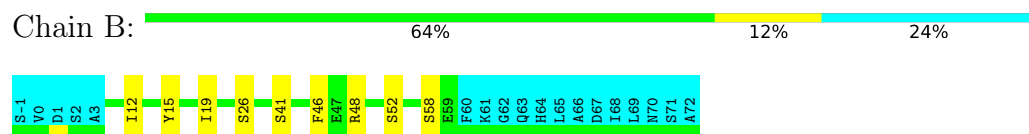
4.1 Average score per residue in the NMR ensemble

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.

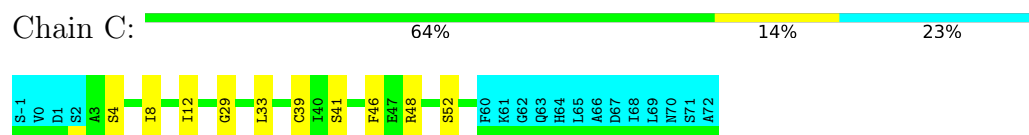
- Molecule 1: Ubiquitin-like protein MDY2



- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2



- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2

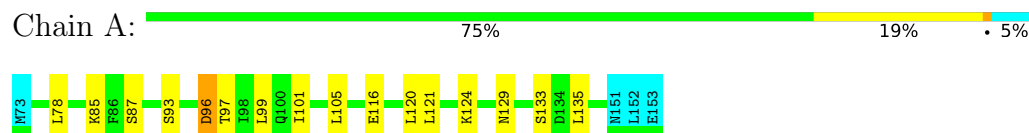


4.2 Scores per residue for each member of the ensemble

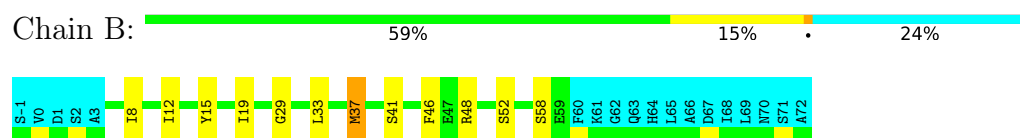
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

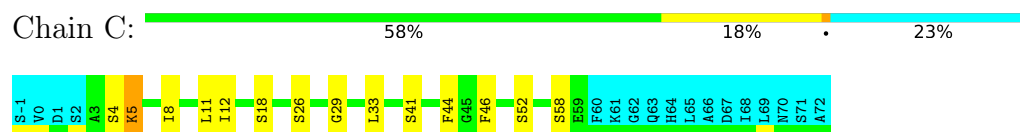
- Molecule 1: Ubiquitin-like protein MDY2



- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2

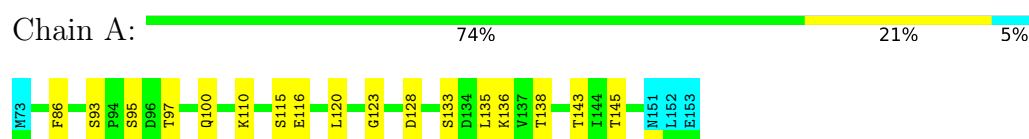


- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2

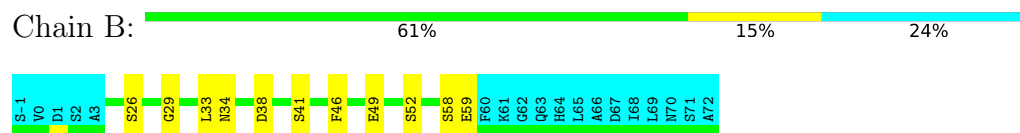


4.2.2 Score per residue for model 2

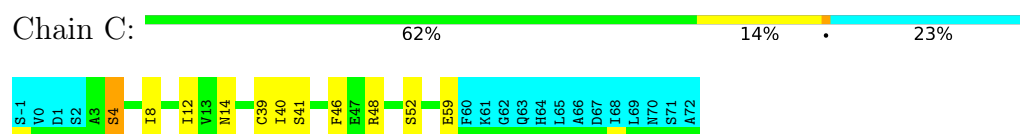
- Molecule 1: Ubiquitin-like protein MDY2



- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2

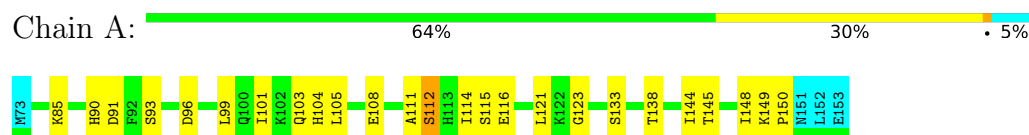


- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2

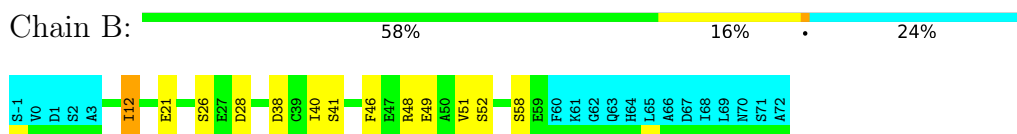


4.2.3 Score per residue for model 3

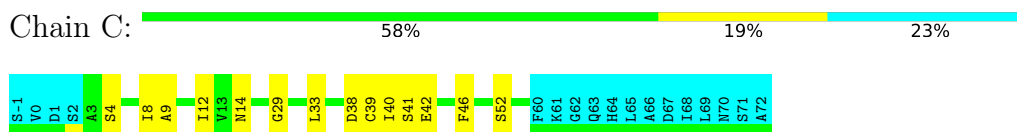
- Molecule 1: Ubiquitin-like protein MDY2



- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2

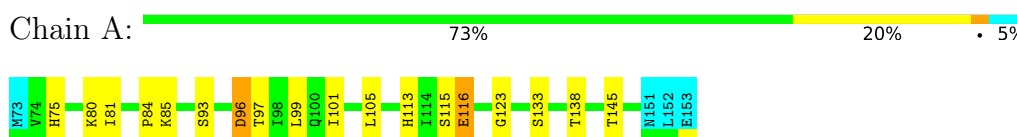


- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2

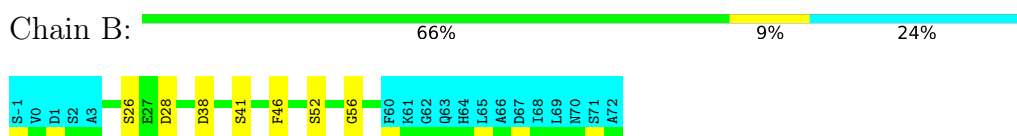


4.2.4 Score per residue for model 4

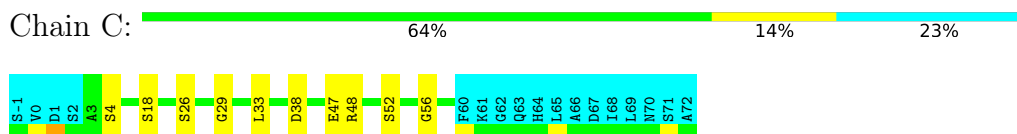
- Molecule 1: Ubiquitin-like protein MDY2



- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2

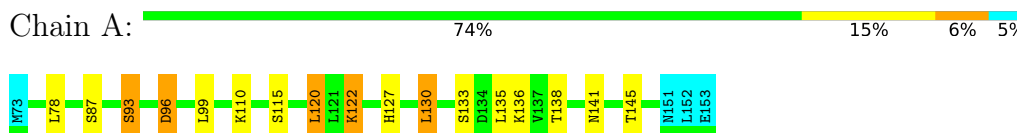


- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2



4.2.5 Score per residue for model 5

- Molecule 1: Ubiquitin-like protein MDY2

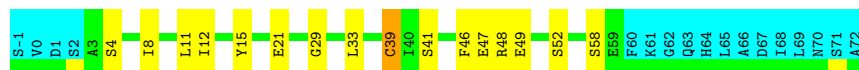


- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2





- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2



4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin-like protein MDY2



- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2



- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2



4.2.7 Score per residue for model 7

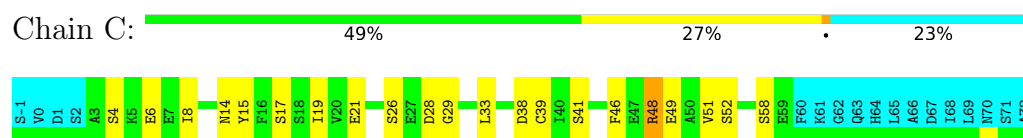
- Molecule 1: Ubiquitin-like protein MDY2



- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2

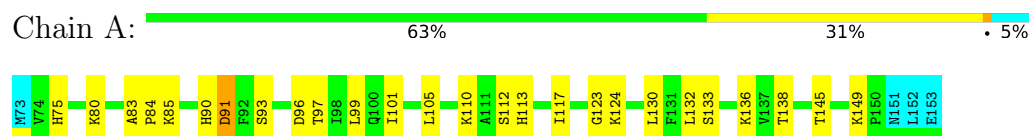


- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2

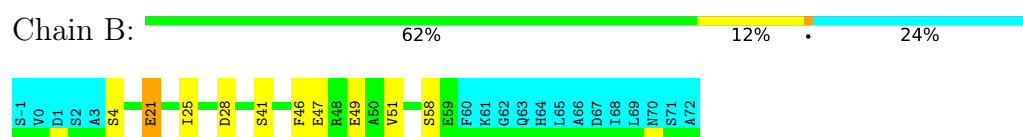


4.2.8 Score per residue for model 8 (medoid)

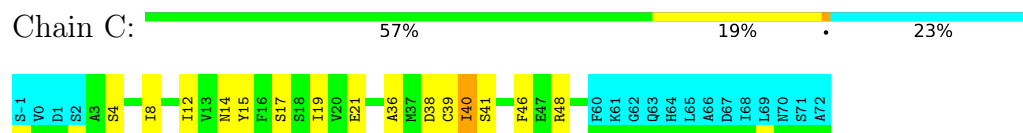
- Molecule 1: Ubiquitin-like protein MDY2



- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2

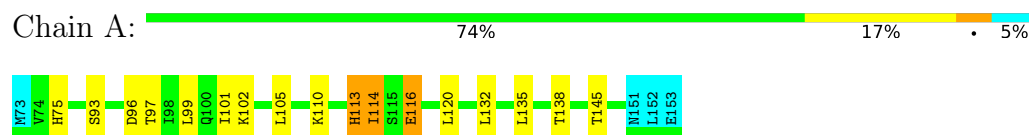


- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2

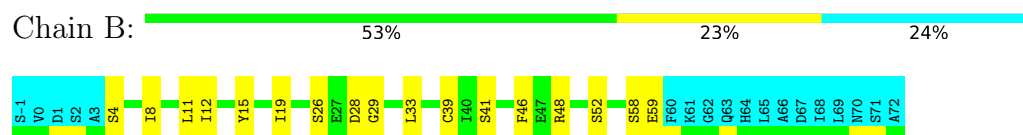


4.2.9 Score per residue for model 9

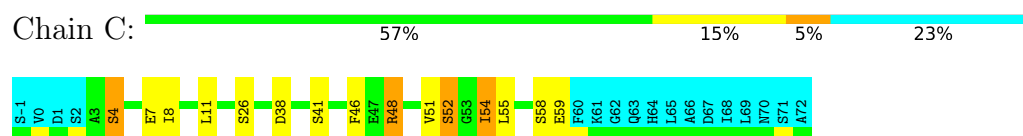
- Molecule 1: Ubiquitin-like protein MDY2



- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2

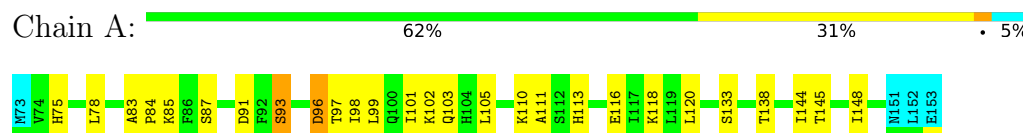


- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2

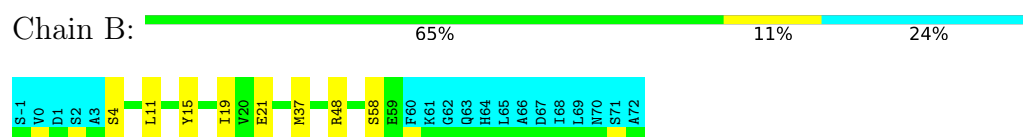


4.2.10 Score per residue for model 10

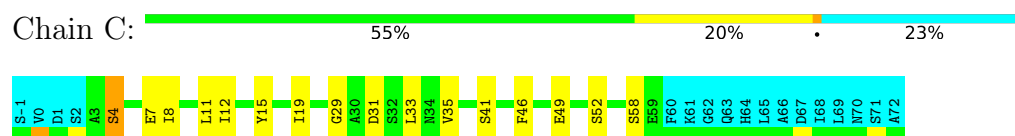
- Molecule 1: Ubiquitin-like protein MDY2



- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2



- Molecule 2: Small glutamine-rich tetratricopeptide repeat-containing protein 2



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, experimentally driven docking*.

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure solution	2.3
ARIA	refinement	2.3
HADDOCK	structure solution	2.1

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	1621
Number of shifts mapped to atoms	1621
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	60%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	610	659	654	6±3
2	B	421	410	410	4±2
2	C	426	415	415	6±2
All	All	14570	14840	14790	133

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:41:SER:HA	2:C:46:PHE:CE1	0.72	2.19	10	9
1:A:123:GLY:HA2	2:C:39:CYS:SG	0.64	2.32	6	5
2:B:8:ILE:O	2:B:12:ILE:HG13	0.61	1.94	9	3
2:B:41:SER:HA	2:B:46:PHE:CE1	0.59	2.32	1	9
2:C:8:ILE:O	2:C:12:ILE:HG13	0.55	2.00	1	3
2:C:29:GLY:O	2:C:33:LEU:HG	0.55	2.01	6	7
2:B:15:TYR:O	2:B:19:ILE:HG12	0.54	2.03	1	6
2:B:12:ILE:HD12	2:C:12:ILE:HG12	0.54	1.79	5	1
1:A:101:ILE:O	1:A:105:LEU:HG	0.53	2.02	8	7
2:C:12:ILE:HG21	2:C:40:ILE:HD13	0.53	1.78	3	1
1:A:111:ALA:HB2	1:A:148:ILE:HD13	0.53	1.80	10	3
1:A:123:GLY:HA3	2:C:38:ASP:CB	0.52	2.34	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:32:SER:HB3	2:C:39:CYS:SG	0.52	2.44	5	1
1:A:127:HIS:HB2	1:A:130:LEU:HD13	0.51	1.83	5	1
1:A:93:SER:O	1:A:96:ASP:HB2	0.50	2.06	3	6
2:B:8:ILE:O	2:B:12:ILE:HG12	0.50	2.06	5	1
2:B:29:GLY:O	2:B:33:LEU:HG	0.50	2.07	1	3
2:C:15:TYR:O	2:C:19:ILE:HG12	0.49	2.08	10	4
2:B:37:MET:SD	2:B:48:ARG:HD2	0.48	2.48	1	2
2:B:8:ILE:HG13	2:C:15:TYR:CE2	0.48	2.43	5	1
1:A:123:GLY:O	2:C:39:CYS:HA	0.48	2.09	3	1
2:B:15:TYR:CE1	2:C:8:ILE:HG13	0.47	2.45	1	1
2:B:12:ILE:HG21	2:B:40:ILE:HD13	0.47	1.85	3	1
1:A:113:HIS:O	1:A:117:ILE:HG13	0.47	2.09	8	1
1:A:104:HIS:O	1:A:108:GLU:HG2	0.47	2.10	7	2
1:A:81:ILE:O	1:A:85:LYS:HG2	0.47	2.10	4	1
1:A:93:SER:O	1:A:132:LEU:HD12	0.47	2.10	8	3
2:B:24:GLU:O	2:C:5:LYS:HE2	0.47	2.09	6	1
1:A:78:LEU:O	1:A:87:SER:HA	0.46	2.10	10	3
2:C:38:ASP:OD2	2:C:48:ARG:HD3	0.46	2.11	9	1
1:A:83:ALA:HA	1:A:84:PRO:C	0.46	2.35	8	2
2:B:21:GLU:OE1	2:B:21:GLU:HA	0.46	2.10	8	1
2:C:7:GLU:HG3	2:C:54:ILE:O	0.45	2.11	9	1
1:A:80:LYS:HG2	1:A:84:PRO:O	0.45	2.12	8	2
1:A:113:HIS:HB3	1:A:116:GLU:CD	0.45	2.36	9	1
1:A:115:SER:HB3	1:A:116:GLU:OE2	0.45	2.10	4	1
1:A:120:LEU:HD21	2:B:35:VAL:HG11	0.45	1.87	7	2
2:C:4:SER:O	2:C:8:ILE:HG12	0.45	2.11	2	5
2:C:36:ALA:O	2:C:40:ILE:HD12	0.44	2.13	8	1
2:C:41:SER:HB3	2:C:46:PHE:O	0.44	2.13	9	1
2:C:8:ILE:O	2:C:12:ILE:HD13	0.44	2.13	2	1
1:A:120:LEU:HD11	2:C:39:CYS:SG	0.44	2.53	5	1
2:C:5:LYS:HB2	2:C:44:PHE:CE1	0.43	2.48	1	1
1:A:122:LYS:HG2	1:A:141:ASN:ND2	0.43	2.28	5	1
1:A:98:ILE:O	1:A:102:LYS:HG3	0.43	2.14	10	1
1:A:121:LEU:HD13	1:A:144:ILE:HD13	0.43	1.89	3	1
1:A:121:LEU:O	1:A:124:LYS:HB3	0.42	2.13	1	1
1:A:103:GLN:OE1	1:A:103:GLN:HA	0.42	2.15	10	2
1:A:112:SER:OG	1:A:150:PRO:HA	0.42	2.14	3	1
1:A:115:SER:HB2	1:A:116:GLU:OE2	0.42	2.14	7	1
1:A:120:LEU:HG	2:C:35:VAL:HG22	0.41	1.92	10	1
2:B:15:TYR:CD2	2:C:8:ILE:HG21	0.41	2.51	10	1
2:B:38:ASP:OD1	2:B:48:ARG:HD3	0.41	2.15	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:8:ILE:O	2:B:12:ILE:HD13	0.41	2.16	1	1
2:B:15:TYR:CZ	2:C:8:ILE:HG13	0.41	2.51	1	1
2:C:9:ALA:HB1	2:C:46:PHE:CE1	0.41	2.51	3	1
1:A:102:LYS:HD3	1:A:114:ILE:HG13	0.41	1.92	9	1
1:A:149:LYS:HD3	2:B:38:ASP:OD2	0.40	2.16	3	1
1:A:147:MET:HE2	2:B:39:CYS:SG	0.40	2.56	7	1
1:A:86:PHE:CZ	1:A:110:LYS:HB3	0.40	2.50	2	1
2:C:48:ARG:O	2:C:51:VAL:HG13	0.40	2.17	7	1
2:C:17:SER:O	2:C:21:GLU:HB2	0.40	2.16	8	1
2:C:4:SER:HB2	2:C:7:GLU:OE1	0.40	2.16	10	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	77/81 (95%)	73±1 (95±2%)	4±2 (5±2%)	0±0 (0±1%)	31	76
2	B	56/74 (76%)	52±2 (93±4%)	4±2 (6±4%)	0±0 (0±1%)	44	80
2	C	57/74 (77%)	54±2 (95±4%)	3±2 (5±3%)	0±1 (1±1%)	26	74
All	All	1900/2290 (83%)	1793 (94%)	100 (5%)	7 (0%)	31	76

All 5 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	136	LYS	3
2	C	56	GLY	1
2	B	59	GLU	1
2	C	51	VAL	1
2	C	59	GLU	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	73/77 (95%)	61±2 (83±3%)	12±2 (17±3%)	4	38
2	B	46/60 (77%)	40±2 (87±4%)	6±2 (13±4%)	6	47
2	C	46/60 (77%)	40±2 (87±5%)	6±2 (13±5%)	6	45
All	All	1650/1970 (84%)	1405 (85%)	245 (15%)	5	43

All 76 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	99	LEU	9
1	A	138	THR	9
1	A	145	THR	9
1	A	96	ASP	8
1	A	116	GLU	8
1	A	133	SER	8
2	C	52	SER	8
1	A	97	THR	7
2	B	52	SER	7
2	B	58	SER	7
2	B	26	SER	6
2	C	48	ARG	6
1	A	85	LYS	5
1	A	135	LEU	5
2	C	4	SER	5
2	C	11	LEU	5
2	C	26	SER	5
2	C	58	SER	5
2	B	49	GLU	5
2	C	14	ASN	5
2	B	28	ASP	5
1	A	110	LYS	5
1	A	120	LEU	4
1	A	115	SER	4
1	A	91	ASP	4
1	A	75	HIS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	113	HIS	4
2	B	4	SER	4
2	C	49	GLU	4
1	A	93	SER	3
1	A	95	SER	3
2	B	38	ASP	3
1	A	90	HIS	3
1	A	112	SER	3
2	B	21	GLU	3
2	B	48	ARG	3
2	B	51	VAL	3
2	B	11	LEU	3
2	B	47	GLU	3
2	C	18	SER	2
1	A	143	THR	2
2	C	40	ILE	2
1	A	114	ILE	2
2	C	47	GLU	2
1	A	130	LEU	2
2	C	21	GLU	2
1	A	144	ILE	2
1	A	129	ASN	1
2	B	37	MET	1
2	C	5	LYS	1
1	A	100	GLN	1
1	A	128	ASP	1
2	B	34	ASN	1
2	B	59	GLU	1
2	C	59	GLU	1
2	B	12	ILE	1
2	C	42	GLU	1
1	A	122	LYS	1
2	C	39	CYS	1
1	A	78	LEU	1
1	A	126	LEU	1
1	A	146	VAL	1
1	A	89	GLU	1
2	B	41	SER	1
2	C	6	GLU	1
2	C	17	SER	1
2	C	28	ASP	1
1	A	124	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	149	LYS	1
2	B	25	ILE	1
2	C	12	ILE	1
2	B	39	CYS	1
2	C	54	ILE	1
2	C	55	LEU	1
1	A	118	LYS	1
2	C	31	ASP	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 60% for the well-defined parts and 54% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1621
Number of shifts mapped to atoms	1621
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	132	-0.34 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	127	0.12 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	75	0.26 ± 0.17	None needed (< 0.5 ppm)
^{15}N	128	0.22 ± 0.39	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 60%, i.e. 1515 atoms were assigned a chemical shift out of a possible 2535. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	571/951 (60%)	254/385 (66%)	196/380 (52%)	121/186 (65%)
Sidechain	900/1436 (63%)	612/939 (65%)	281/464 (61%)	7/33 (21%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	44/148 (30%)	31/73 (42%)	13/65 (20%)	0/10 (0%)
Overall	1515/2535 (60%)	897/1397 (64%)	490/909 (54%)	128/229 (56%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 54%, i.e. 1621 atoms were assigned a chemical shift out of a possible 3029. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	610/1148 (53%)	275/465 (59%)	207/458 (45%)	128/225 (57%)
Sidechain	958/1697 (56%)	652/1110 (59%)	298/547 (54%)	8/40 (20%)
Aromatic	53/184 (29%)	36/91 (40%)	17/79 (22%)	0/14 (0%)
Overall	1621/3029 (54%)	963/1666 (58%)	522/1084 (48%)	136/279 (49%)

7.1.4 Statistically unusual chemical shifts ⓘ

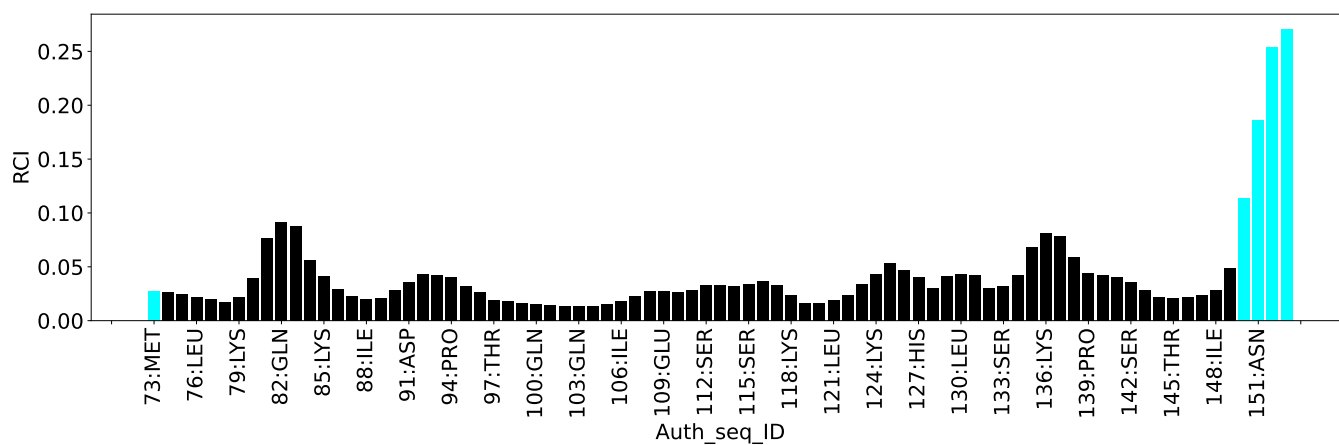
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	80	LYS	HB2	0.34	0.58 – 2.97	-6.0

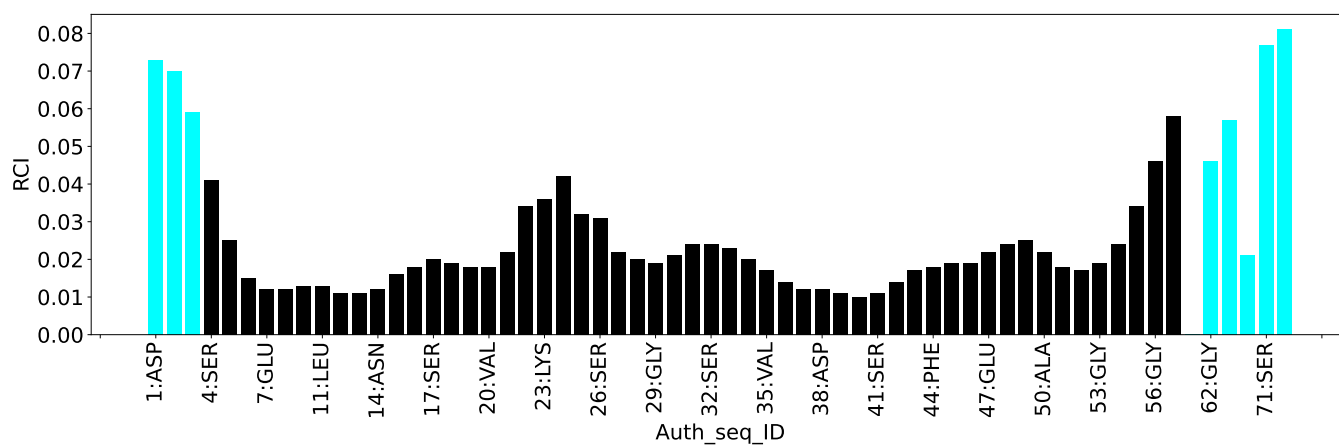
7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



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	4346
Intra-residue ($ i-j =0$)	1583
Sequential ($ i-j =1$)	940
Medium range ($ i-j >1$ and $ i-j <5$)	703
Long range ($ i-j \geq 5$)	833
Inter-chain	135
Hydrogen bond restraints	152
Disulfide bond restraints	0
Total dihedral-angle restraints	330
Number of unmapped restraints	0
Number of restraints per residue	20.4
Number of long range restraints per residue ¹	3.8

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)	82.6	0.2
0.2-0.5 (Medium)	173.5	0.5
>0.5 (Large)	299.0	8.24

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	11.4	8.76
10.0-20.0 (Medium)	0.1	13.56
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

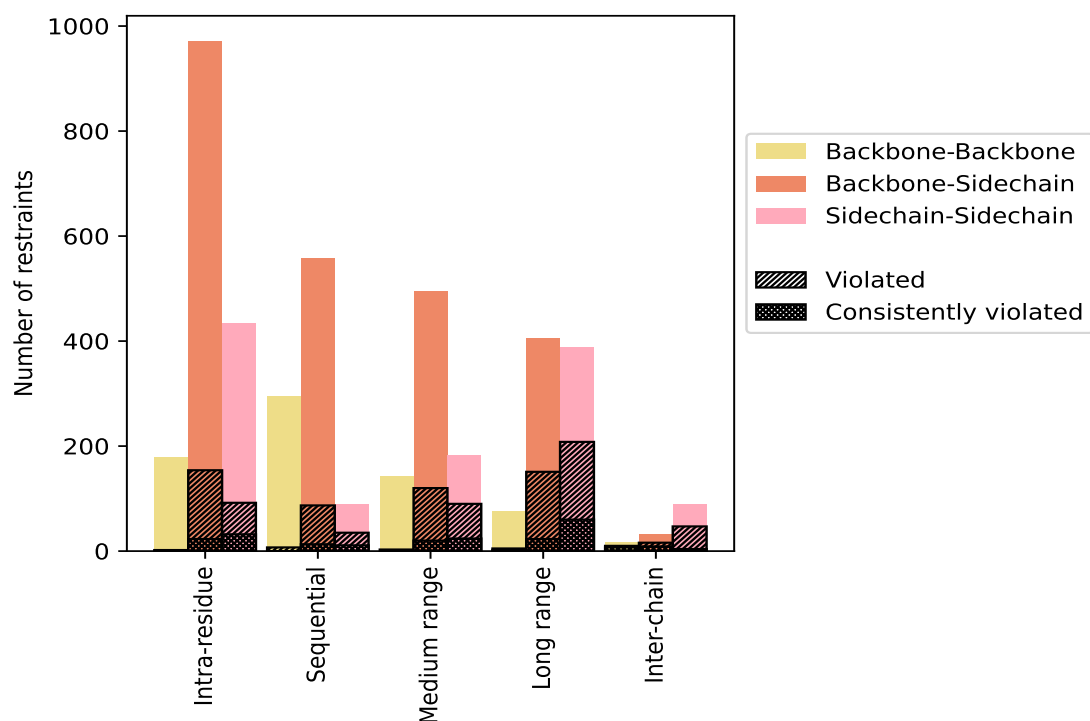
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	1583	36.4	248	15.7	5.7	56	3.5	1.3
Backbone-Backbone	179	4.1	2	1.1	0.0	1	0.6	0.0
Backbone-Sidechain	971	22.3	154	15.9	3.5	23	2.4	0.5
Sidechain-Sidechain	433	10.0	92	21.2	2.1	32	7.4	0.7
Sequential ($i-j =1$)	940	21.6	129	13.7	3.0	24	2.6	0.6
Backbone-Backbone	294	6.8	7	2.4	0.2	0	0.0	0.0
Backbone-Sidechain	558	12.8	87	15.6	2.0	13	2.3	0.3
Sidechain-Sidechain	88	2.0	35	39.8	0.8	11	12.5	0.3
Medium range ($i-j >1$ & $i-j <5$)	703	16.2	209	29.7	4.8	44	6.3	1.0
Backbone-Backbone	142	3.3	3	2.1	0.1	0	0.0	0.0
Backbone-Sidechain	379	8.7	116	30.6	2.7	20	5.3	0.5
Sidechain-Sidechain	182	4.2	90	49.5	2.1	24	13.2	0.6
Long range ($i-j \geq 5$)	833	19.2	358	43.0	8.2	85	10.2	2.0
Backbone-Backbone	75	1.7	5	6.7	0.1	2	2.7	0.0
Backbone-Sidechain	370	8.5	145	39.2	3.3	23	6.2	0.5
Sidechain-Sidechain	388	8.9	208	53.6	4.8	60	15.5	1.4
Inter-chain	135	3.1	73	54.1	1.7	20	14.8	0.5
Backbone-Backbone	16	0.4	10	62.5	0.2	7	43.8	0.2
Backbone-Sidechain	31	0.7	16	51.6	0.4	9	29.0	0.2
Sidechain-Sidechain	88	2.0	47	53.4	1.1	4	4.5	0.1
Hydrogen bond	152	3.5	10	6.6	0.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	4346	100.0	1027	23.6	23.6	229	5.3	5.3
Backbone-Backbone	706	16.2	27	3.8	0.6	10	1.4	0.2
Backbone-Sidechain	2461	56.6	528	21.5	12.1	88	3.6	2.0
Sidechain-Sidechain	1179	27.1	472	40.0	10.9	131	11.1	3.0

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 disulfid bonds are counted in their appropriate category on the x-axis

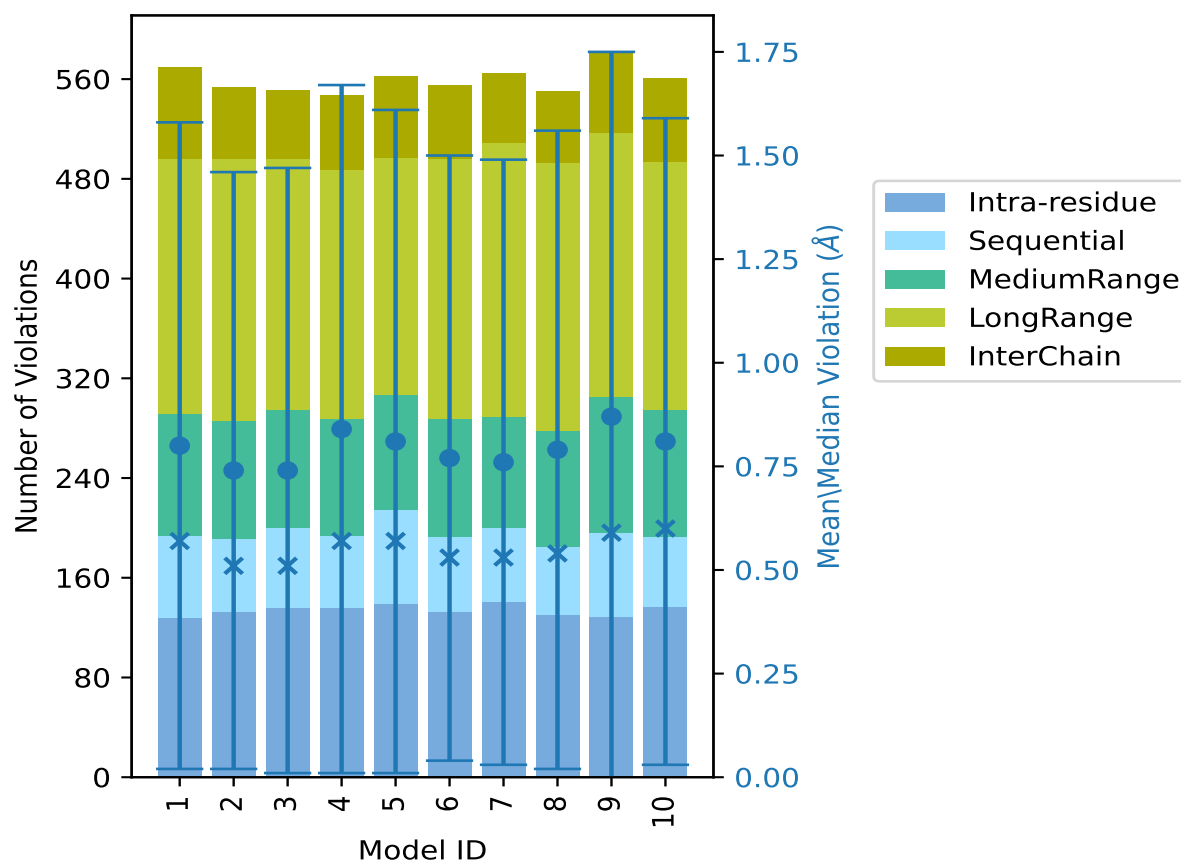
9.2 Distance violation statistics for each model [i](#)

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	128	66	98	204	73	569	0.8	8.03	0.78	0.57
2	133	58	95	210	57	553	0.74	7.17	0.72	0.51
3	136	64	95	201	55	551	0.74	7.33	0.73	0.51
4	136	58	94	199	60	547	0.84	7.53	0.83	0.57
5	139	75	93	190	65	562	0.81	7.04	0.8	0.57
6	133	60	95	208	59	555	0.77	7.25	0.73	0.53
7	141	59	89	220	56	565	0.76	7.3	0.73	0.53
8	130	55	93	215	57	550	0.79	7.56	0.77	0.54
9	129	67	109	212	65	582	0.87	7.41	0.88	0.59
10	137	56	102	199	67	561	0.81	8.24	0.78	0.6

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3177(IR:1335, SQ:811, MR:494, LR:475, IC:62) 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	%
56	36	46	53	13	204	1	10.0
28	20	23	28	5	104	2	20.0
18	8	17	31	5	79	3	30.0

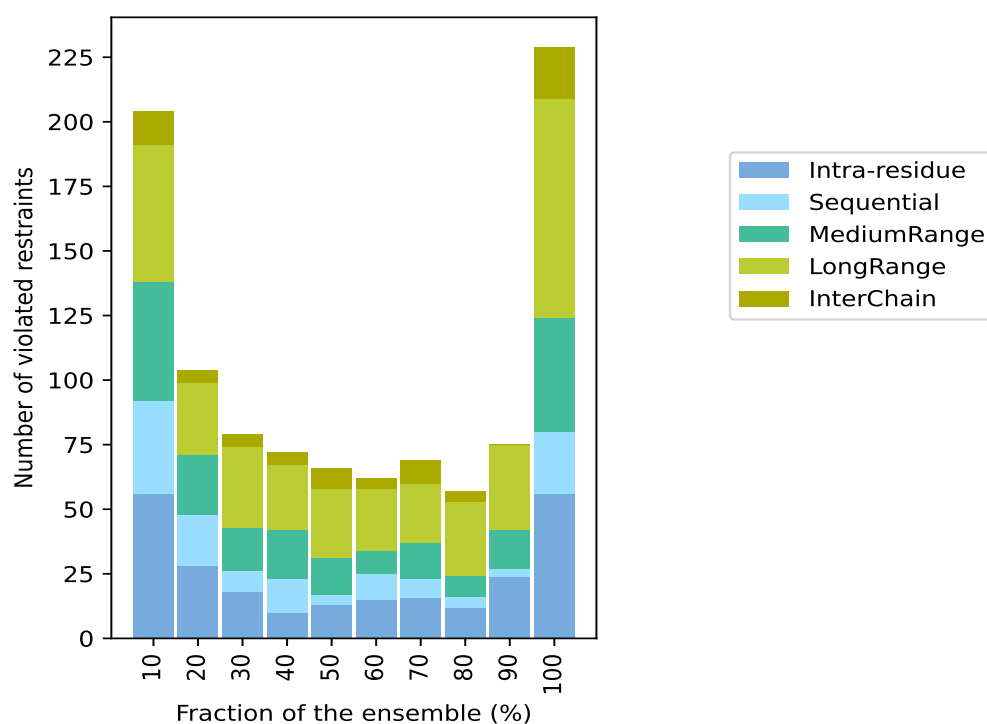
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
10	13	19	25	5	72	4	40.0
13	4	14	27	8	66	5	50.0
15	10	9	24	4	62	6	60.0
16	7	14	23	9	69	7	70.0
12	4	8	29	4	57	8	80.0
24	3	15	33	0	75	9	90.0
56	24	44	85	20	229	10	100.0

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

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

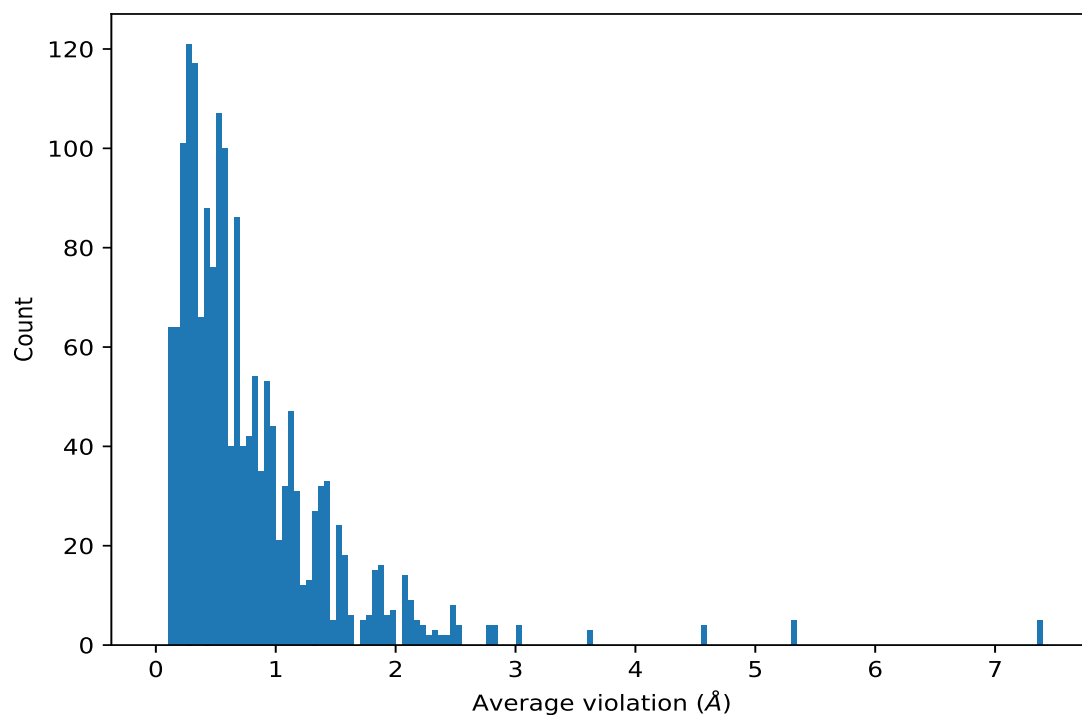


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4172)	1:122:A:LYS:C	2:35:B:VAL:HG11	10	7.36	0.62	7.37
(1,4172)	1:122:A:LYS:C	2:35:B:VAL:HG13	10	7.36	0.62	7.37
(1,4172)	1:122:A:LYS:H	2:35:B:VAL:HG13	10	7.36	0.62	7.37
(1,4172)	1:122:A:LYS:HD2	2:39:B:CYS:SG	10	7.36	0.62	7.37
(1,4172)	1:122:A:LYS:C	2:35:B:VAL:HG12	10	7.36	0.62	7.37
(1,4174)	1:124:A:LYS:O	2:35:B:VAL:HG13	10	5.31	0.43	5.14
(1,4174)	1:124:A:LYS:C	2:35:B:VAL:HG12	10	5.31	0.43	5.14
(1,4174)	1:124:A:LYS:C	2:35:B:VAL:HG13	10	5.31	0.43	5.14
(1,4174)	1:124:A:LYS:O	2:35:B:VAL:HG12	10	5.31	0.43	5.14
(1,4174)	1:124:A:LYS:C	2:35:B:VAL:HG11	10	5.31	0.43	5.14
(1,4173)	1:123:A:GLY:HA2	2:35:B:VAL:HG11	10	4.6	0.46	4.54
(1,4173)	1:123:A:GLY:O	2:35:B:VAL:HG13	10	4.6	0.46	4.54
(1,4173)	1:123:A:GLY:O	2:35:B:VAL:HG11	10	4.6	0.46	4.54
(1,4173)	1:123:A:GLY:O	2:35:B:VAL:HG12	10	4.6	0.46	4.54
(1,708)	1:122:A:LYS:HE3	1:121:A:LEU:HD12	10	3.61	1.21	3.88

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,708)	1:122:A:LYS:HE3	1:121:A:LEU:HD13	10	3.61	1.21	3.88
(1,708)	1:122:A:LYS:HE3	1:121:A:LEU:HD11	10	3.61	1.21	3.88
(1,792)	1:134:A:ASP:HB2	1:130:A:LEU:HD22	10	3.01	0.35	3.12
(1,792)	1:134:A:ASP:HB2	1:130:A:LEU:HD23	10	3.01	0.35	3.12
(1,792)	1:134:A:ASP:HB2	1:130:A:LEU:HD21	10	3.01	0.35	3.12
(1,1629)	1:105:A:LEU:HD11	1:90:A:HIS:HE1	10	2.82	0.98	3.17
(1,1629)	1:105:A:LEU:HD13	1:90:A:HIS:HE1	10	2.82	0.98	3.17
(1,1629)	1:105:A:LEU:HD11	1:104:A:HIS:HE1	10	2.82	0.98	3.17
(1,1629)	1:105:A:LEU:HD12	1:90:A:HIS:HE1	10	2.82	0.98	3.17
(1,135)	1:125:A:VAL:HG21	1:118:A:LYS:HE3	10	2.53	1.67	1.84
(1,135)	1:125:A:VAL:HG23	1:118:A:LYS:HE3	10	2.53	1.67	1.84
(1,135)	1:125:A:VAL:HG22	1:118:A:LYS:HE3	10	2.53	1.67	1.84
(1,82)	1:148:A:ILE:HG21	1:150:A:PRO:HD2	10	2.45	0.23	2.49
(1,82)	1:148:A:ILE:HG22	1:150:A:PRO:HD2	10	2.45	0.23	2.49
(1,82)	1:148:A:ILE:HG23	1:150:A:PRO:HD2	10	2.45	0.23	2.49
(1,2616)	2:51:B:VAL:HG23	2:46:B:PHE:HZ	10	2.45	0.43	2.41
(1,2616)	2:51:B:VAL:HG21	2:46:B:PHE:HZ	10	2.45	0.43	2.41
(1,2616)	2:51:B:VAL:HG22	2:46:B:PHE:HZ	10	2.45	0.43	2.41
(1,2617)	2:51:C:VAL:HG23	2:46:C:PHE:HZ	10	2.39	0.84	2.24
(1,2617)	2:51:C:VAL:HG22	2:46:C:PHE:HZ	10	2.39	0.84	2.24
(1,705)	1:122:A:LYS:HE3	1:122:A:LYS:HB3	10	2.3	0.55	2.46
(1,1660)	1:125:A:VAL:HG21	1:118:A:LYS:HE3	10	2.24	1.09	1.78
(1,1660)	1:125:A:VAL:HG23	1:118:A:LYS:HE3	10	2.24	1.09	1.78
(1,1660)	1:125:A:VAL:HG22	1:118:A:LYS:HE3	10	2.24	1.09	1.78
(1,1660)	1:124:A:LYS:HE2	1:135:A:LEU:HD21	10	2.24	1.09	1.78
(1,57)	1:81:A:ILE:HD12	1:145:A:THR:HB	10	2.16	0.61	2.17
(1,57)	1:81:A:ILE:HD11	1:145:A:THR:HB	10	2.16	0.61	2.17
(1,57)	1:81:A:ILE:HD13	1:145:A:THR:HB	10	2.16	0.61	2.17
(1,157)	1:99:A:LEU:HD21	1:103:A:GLN:HE22	10	2.14	0.62	2.15
(1,157)	1:99:A:LEU:HD23	1:103:A:GLN:HE22	10	2.14	0.62	2.15
(1,157)	1:99:A:LEU:HD22	1:103:A:GLN:HE22	10	2.14	0.62	2.15
(1,3737)	2:54:C:ILE:HD11	2:13:C:VAL:HG23	10	2.14	0.21	2.14
(1,3737)	2:54:C:ILE:HD11	2:13:C:VAL:HG21	10	2.14	0.21	2.14
(1,3737)	2:54:C:ILE:HD12	2:13:C:VAL:HG21	10	2.14	0.21	2.14
(1,3737)	2:54:C:ILE:HD12	2:13:C:VAL:HG23	10	2.14	0.21	2.14
(1,3737)	2:54:C:ILE:HD13	2:13:C:VAL:HG22	10	2.14	0.21	2.14
(1,860)	1:80:A:LYS:H	1:79:A:LYS:HD3	10	2.12	0.51	2.33
(1,3576)	2:33:B:LEU:HD22	2:19:B:ILE:HG21	10	2.09	0.25	2.18
(1,3576)	2:33:B:LEU:HD22	2:19:B:ILE:HG23	10	2.09	0.25	2.18
(1,3576)	2:33:B:LEU:HD21	2:19:B:ILE:HG22	10	2.09	0.25	2.18
(1,3576)	2:33:B:LEU:HD23	2:19:B:ILE:HG21	10	2.09	0.25	2.18
(1,3576)	2:33:B:LEU:HD21	2:12:B:ILE:HG23	10	2.09	0.25	2.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3576)	2:33:B:LEU:HD21	2:19:B:ILE:HG23	10	2.09	0.25	2.18
(1,3780)	2:13:B:VAL:HG21	2:16:B:PHE:HE2	10	2.08	0.45	2.12
(1,3780)	2:13:B:VAL:HG23	2:16:B:PHE:HE2	10	2.08	0.45	2.12
(1,3780)	2:13:B:VAL:HG22	2:16:C:PHE:HE1	10	2.08	0.45	2.12
(1,3780)	2:13:B:VAL:HG22	2:16:B:PHE:HE2	10	2.08	0.45	2.12
(1,3780)	2:13:B:VAL:HG23	2:16:B:PHE:HE1	10	2.08	0.45	2.12
(1,2642)	2:25:B:ILE:HD12	2:20:B:VAL:HG12	10	1.99	0.71	2.06
(1,2642)	2:25:B:ILE:HD13	2:20:B:VAL:HG11	10	1.99	0.71	2.06
(1,2642)	2:25:B:ILE:HD12	2:20:B:VAL:HG13	10	1.99	0.71	2.06
(1,2642)	2:25:B:ILE:HD11	2:20:B:VAL:HG11	10	1.99	0.71	2.06
(1,3736)	2:54:B:ILE:HD13	2:13:B:VAL:HG21	10	1.95	0.21	1.96
(1,3736)	2:54:B:ILE:HD12	2:13:B:VAL:HG23	10	1.95	0.21	1.96
(1,3736)	2:54:B:ILE:HD13	2:13:B:VAL:HG23	10	1.95	0.21	1.96
(1,3736)	2:54:B:ILE:HD11	2:13:B:VAL:HG23	10	1.95	0.21	1.96
(1,3736)	2:54:B:ILE:HD13	2:13:B:VAL:HG22	10	1.95	0.21	1.96
(1,3781)	2:13:C:VAL:HG22	2:16:C:PHE:HE2	10	1.89	0.26	1.85
(1,3781)	2:13:C:VAL:HG23	2:16:C:PHE:HE2	10	1.89	0.26	1.85
(1,3781)	2:13:C:VAL:HG23	2:16:B:PHE:HE1	10	1.89	0.26	1.85
(1,2246)	2:11:B:LEU:HA	2:12:B:ILE:HD12	10	1.88	1.07	1.82
(1,2246)	2:11:B:LEU:HA	2:12:B:ILE:HD13	10	1.88	1.07	1.82
(1,2246)	2:11:B:LEU:HA	2:12:B:ILE:HD11	10	1.88	1.07	1.82
(1,834)	1:85:A:LYS:HE3	1:82:A:GLN:HA	10	1.88	0.39	1.83
(1,2088)	2:8:B:ILE:HD11	2:19:C:ILE:HG12	10	1.86	0.52	1.78
(1,2088)	2:8:B:ILE:HD12	2:19:C:ILE:HG12	10	1.86	0.52	1.78
(1,2088)	2:8:B:ILE:HD13	2:19:C:ILE:HG12	10	1.86	0.52	1.78
(1,1457)	1:120:A:LEU:HD22	1:118:A:LYS:HE3	10	1.85	1.05	1.49
(1,1457)	1:120:A:LEU:HD23	1:118:A:LYS:HE3	10	1.85	1.05	1.49
(1,1457)	1:120:A:LEU:HD21	1:118:A:LYS:HE3	10	1.85	1.05	1.49
(1,2089)	2:8:C:ILE:HD11	2:19:B:ILE:HG12	10	1.84	0.63	1.79
(1,2089)	2:8:C:ILE:HD13	2:19:B:ILE:HG12	10	1.84	0.63	1.79
(1,2089)	2:8:C:ILE:HD12	2:19:B:ILE:HG12	10	1.84	0.63	1.79
(1,3577)	2:33:C:LEU:HD21	2:19:C:ILE:HG21	10	1.83	0.33	1.95
(1,3577)	2:33:C:LEU:HD23	2:19:C:ILE:HG23	10	1.83	0.33	1.95
(1,3577)	2:33:C:LEU:HD23	2:19:C:ILE:HG21	10	1.83	0.33	1.95
(1,3577)	2:33:C:LEU:HD22	2:19:C:ILE:HG21	10	1.83	0.33	1.95
(1,3577)	2:33:C:LEU:HD21	2:12:C:ILE:HG22	10	1.83	0.33	1.95
(1,698)	1:79:A:LYS:HE3	1:81:A:ILE:HG21	10	1.83	0.85	1.72
(1,698)	1:79:A:LYS:HE3	1:81:A:ILE:HG23	10	1.83	0.85	1.72
(1,179)	1:120:A:LEU:HD21	1:147:A:MET:HG3	10	1.83	0.83	2.18
(1,179)	1:120:A:LEU:HD22	1:147:A:MET:HG3	10	1.83	0.83	2.18
(1,179)	1:120:A:LEU:HD23	1:147:A:MET:HG3	10	1.83	0.83	2.18
(1,2643)	2:25:C:ILE:HD11	2:20:C:VAL:HG13	10	1.81	0.34	1.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2643)	2:25:C:ILE:HD11	2:20:C:VAL:HG11	10	1.81	0.34	1.72
(1,1141)	1:82:A:GLN:H	1:80:A:LYS:HG2	10	1.76	0.94	2.33
(1,2644)	2:20:B:VAL:HG11	2:33:B:LEU:HD22	10	1.75	0.34	1.74
(1,2644)	2:20:B:VAL:HG13	2:33:B:LEU:HD21	10	1.75	0.34	1.74
(1,2644)	2:20:B:VAL:HG12	2:33:B:LEU:HD23	10	1.75	0.34	1.74
(1,1446)	1:97:A:THR:HG22	1:96:A:ASP:HB3	10	1.73	0.38	1.9
(1,1446)	1:97:A:THR:HG21	1:100:A:GLN:HG3	10	1.73	0.38	1.9
(1,1446)	1:97:A:THR:HG23	1:96:A:ASP:HB3	10	1.73	0.38	1.9
(1,1356)	1:151:A:ASN:HA	1:151:A:ASN:HD22	10	1.72	0.5	1.64
(1,2628)	2:37:B:MET:HB3	2:17:B:SER:HB3	10	1.65	0.69	1.74
(1,3741)	2:25:C:ILE:HD12	2:19:C:ILE:HD11	10	1.65	0.52	1.61
(1,3741)	2:19:C:ILE:HD12	2:8:B:ILE:HG22	10	1.65	0.52	1.61
(1,2247)	2:11:C:LEU:HA	2:12:C:ILE:HD11	10	1.59	1.18	0.87
(1,2247)	2:11:C:LEU:HA	2:12:C:ILE:HD12	10	1.59	1.18	0.87
(1,2247)	2:11:C:LEU:HA	2:12:C:ILE:HD13	10	1.59	1.18	0.87
(1,3572)	2:33:B:LEU:HD22	2:19:B:ILE:HB	10	1.58	0.25	1.66
(1,3572)	2:33:B:LEU:HD21	2:19:B:ILE:HB	10	1.58	0.25	1.66
(1,3572)	2:33:B:LEU:HD23	2:19:B:ILE:HB	10	1.58	0.25	1.66
(1,3740)	2:19:B:ILE:HD12	2:8:C:ILE:HG21	10	1.57	0.27	1.56
(1,3740)	2:19:B:ILE:HD13	2:8:C:ILE:HG21	10	1.57	0.27	1.56
(1,3740)	2:19:B:ILE:HD13	2:8:C:ILE:HG23	10	1.57	0.27	1.56
(1,3740)	2:19:B:ILE:HD11	2:8:C:ILE:HG21	10	1.57	0.27	1.56
(1,3740)	2:25:B:ILE:HD13	2:19:B:ILE:HD11	10	1.57	0.27	1.56
(1,1353)	1:121:A:LEU:HD13	1:141:A:ASN:HD21	10	1.56	0.85	1.4
(1,1353)	1:121:A:LEU:HD12	1:141:A:ASN:HD21	10	1.56	0.85	1.4
(1,2553)	2:35:C:VAL:HG12	2:37:C:MET:HB3	10	1.55	0.58	1.5
(1,2553)	2:35:C:VAL:HG11	2:37:C:MET:HB3	10	1.55	0.58	1.5
(1,2553)	2:35:C:VAL:HG13	2:37:C:MET:HB3	10	1.55	0.58	1.5
(1,52)	1:81:A:ILE:HD12	1:81:A:ILE:H	10	1.54	0.48	1.62
(1,52)	1:81:A:ILE:HD13	1:81:A:ILE:H	10	1.54	0.48	1.62
(1,52)	1:81:A:ILE:HD11	1:81:A:ILE:H	10	1.54	0.48	1.62
(1,4182)	1:120:A:LEU:HD23	2:38:C:ASP:H	10	1.54	0.44	1.6
(1,4182)	1:120:A:LEU:HD21	2:38:B:ASP:H	10	1.54	0.44	1.6
(1,4182)	1:120:A:LEU:HD22	2:31:B:ASP:H	10	1.54	0.44	1.6
(1,4182)	1:120:A:LEU:HD23	2:38:B:ASP:H	10	1.54	0.44	1.6
(1,4182)	1:120:A:LEU:HD21	2:31:B:ASP:H	10	1.54	0.44	1.6
(1,4182)	1:120:A:LEU:HD22	2:38:B:ASP:H	10	1.54	0.44	1.6
(1,4182)	1:120:A:LEU:HD22	2:38:C:ASP:H	10	1.54	0.44	1.6
(1,2629)	2:37:C:MET:HB3	2:17:C:SER:HB3	10	1.52	0.96	1.63
(1,3934)	2:55:B:LEU:HD12	2:7:B:GLU:HG2	10	1.5	0.64	1.33
(1,3934)	2:55:B:LEU:HD11	2:7:B:GLU:HG2	10	1.5	0.64	1.33
(1,3934)	2:55:B:LEU:HD13	2:7:B:GLU:HG2	10	1.5	0.64	1.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3626)	2:41:B:SER:HB3	2:9:B:ALA:HB3	10	1.47	0.2	1.45
(1,3626)	2:41:B:SER:HB3	2:9:B:ALA:HB1	10	1.47	0.2	1.45
(1,3626)	2:41:B:SER:HB3	2:43:B:ALA:HB2	10	1.47	0.2	1.45
(1,4052)	2:55:B:LEU:HD22	2:8:B:ILE:H	10	1.46	0.5	1.36
(1,4052)	2:55:B:LEU:HD21	2:8:B:ILE:H	10	1.46	0.5	1.36
(1,3542)	2:51:B:VAL:HG23	2:49:B:GLU:HG3	10	1.45	0.52	1.44
(1,3542)	2:51:B:VAL:HG21	2:49:B:GLU:HG3	10	1.45	0.52	1.44
(1,3542)	2:51:B:VAL:HG22	2:13:B:VAL:HB	10	1.45	0.52	1.44
(1,3542)	2:51:B:VAL:HG21	2:13:B:VAL:HB	10	1.45	0.52	1.44
(1,2645)	2:20:C:VAL:HG12	2:33:C:LEU:HD21	10	1.45	0.4	1.31
(1,2645)	2:20:C:VAL:HG13	2:33:C:LEU:HD22	10	1.45	0.4	1.31
(1,2645)	2:20:C:VAL:HG12	2:33:C:LEU:HD22	10	1.45	0.4	1.31
(1,2063)	2:55:C:LEU:HD21	2:14:C:ASN:HB2	10	1.44	0.42	1.43
(1,2063)	2:55:C:LEU:HD23	2:14:C:ASN:HB2	10	1.44	0.42	1.43
(1,2063)	2:55:C:LEU:HD22	2:14:C:ASN:HB2	10	1.44	0.42	1.43
(1,2546)	2:20:B:VAL:HG21	2:30:B:ALA:HB3	10	1.44	0.35	1.46
(1,2546)	2:20:B:VAL:HG22	2:30:B:ALA:HB2	10	1.44	0.35	1.46
(1,2546)	2:20:B:VAL:HG22	2:30:B:ALA:HB3	10	1.44	0.35	1.46
(1,1651)	1:88:A:ILE:HG21	1:89:A:GLU:HG3	10	1.43	0.27	1.45
(1,1651)	1:88:A:ILE:HG22	1:89:A:GLU:HG3	10	1.43	0.27	1.45
(1,1651)	1:88:A:ILE:HG23	1:78:A:LEU:HB3	10	1.43	0.27	1.45
(1,2547)	2:20:C:VAL:HG21	2:30:C:ALA:HB2	10	1.43	0.22	1.48
(1,2547)	2:20:C:VAL:HG22	2:30:C:ALA:HB3	10	1.43	0.22	1.48
(1,2547)	2:20:C:VAL:HG23	2:30:C:ALA:HB1	10	1.43	0.22	1.48
(1,2547)	2:20:C:VAL:HG21	2:30:C:ALA:HB3	10	1.43	0.22	1.48
(1,2639)	2:35:C:VAL:HG21	2:37:C:MET:HB3	10	1.38	0.54	1.21
(1,2639)	2:35:C:VAL:HG22	2:37:C:MET:HB3	10	1.38	0.54	1.21
(1,2639)	2:35:C:VAL:HG23	2:37:C:MET:HB3	10	1.38	0.54	1.21
(1,1653)	1:126:A:LEU:HD13	1:126:A:LEU:HB3	10	1.38	0.12	1.42
(1,1653)	1:126:A:LEU:HD11	1:126:A:LEU:HB3	10	1.38	0.12	1.42
(1,1653)	1:126:A:LEU:HD12	1:124:A:LYS:HD3	10	1.38	0.12	1.42
(1,2158)	2:13:B:VAL:HG22	2:48:B:ARG:HD3	10	1.38	0.53	1.43
(1,2158)	2:13:B:VAL:HG21	2:48:B:ARG:HD3	10	1.38	0.53	1.43
(1,2158)	2:13:B:VAL:HG23	2:48:B:ARG:HD3	10	1.38	0.53	1.43
(1,4187)	1:81:A:ILE:HG23	2:39:B:CYS:H	10	1.38	0.24	1.4
(1,4187)	1:81:A:ILE:HG21	2:39:B:CYS:H	10	1.38	0.24	1.4
(1,4187)	1:81:A:ILE:HG23	2:36:C:ALA:H	10	1.38	0.24	1.4
(1,4187)	1:81:A:ILE:HG22	2:39:B:CYS:H	10	1.38	0.24	1.4
(1,1434)	1:83:A:ALA:HB2	1:84:A:PRO:HG2	10	1.36	0.14	1.37
(1,1434)	1:83:A:ALA:HB1	1:84:A:PRO:HG2	10	1.36	0.14	1.37
(1,1434)	1:83:A:ALA:HB3	1:82:A:GLN:HB2	10	1.36	0.14	1.37
(1,3627)	2:41:C:SER:HB3	2:9:C:ALA:HB2	10	1.36	0.24	1.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3627)	2:41:C:SER:HB3	2:9:C:ALA:HB3	10	1.36	0.24	1.25
(1,2883)	2:13:C:VAL:HG13	2:41:C:SER:HB3	10	1.35	0.27	1.34
(1,2883)	2:13:C:VAL:HG11	2:41:C:SER:HB3	10	1.35	0.27	1.34
(1,2883)	2:13:C:VAL:HG12	2:41:C:SER:HB3	10	1.35	0.27	1.34
(1,185)	1:130:A:LEU:HD22	1:131:A:PHE:H	10	1.35	0.11	1.33
(1,185)	1:130:A:LEU:HD23	1:131:A:PHE:H	10	1.35	0.11	1.33
(1,3573)	2:33:C:LEU:HD21	2:19:C:ILE:HB	10	1.34	0.32	1.28
(1,3573)	2:33:C:LEU:HD22	2:19:C:ILE:HB	10	1.34	0.32	1.28
(1,4053)	2:55:C:LEU:HD21	2:8:C:ILE:H	10	1.34	0.49	1.61
(1,4053)	2:55:C:LEU:HD23	2:8:C:ILE:H	10	1.34	0.49	1.61
(1,4053)	2:55:C:LEU:HD22	2:8:C:ILE:H	10	1.34	0.49	1.61
(1,4053)	2:55:C:LEU:HD11	2:50:C:ALA:H	10	1.34	0.49	1.61
(1,700)	1:79:A:LYS:HE3	1:81:A:ILE:HA	10	1.33	0.71	1.48
(1,25)	1:144:A:ILE:HD12	1:120:A:LEU:H	10	1.33	0.57	1.34
(1,25)	1:144:A:ILE:HD11	1:120:A:LEU:H	10	1.33	0.57	1.34
(1,3719)	2:54:C:ILE:HG23	2:13:C:VAL:HG22	10	1.33	0.58	1.16
(1,3719)	2:54:C:ILE:HG21	2:13:C:VAL:HG23	10	1.33	0.58	1.16
(1,3719)	2:54:C:ILE:HG22	2:13:C:VAL:HG23	10	1.33	0.58	1.16
(1,3719)	2:54:C:ILE:HG23	2:13:C:VAL:HG23	10	1.33	0.58	1.16
(1,3935)	2:55:C:LEU:HD12	2:7:C:GLU:HG2	10	1.32	0.45	1.48
(1,3935)	2:55:C:LEU:HD13	2:7:C:GLU:HG2	10	1.32	0.45	1.48
(1,3935)	2:55:C:LEU:HD11	2:7:C:GLU:HG2	10	1.32	0.45	1.48
(1,630)	1:78:A:LEU:HB2	1:146:A:VAL:HG22	10	1.29	0.21	1.3
(1,630)	1:78:A:LEU:HB2	1:146:A:VAL:HG23	10	1.29	0.21	1.3
(1,150)	1:78:A:LEU:HD13	1:92:A:PHE:HZ	10	1.24	0.49	1.25
(1,150)	1:78:A:LEU:HD11	1:92:A:PHE:HZ	10	1.24	0.49	1.25
(1,3718)	2:54:B:ILE:HG23	2:13:B:VAL:HG21	10	1.24	0.21	1.15
(1,3718)	2:54:B:ILE:HG22	2:13:B:VAL:HG23	10	1.24	0.21	1.15
(1,3718)	2:54:B:ILE:HG22	2:13:B:VAL:HG22	10	1.24	0.21	1.15
(1,3718)	2:54:B:ILE:HG21	2:13:B:VAL:HG22	10	1.24	0.21	1.15
(1,736)	1:114:A:ILE:HG12	1:102:A:LYS:HB3	10	1.21	0.51	1.04
(1,4180)	1:147:A:MET:HE1	2:38:B:ASP:H	10	1.2	0.33	1.27
(1,4180)	1:147:A:MET:HE3	2:38:B:ASP:H	10	1.2	0.33	1.27
(1,4180)	1:147:A:MET:HE1	2:38:C:ASP:H	10	1.2	0.33	1.27
(1,4180)	1:147:A:MET:HE2	2:38:B:ASP:H	10	1.2	0.33	1.27
(1,4181)	1:120:A:LEU:HD12	2:38:C:ASP:H	10	1.2	0.53	1.44
(1,4181)	1:120:A:LEU:HD11	2:31:B:ASP:H	10	1.2	0.53	1.44
(1,4181)	1:120:A:LEU:HD12	2:31:B:ASP:H	10	1.2	0.53	1.44
(1,4181)	1:120:A:LEU:HD11	2:38:C:ASP:H	10	1.2	0.53	1.44
(1,2882)	2:13:B:VAL:HG12	2:41:B:SER:HB3	10	1.18	0.29	1.08
(1,2882)	2:13:B:VAL:HG13	2:41:B:SER:HB3	10	1.18	0.29	1.08
(1,174)	1:132:A:LEU:HD22	1:92:A:PHE:HA	10	1.17	0.11	1.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,174)	1:132:A:LEU:HD21	1:92:A:PHE:HA	10	1.17	0.11	1.16
(1,3621)	2:40:C:ILE:HA	2:36:B:ALA:HB1	10	1.17	0.34	1.06
(1,3621)	2:40:C:ILE:HA	2:36:B:ALA:HB3	10	1.17	0.34	1.06
(1,3621)	2:40:C:ILE:HA	2:36:B:ALA:HB2	10	1.17	0.34	1.06
(1,1021)	1:103:A:GLN:HG3	1:103:A:GLN:H	10	1.17	0.18	1.12
(1,3555)	2:25:C:ILE:HD12	2:5:B:LYS:HB3	10	1.17	0.19	1.18
(1,3555)	2:25:C:ILE:HD12	2:19:C:ILE:HB	10	1.17	0.19	1.18
(1,3555)	2:25:C:ILE:HD11	2:19:C:ILE:HB	10	1.17	0.19	1.18
(1,3672)	2:12:B:ILE:HG23	2:11:B:LEU:H	10	1.15	0.28	1.23
(1,3672)	2:12:B:ILE:HG21	2:11:B:LEU:H	10	1.15	0.28	1.23
(1,3672)	2:12:B:ILE:HG22	2:11:B:LEU:H	10	1.15	0.28	1.23
(1,2083)	2:25:C:ILE:HD12	2:19:C:ILE:HG21	10	1.14	0.24	1.1
(1,2083)	2:25:C:ILE:HD12	2:19:C:ILE:HG23	10	1.14	0.24	1.1
(1,2083)	2:25:C:ILE:HD12	2:19:C:ILE:HG22	10	1.14	0.24	1.1
(1,782)	1:98:A:ILE:HG23	1:98:A:ILE:HG12	10	1.14	0.05	1.16
(1,782)	1:98:A:ILE:HG22	1:98:A:ILE:HG12	10	1.14	0.05	1.16
(1,782)	1:98:A:ILE:HG21	1:98:A:ILE:HG12	10	1.14	0.05	1.16
(1,3874)	2:15:B:TYR:HA	2:12:C:ILE:HD12	10	1.14	0.45	1.1
(1,3874)	2:15:B:TYR:HA	2:12:C:ILE:HD13	10	1.14	0.45	1.1
(1,3874)	2:15:B:TYR:HA	2:12:B:ILE:HD11	10	1.14	0.45	1.1
(1,2062)	2:55:B:LEU:HD22	2:14:B:ASN:HB2	10	1.13	0.44	1.16
(1,2062)	2:55:B:LEU:HD21	2:14:B:ASN:HB2	10	1.13	0.44	1.16
(1,176)	1:132:A:LEU:HD22	1:96:A:ASP:HB2	10	1.12	0.53	0.94
(1,176)	1:132:A:LEU:HD21	1:96:A:ASP:HB2	10	1.12	0.53	0.94
(1,151)	1:135:A:LEU:HD12	1:135:A:LEU:H	10	1.11	0.15	1.05
(1,151)	1:135:A:LEU:HD11	1:135:A:LEU:H	10	1.11	0.15	1.05
(1,2534)	2:36:B:ALA:HB2	2:40:C:ILE:HG13	10	1.11	0.6	0.82
(1,2534)	2:36:B:ALA:HB3	2:40:C:ILE:HG13	10	1.11	0.6	0.82
(1,2534)	2:36:B:ALA:HB1	2:40:C:ILE:HG13	10	1.11	0.6	0.82
(1,2082)	2:25:B:ILE:HD13	2:19:B:ILE:HG21	10	1.1	0.33	1.1
(1,2082)	2:25:B:ILE:HD13	2:19:B:ILE:HG23	10	1.1	0.33	1.1
(1,2082)	2:25:B:ILE:HD11	2:19:B:ILE:HG23	10	1.1	0.33	1.1
(1,2082)	2:25:B:ILE:HD13	2:19:B:ILE:HG22	10	1.1	0.33	1.1
(1,2082)	2:25:B:ILE:HD11	2:19:B:ILE:HG21	10	1.1	0.33	1.1
(1,3313)	2:26:C:SER:H	2:44:B:PHE:HD1	10	1.1	0.35	1.02
(1,1449)	1:78:A:LEU:HD11	1:90:A:HIS:H	10	1.09	0.37	1.12
(1,1449)	1:78:A:LEU:HD12	1:90:A:HIS:H	10	1.09	0.37	1.12
(1,2638)	2:35:B:VAL:HG22	2:37:B:MET:HB3	10	1.09	0.28	1.0
(1,2638)	2:35:B:VAL:HG21	2:37:B:MET:HB3	10	1.09	0.28	1.0
(1,2638)	2:35:B:VAL:HG23	2:37:B:MET:HB3	10	1.09	0.28	1.0
(1,3608)	2:38:B:ASP:HA	2:40:B:ILE:HD13	10	1.08	0.17	1.08
(1,3608)	2:38:B:ASP:HA	2:40:B:ILE:HD11	10	1.08	0.17	1.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3608)	2:38:B:ASP:HA	2:13:B:VAL:HG22	10	1.08	0.17	1.08
(1,3673)	2:12:C:ILE:HG22	2:11:C:LEU:H	10	1.06	0.34	0.92
(1,3673)	2:12:C:ILE:HG23	2:11:C:LEU:H	10	1.06	0.34	0.92
(1,3673)	2:12:C:ILE:HG21	2:11:C:LEU:H	10	1.06	0.34	0.92
(1,3553)	2:25:C:ILE:HD12	2:24:C:GLU:HB3	10	1.06	0.33	0.98
(1,3554)	2:25:B:ILE:HD13	2:5:C:LYS:HB3	10	1.05	0.37	1.19
(1,3554)	2:25:B:ILE:HD13	2:19:B:ILE:HB	10	1.05	0.37	1.19
(1,3554)	2:25:B:ILE:HD11	2:19:B:ILE:HB	10	1.05	0.37	1.19
(1,3554)	2:25:B:ILE:HD12	2:5:C:LYS:HB3	10	1.05	0.37	1.19
(1,2545)	2:51:C:VAL:HG12	2:55:C:LEU:HG	10	1.02	0.8	0.75
(1,3183)	2:12:C:ILE:HD11	2:9:C:ALA:H	10	1.02	0.25	0.96
(1,3183)	2:12:C:ILE:HD13	2:9:C:ALA:H	10	1.02	0.25	0.96
(1,3183)	2:12:C:ILE:HD12	2:9:C:ALA:H	10	1.02	0.25	0.96
(1,1423)	1:119:A:LEU:HD22	1:117:A:ILE:HB	10	1.01	0.39	0.94
(1,1423)	1:119:A:LEU:HD21	1:126:A:LEU:HB3	10	1.01	0.39	0.94
(1,1423)	1:119:A:LEU:HD23	1:117:A:ILE:HB	10	1.01	0.39	0.94
(1,1423)	1:119:A:LEU:HD21	1:117:A:ILE:HB	10	1.01	0.39	0.94
(1,13)	1:119:A:LEU:HD21	1:98:A:ILE:HA	10	0.99	0.75	0.76
(1,3875)	2:15:C:TYR:HA	2:12:B:ILE:HD13	10	0.98	0.32	0.99
(1,3875)	2:15:C:TYR:HA	2:12:C:ILE:HD11	10	0.98	0.32	0.99
(1,3875)	2:15:C:TYR:HA	2:12:B:ILE:HD11	10	0.98	0.32	0.99
(1,3875)	2:15:C:TYR:HA	2:12:B:ILE:HD12	10	0.98	0.32	0.99
(1,3875)	2:15:C:TYR:HA	2:12:C:ILE:HD12	10	0.98	0.32	0.99
(1,2532)	2:36:B:ALA:HB1	2:35:B:VAL:HB	10	0.98	0.1	0.97
(1,2532)	2:36:B:ALA:HB3	2:35:B:VAL:HB	10	0.98	0.1	0.97
(1,2533)	2:36:C:ALA:HB2	2:35:C:VAL:HB	10	0.98	0.11	1.0
(1,2533)	2:36:C:ALA:HB3	2:35:C:VAL:HB	10	0.98	0.11	1.0
(1,4081)	2:13:C:VAL:H	2:41:C:SER:HA	10	0.98	0.3	0.98
(1,3620)	2:40:B:ILE:HA	2:36:C:ALA:HB2	10	0.97	0.21	0.9
(1,3620)	2:40:B:ILE:HA	2:36:C:ALA:HB3	10	0.97	0.21	0.9
(1,3794)	2:17:B:SER:HA	2:19:B:ILE:HG23	10	0.96	0.16	0.92
(1,3794)	2:17:B:SER:HA	2:19:B:ILE:HG22	10	0.96	0.16	0.92
(1,3794)	2:17:B:SER:HA	2:19:B:ILE:HG21	10	0.96	0.16	0.92
(1,3794)	2:18:B:SER:HB3	2:19:B:ILE:HG22	10	0.96	0.16	0.92
(1,720)	1:148:A:ILE:HD13	1:86:A:PHE:HZ	10	0.96	0.72	0.8
(1,720)	1:148:A:ILE:HD11	1:86:A:PHE:HZ	10	0.96	0.72	0.8
(1,720)	1:148:A:ILE:HD12	1:86:A:PHE:HZ	10	0.96	0.72	0.8
(1,3552)	2:25:B:ILE:HD13	2:24:B:GLU:HB3	10	0.94	0.37	0.94
(1,3552)	2:25:B:ILE:HD11	2:24:B:GLU:HB3	10	0.94	0.37	0.94
(1,3552)	2:25:B:ILE:HD12	2:24:B:GLU:HB3	10	0.94	0.37	0.94
(1,2127)	2:54:C:ILE:HB	2:13:C:VAL:HG22	10	0.94	0.29	0.85
(1,2127)	2:54:C:ILE:HB	2:13:C:VAL:HG23	10	0.94	0.29	0.85

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2127)	2:54:C:ILE:HB	2:13:C:VAL:HG21	10	0.94	0.29	0.85
(1,3546)	2:51:B:VAL:HG23	2:50:B:ALA:HB2	10	0.94	0.1	0.96
(1,3546)	2:51:B:VAL:HG23	2:55:B:LEU:HG	10	0.94	0.1	0.96
(1,3546)	2:51:B:VAL:HG22	2:50:B:ALA:HB2	10	0.94	0.1	0.96
(1,3546)	2:51:B:VAL:HG23	2:50:B:ALA:HB3	10	0.94	0.1	0.96
(1,3546)	2:51:B:VAL:HG22	2:55:B:LEU:HG	10	0.94	0.1	0.96
(1,3546)	2:51:B:VAL:HG21	2:50:B:ALA:HB2	10	0.94	0.1	0.96
(1,3795)	2:17:C:SER:HA	2:19:C:ILE:HG23	10	0.92	0.18	0.9
(1,3795)	2:17:C:SER:HA	2:19:C:ILE:HG22	10	0.92	0.18	0.9
(1,3795)	2:17:C:SER:HA	2:19:C:ILE:HG21	10	0.92	0.18	0.9
(1,3547)	2:51:C:VAL:HG23	2:50:C:ALA:HB3	10	0.92	0.2	1.02
(1,3547)	2:51:C:VAL:HG22	2:55:C:LEU:HG	10	0.92	0.2	1.02
(1,3547)	2:51:C:VAL:HG23	2:50:C:ALA:HB2	10	0.92	0.2	1.02
(1,3547)	2:51:C:VAL:HG22	2:50:C:ALA:HB1	10	0.92	0.2	1.02
(1,3547)	2:51:C:VAL:HG23	2:55:C:LEU:HG	10	0.92	0.2	1.02
(1,3547)	2:51:C:VAL:HG22	2:50:C:ALA:HB3	10	0.92	0.2	1.02
(1,3745)	2:40:C:ILE:HD13	2:36:C:ALA:HB3	10	0.92	0.39	0.89
(1,3745)	2:40:C:ILE:HD12	2:36:B:ALA:HB2	10	0.92	0.39	0.89
(1,3745)	2:40:C:ILE:HD11	2:36:C:ALA:HB1	10	0.92	0.39	0.89
(1,3745)	2:40:C:ILE:HD12	2:36:C:ALA:HB3	10	0.92	0.39	0.89
(1,3745)	2:40:C:ILE:HD11	2:36:C:ALA:HB3	10	0.92	0.39	0.89
(1,3745)	2:40:C:ILE:HD13	2:36:B:ALA:HB2	10	0.92	0.39	0.89
(1,672)	1:121:A:LEU:HD23	1:144:A:ILE:HA	10	0.92	0.22	0.98
(1,672)	1:121:A:LEU:HD21	1:144:A:ILE:HA	10	0.92	0.22	0.98
(1,2552)	2:35:B:VAL:HG12	2:37:B:MET:HB3	10	0.9	0.51	0.8
(1,2552)	2:35:B:VAL:HG11	2:37:B:MET:HB3	10	0.9	0.51	0.8
(1,2552)	2:35:B:VAL:HG13	2:37:B:MET:HB3	10	0.9	0.51	0.8
(1,118)	1:97:A:THR:HG22	1:97:A:THR:H	10	0.88	0.42	1.06
(1,118)	1:97:A:THR:HG23	1:97:A:THR:H	10	0.88	0.42	1.06
(1,2250)	2:11:B:LEU:HA	2:55:B:LEU:HB3	10	0.88	0.24	0.98
(1,1338)	1:99:A:LEU:HD11	1:103:A:GLN:HE21	10	0.87	0.59	0.71
(1,1338)	1:99:A:LEU:HD13	1:103:A:GLN:HE21	10	0.87	0.59	0.71
(1,3221)	2:34:C:ASN:HA	2:17:C:SER:H	10	0.87	0.23	0.86
(1,3312)	2:26:B:SER:H	2:44:C:PHE:HD1	10	0.86	0.43	0.7
(1,2061)	2:55:C:LEU:HD21	2:14:C:ASN:H	10	0.86	0.42	0.84
(1,2061)	2:55:C:LEU:HD23	2:14:C:ASN:H	10	0.86	0.42	0.84
(1,2061)	2:55:C:LEU:HD22	2:14:C:ASN:H	10	0.86	0.42	0.84
(1,2640)	2:33:B:LEU:HD11	2:20:B:VAL:HG12	10	0.86	0.38	0.86
(1,2640)	2:33:B:LEU:HD12	2:20:B:VAL:HG13	10	0.86	0.38	0.86
(1,2640)	2:33:B:LEU:HD12	2:20:B:VAL:HG11	10	0.86	0.38	0.86
(1,2640)	2:33:B:LEU:HD12	2:20:B:VAL:HG12	10	0.86	0.38	0.86
(1,2640)	2:33:B:LEU:HD11	2:20:B:VAL:HG11	10	0.86	0.38	0.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,54)	1:81:A:ILE:HD12	1:82:A:GLN:H	10	0.86	0.26	0.86
(1,54)	1:81:A:ILE:HD11	1:82:A:GLN:H	10	0.86	0.26	0.86
(1,54)	1:81:A:ILE:HD13	1:82:A:GLN:H	10	0.86	0.26	0.86
(1,1648)	1:135:A:LEU:HA	1:135:A:LEU:HD12	10	0.86	0.19	0.75
(1,1648)	1:136:A:LYS:HA	1:135:A:LEU:HD12	10	0.86	0.19	0.75
(1,1648)	1:136:A:LYS:HA	1:135:A:LEU:HD11	10	0.86	0.19	0.75
(1,3830)	2:40:B:ILE:HD13	2:13:B:VAL:HB	10	0.84	0.42	0.88
(1,3830)	2:40:B:ILE:HD11	2:13:B:VAL:HB	10	0.84	0.42	0.88
(1,3049)	2:50:C:ALA:H	2:13:C:VAL:HG13	10	0.83	0.36	0.69
(1,3049)	2:50:C:ALA:H	2:13:C:VAL:HG11	10	0.83	0.36	0.69
(1,3049)	2:50:C:ALA:H	2:13:C:VAL:HG12	10	0.83	0.36	0.69
(1,4188)	1:79:A:LYS:HE2	2:35:C:VAL:H	10	0.82	0.05	0.8
(1,1441)	1:77:A:THR:HG23	1:143:A:THR:HA	10	0.81	0.12	0.8
(1,1441)	1:77:A:THR:HG22	1:143:A:THR:HA	10	0.81	0.12	0.8
(1,1441)	1:77:A:THR:HG23	1:79:A:LYS:HA	10	0.81	0.12	0.8
(1,2243)	2:11:C:LEU:HA	2:54:C:ILE:HB	10	0.81	0.26	0.74
(1,47)	1:88:A:ILE:HD13	1:105:A:LEU:HA	10	0.81	0.3	0.69
(1,47)	1:88:A:ILE:HD11	1:105:A:LEU:HA	10	0.81	0.3	0.69
(1,2242)	2:11:B:LEU:HA	2:54:B:ILE:HB	10	0.8	0.12	0.79
(1,2564)	2:33:B:LEU:HD13	2:19:B:ILE:HG21	10	0.8	0.37	0.84
(1,2564)	2:33:B:LEU:HD12	2:19:B:ILE:HG22	10	0.8	0.37	0.84
(1,2564)	2:33:B:LEU:HD11	2:19:B:ILE:HG23	10	0.8	0.37	0.84
(1,2564)	2:33:B:LEU:HD12	2:19:B:ILE:HG21	10	0.8	0.37	0.84
(1,2564)	2:33:B:LEU:HD13	2:19:B:ILE:HG23	10	0.8	0.37	0.84
(1,2564)	2:33:B:LEU:HD11	2:19:B:ILE:HG21	10	0.8	0.37	0.84
(1,2182)	2:9:B:ALA:HA	2:40:B:ILE:HG21	10	0.76	0.24	0.78
(1,2182)	2:9:B:ALA:HA	2:40:B:ILE:HG22	10	0.76	0.24	0.78
(1,2182)	2:9:B:ALA:HA	2:40:B:ILE:HG23	10	0.76	0.24	0.78
(1,4080)	2:13:B:VAL:H	2:41:B:SER:HA	10	0.76	0.08	0.76
(1,2251)	2:11:C:LEU:HA	2:55:C:LEU:HB3	10	0.75	0.11	0.72
(1,2544)	2:51:B:VAL:HG12	2:55:B:LEU:HG	10	0.75	0.4	0.64
(1,2544)	2:51:B:VAL:HG11	2:55:B:LEU:HG	10	0.75	0.4	0.64
(1,2544)	2:51:B:VAL:HG13	2:55:B:LEU:HG	10	0.75	0.4	0.64
(1,3609)	2:38:C:ASP:HA	2:40:C:ILE:HD12	10	0.75	0.23	0.76
(1,3609)	2:38:C:ASP:HA	2:40:C:ILE:HD11	10	0.75	0.23	0.76
(1,3609)	2:38:C:ASP:HA	2:40:C:ILE:HD13	10	0.75	0.23	0.76
(1,3609)	2:38:C:ASP:HA	2:13:C:VAL:HG23	10	0.75	0.23	0.76
(1,3609)	2:38:C:ASP:HA	2:13:C:VAL:HG21	10	0.75	0.23	0.76
(1,36)	1:106:A:ILE:HD11	1:106:A:ILE:HA	10	0.74	0.1	0.76
(1,36)	1:106:A:ILE:HD13	1:106:A:ILE:HA	10	0.74	0.1	0.76
(1,36)	1:106:A:ILE:HD12	1:106:A:ILE:HA	10	0.74	0.1	0.76
(1,717)	1:120:A:LEU:HG	1:125:A:VAL:HA	10	0.74	0.34	0.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3770)	2:20:B:VAL:HG23	2:19:B:ILE:HA	10	0.74	0.26	0.74
(1,3770)	2:30:B:ALA:HA	2:20:B:VAL:HG22	10	0.74	0.26	0.74
(1,3770)	2:20:B:VAL:HG21	2:19:B:ILE:HA	10	0.74	0.26	0.74
(1,2064)	2:55:B:LEU:HD22	2:51:B:VAL:HB	10	0.71	0.39	0.6
(1,2064)	2:55:B:LEU:HD21	2:51:B:VAL:HB	10	0.71	0.39	0.6
(1,4050)	2:54:B:ILE:HB	2:50:B:ALA:H	10	0.71	0.23	0.78
(1,3771)	2:20:C:VAL:HG23	2:19:C:ILE:HA	10	0.71	0.2	0.77
(1,3771)	2:30:C:ALA:HA	2:20:C:VAL:HG22	10	0.71	0.2	0.77
(1,3771)	2:30:C:ALA:HA	2:20:C:VAL:HG23	10	0.71	0.2	0.77
(1,3771)	2:30:C:ALA:HA	2:20:C:VAL:HG21	10	0.71	0.2	0.77
(1,3119)	2:48:C:ARG:HB3	2:49:C:GLU:H	10	0.71	0.19	0.64
(1,4084)	2:14:B:ASN:H	2:12:B:ILE:HG23	10	0.71	0.33	0.62
(1,4084)	2:14:B:ASN:H	2:12:B:ILE:HG21	10	0.71	0.33	0.62
(1,4084)	2:14:B:ASN:H	2:12:B:ILE:HG22	10	0.71	0.33	0.62
(1,4084)	2:55:B:LEU:HD21	2:14:B:ASN:H	10	0.71	0.33	0.62
(1,3069)	2:39:C:CYS:H	2:35:C:VAL:HB	10	0.7	0.09	0.72
(1,4085)	2:14:C:ASN:H	2:12:C:ILE:HG23	10	0.7	0.31	0.68
(1,4085)	2:14:C:ASN:H	2:12:C:ILE:HG22	10	0.7	0.31	0.68
(1,1454)	1:105:A:LEU:HD22	1:105:A:LEU:HB2	10	0.69	0.06	0.7
(1,1454)	1:105:A:LEU:HD23	1:105:A:LEU:HB2	10	0.69	0.06	0.7
(1,1454)	1:78:A:LEU:HD21	1:78:A:LEU:HB3	10	0.69	0.06	0.7
(1,1454)	1:78:A:LEU:HD22	1:78:A:LEU:HB3	10	0.69	0.06	0.7
(1,2694)	2:54:B:ILE:HG23	2:46:B:PHE:HB2	10	0.68	0.21	0.7
(1,2694)	2:54:B:ILE:HG22	2:46:B:PHE:HB2	10	0.68	0.21	0.7
(1,2694)	2:54:B:ILE:HG21	2:46:B:PHE:HB2	10	0.68	0.21	0.7
(1,4175)	1:125:A:VAL:HG12	2:39:C:CYS:HG	10	0.68	0.42	0.8
(1,4175)	1:125:A:VAL:HG13	2:31:B:ASP:HB3	10	0.68	0.42	0.8
(1,4175)	1:125:A:VAL:HG21	2:31:B:ASP:HB3	10	0.68	0.42	0.8
(1,4175)	1:125:A:VAL:HG22	2:39:C:CYS:HG	10	0.68	0.42	0.8
(1,4175)	1:125:A:VAL:HG21	2:31:B:ASP:OD2	10	0.68	0.42	0.8
(1,4175)	1:125:A:VAL:H	2:42:C:GLU:OE2	10	0.68	0.42	0.8
(1,4175)	1:125:A:VAL:HB	2:39:C:CYS:HG	10	0.68	0.42	0.8
(1,3220)	2:34:B:ASN:HA	2:17:B:SER:H	10	0.68	0.23	0.68
(1,2126)	2:54:B:ILE:HB	2:13:B:VAL:HG21	10	0.66	0.21	0.66
(1,2126)	2:54:B:ILE:HB	2:13:B:VAL:HG23	10	0.66	0.21	0.66
(1,2126)	2:54:B:ILE:HB	2:13:B:VAL:HG22	10	0.66	0.21	0.66
(1,1010)	1:98:A:ILE:H	1:98:A:ILE:HG13	10	0.65	0.06	0.65
(1,3118)	2:48:B:ARG:HB3	2:49:B:GLU:H	10	0.63	0.14	0.66
(1,2499)	2:25:C:ILE:HG22	2:20:C:VAL:HG13	10	0.62	0.27	0.6
(1,2499)	2:25:C:ILE:HG21	2:20:C:VAL:HG11	10	0.62	0.27	0.6
(1,2499)	2:25:C:ILE:HG21	2:20:C:VAL:HG13	10	0.62	0.27	0.6
(1,2499)	2:25:C:ILE:HG23	2:20:C:VAL:HG13	10	0.62	0.27	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1623)	1:126:A:LEU:HG	1:124:A:LYS:HE3	10	0.61	0.24	0.66
(1,1623)	1:126:A:LEU:HG	1:127:A:HIS:HB2	10	0.61	0.24	0.66
(1,979)	1:101:A:ILE:HG12	1:101:A:ILE:H	10	0.59	0.05	0.58
(1,1270)	1:108:A:GLU:H	1:106:A:ILE:HG21	10	0.58	0.07	0.62
(1,1270)	1:108:A:GLU:H	1:106:A:ILE:HG23	10	0.58	0.07	0.62
(1,1272)	1:111:A:ALA:H	1:106:A:ILE:HD11	10	0.58	0.18	0.62
(1,1272)	1:111:A:ALA:H	1:106:A:ILE:HD13	10	0.58	0.18	0.62
(1,1272)	1:111:A:ALA:H	1:106:A:ILE:HD12	10	0.58	0.18	0.62
(1,2090)	2:8:B:ILE:HD12	2:3:B:ALA:HB3	10	0.57	0.21	0.6
(1,2090)	2:8:B:ILE:HD12	2:3:B:ALA:HB1	10	0.57	0.21	0.6
(1,2090)	2:8:B:ILE:HD11	2:3:B:ALA:HB2	10	0.57	0.21	0.6
(1,2090)	2:8:B:ILE:HD11	2:3:B:ALA:HB3	10	0.57	0.21	0.6
(1,2090)	2:8:B:ILE:HD13	2:3:B:ALA:HB3	10	0.57	0.21	0.6
(1,3622)	2:12:B:ILE:HA	2:13:B:VAL:HG13	10	0.57	0.14	0.56
(1,3622)	2:40:B:ILE:HA	2:33:C:LEU:HG	10	0.57	0.14	0.56
(1,2565)	2:33:C:LEU:HD13	2:19:C:ILE:HG21	10	0.56	0.25	0.56
(1,2565)	2:33:C:LEU:HD11	2:19:C:ILE:HG23	10	0.56	0.25	0.56
(1,2565)	2:33:C:LEU:HD13	2:19:C:ILE:HG22	10	0.56	0.25	0.56
(1,2565)	2:33:C:LEU:HD12	2:19:C:ILE:HG21	10	0.56	0.25	0.56
(1,2565)	2:33:C:LEU:HD11	2:19:C:ILE:HG21	10	0.56	0.25	0.56
(1,2565)	2:33:C:LEU:HD11	2:19:C:ILE:HG22	10	0.56	0.25	0.56
(1,2535)	2:36:C:ALA:HB3	2:40:B:ILE:HG13	10	0.55	0.2	0.47
(1,2535)	2:36:C:ALA:HB2	2:40:B:ILE:HG13	10	0.55	0.2	0.47
(1,2535)	2:36:C:ALA:HB1	2:40:B:ILE:HG13	10	0.55	0.2	0.47
(1,669)	1:103:A:GLN:HG3	1:99:A:LEU:HD11	10	0.55	0.2	0.49
(1,669)	1:103:A:GLN:HG3	1:99:A:LEU:HD12	10	0.55	0.2	0.49
(1,2482)	2:25:B:ILE:HB	2:19:B:ILE:HG21	10	0.54	0.19	0.56
(1,2482)	2:25:B:ILE:HB	2:19:B:ILE:HG22	10	0.54	0.19	0.56
(1,2482)	2:25:B:ILE:HB	2:19:B:ILE:HG23	10	0.54	0.19	0.56
(1,2483)	2:25:C:ILE:HB	2:19:C:ILE:HG22	10	0.53	0.27	0.5
(1,2483)	2:25:C:ILE:HB	2:19:C:ILE:HG23	10	0.53	0.27	0.5
(1,2483)	2:25:C:ILE:HB	2:19:C:ILE:HG21	10	0.53	0.27	0.5
(1,1654)	1:121:A:LEU:HG	1:121:A:LEU:HD13	10	0.53	0.03	0.53
(1,1654)	1:121:A:LEU:HG	1:121:A:LEU:HD22	10	0.53	0.03	0.53
(1,1654)	1:121:A:LEU:HG	1:121:A:LEU:HD12	10	0.53	0.03	0.53
(1,1654)	1:121:A:LEU:HG	1:121:A:LEU:HD21	10	0.53	0.03	0.53
(1,1654)	1:99:A:LEU:HG	1:99:A:LEU:HD11	10	0.53	0.03	0.53
(1,1784)	1:105:A:LEU:H	1:117:A:ILE:HD13	10	0.53	0.14	0.56
(1,1784)	1:105:A:LEU:H	1:117:A:ILE:HD11	10	0.53	0.14	0.56
(1,2540)	2:36:B:ALA:HB3	2:33:B:LEU:HD13	10	0.52	0.23	0.48
(1,2540)	2:36:B:ALA:HB3	2:33:B:LEU:HD11	10	0.52	0.23	0.48
(1,2540)	2:36:B:ALA:HB2	2:33:B:LEU:HD11	10	0.52	0.23	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1831)	1:148:A:ILE:HD12	1:148:A:ILE:H	10	0.52	0.1	0.52
(1,1831)	1:148:A:ILE:HD13	1:148:A:ILE:H	10	0.52	0.1	0.52
(1,1831)	1:148:A:ILE:HG21	1:148:A:ILE:H	10	0.52	0.1	0.52
(1,1831)	1:148:A:ILE:HG23	1:148:A:ILE:H	10	0.52	0.1	0.52
(1,1831)	1:148:A:ILE:HD11	1:148:A:ILE:H	10	0.52	0.1	0.52
(1,2091)	2:8:C:ILE:HD12	2:3:C:ALA:HB1	10	0.51	0.17	0.56
(1,2091)	2:8:C:ILE:HD11	2:3:C:ALA:HB3	10	0.51	0.17	0.56
(1,2091)	2:8:C:ILE:HD13	2:3:C:ALA:HB1	10	0.51	0.17	0.56
(1,2091)	2:8:C:ILE:HD12	2:3:C:ALA:HB2	10	0.51	0.17	0.56
(1,2091)	2:8:C:ILE:HD11	2:3:C:ALA:HB1	10	0.51	0.17	0.56
(1,1994)	2:36:B:ALA:HB3	2:33:B:LEU:HD21	10	0.5	0.13	0.48
(1,1994)	2:36:B:ALA:HB3	2:33:B:LEU:HD23	10	0.5	0.13	0.48
(1,1994)	2:36:B:ALA:HB2	2:33:B:LEU:HD22	10	0.5	0.13	0.48
(1,4169)	1:81:A:ILE:HD11	2:39:B:CYS:HG	10	0.5	0.19	0.52
(1,4169)	1:81:A:ILE:HD11	2:31:C:ASP:OD2	10	0.5	0.19	0.52
(1,4169)	1:81:A:ILE:HD12	2:31:C:ASP:OD1	10	0.5	0.19	0.52
(1,4169)	1:81:A:ILE:HG22	2:42:B:GLU:HG3	10	0.5	0.19	0.52
(1,4169)	1:81:A:ILE:HD12	2:35:C:VAL:HG11	10	0.5	0.19	0.52
(1,4169)	1:81:A:ILE:HD13	2:31:C:ASP:OD2	10	0.5	0.19	0.52
(1,4169)	1:81:A:ILE:HD12	2:31:C:ASP:OD2	10	0.5	0.19	0.52
(1,4169)	1:81:A:ILE:HD12	2:39:B:CYS:HG	10	0.5	0.19	0.52
(1,4169)	1:81:A:ILE:HD13	2:35:C:VAL:HG13	10	0.5	0.19	0.52
(1,2551)	2:20:C:VAL:HG12	2:19:C:ILE:HB	10	0.5	0.11	0.48
(1,2551)	2:20:C:VAL:HG13	2:19:C:ILE:HB	10	0.5	0.11	0.48
(1,101)	1:77:A:THR:HG23	1:87:A:SER:HB3	10	0.48	0.21	0.46
(1,101)	1:77:A:THR:HG21	1:87:A:SER:HB3	10	0.48	0.21	0.46
(1,2550)	2:20:B:VAL:HG11	2:19:B:ILE:HB	10	0.48	0.07	0.47
(1,2550)	2:20:B:VAL:HG13	2:19:B:ILE:HB	10	0.48	0.07	0.47
(1,2550)	2:20:B:VAL:HG12	2:19:B:ILE:HB	10	0.48	0.07	0.47
(1,980)	1:101:A:ILE:HG13	1:101:A:ILE:H	10	0.46	0.09	0.48
(1,3068)	2:39:B:CYS:H	2:35:B:VAL:HB	10	0.46	0.19	0.5
(1,1458)	1:126:A:LEU:HD23	1:126:A:LEU:HA	10	0.45	0.1	0.48
(1,1458)	1:126:A:LEU:HD21	1:126:A:LEU:HA	10	0.45	0.1	0.48
(1,1458)	1:126:A:LEU:HD22	1:126:A:LEU:HA	10	0.45	0.1	0.48
(1,1995)	2:36:C:ALA:HB1	2:33:C:LEU:HD23	10	0.45	0.13	0.47
(1,1995)	2:36:C:ALA:HB1	2:33:C:LEU:HD21	10	0.45	0.13	0.47
(1,1995)	2:36:C:ALA:HB2	2:33:C:LEU:HD21	10	0.45	0.13	0.47
(1,3420)	2:51:B:VAL:H	2:54:B:ILE:HG12	10	0.43	0.2	0.38
(1,2112)	2:13:B:VAL:HG23	2:51:B:VAL:HB	10	0.42	0.13	0.45
(1,2112)	2:13:B:VAL:HG22	2:51:B:VAL:HB	10	0.42	0.13	0.45
(1,2112)	2:13:B:VAL:HG21	2:51:B:VAL:HB	10	0.42	0.13	0.45
(1,1659)	1:124:A:LYS:HE2	1:124:A:LYS:HD3	10	0.41	0.05	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1659)	1:118:A:LYS:HB2	1:118:A:LYS:HE3	10	0.41	0.05	0.4
(1,3692)	2:9:B:ALA:HA	2:46:B:PHE:HE1	10	0.41	0.15	0.42
(1,3692)	2:9:B:ALA:HA	2:16:C:PHE:HZ	10	0.41	0.15	0.42
(1,4185)	1:120:A:LEU:HG	2:35:C:VAL:H	10	0.4	0.19	0.36
(1,4185)	1:120:A:LEU:HG	2:35:B:VAL:H	10	0.4	0.19	0.36
(1,4186)	1:120:A:LEU:HG	2:35:C:VAL:H	10	0.4	0.19	0.36
(1,4186)	1:120:A:LEU:HG	2:35:B:VAL:H	10	0.4	0.19	0.36
(1,1011)	1:98:A:ILE:H	1:98:A:ILE:HG12	10	0.4	0.09	0.41
(1,67)	1:83:A:ALA:HB2	1:85:A:LYS:H	10	0.39	0.21	0.41
(1,67)	1:83:A:ALA:HB1	1:85:A:LYS:H	10	0.39	0.21	0.41
(1,2492)	2:54:B:ILE:HB	2:54:B:ILE:HG22	10	0.37	0.01	0.38
(1,2492)	2:54:B:ILE:HB	2:54:B:ILE:HG21	10	0.37	0.01	0.38
(1,2492)	2:54:B:ILE:HB	2:54:B:ILE:HG23	10	0.37	0.01	0.38
(1,46)	1:88:A:ILE:HD13	1:88:A:ILE:HG12	10	0.36	0.02	0.38
(1,46)	1:88:A:ILE:HD11	1:88:A:ILE:HG12	10	0.36	0.02	0.38
(1,780)	1:148:A:ILE:HG22	1:148:A:ILE:HB	10	0.36	0.04	0.38
(1,780)	1:148:A:ILE:HG23	1:148:A:ILE:HB	10	0.36	0.04	0.38
(1,780)	1:148:A:ILE:HG21	1:148:A:ILE:HB	10	0.36	0.04	0.38
(1,3750)	2:51:B:VAL:HG12	2:51:B:VAL:HB	10	0.36	0.04	0.36
(1,3750)	2:51:B:VAL:HG11	2:51:B:VAL:HB	10	0.36	0.04	0.36
(1,3750)	2:20:B:VAL:HG22	2:20:B:VAL:HB	10	0.36	0.04	0.36
(1,3750)	2:20:B:VAL:HG23	2:20:B:VAL:HB	10	0.36	0.04	0.36
(1,3750)	2:51:B:VAL:HG13	2:51:B:VAL:HB	10	0.36	0.04	0.36
(1,3760)	2:51:B:VAL:HG12	2:51:B:VAL:HB	10	0.36	0.04	0.36
(1,3760)	2:51:B:VAL:HG11	2:51:B:VAL:HB	10	0.36	0.04	0.36
(1,3760)	2:20:B:VAL:HG11	2:20:B:VAL:HB	10	0.36	0.04	0.36
(1,3760)	2:20:B:VAL:HG22	2:20:B:VAL:HB	10	0.36	0.04	0.36
(1,3760)	2:20:B:VAL:HG12	2:20:B:VAL:HB	10	0.36	0.04	0.36
(1,3760)	2:20:B:VAL:HG23	2:20:B:VAL:HB	10	0.36	0.04	0.36
(1,3760)	2:51:B:VAL:HG13	2:51:B:VAL:HB	10	0.36	0.04	0.36
(1,4177)	1:147:A:MET:HG3	2:35:B:VAL:HG22	10	0.35	0.16	0.33
(1,4177)	1:147:A:MET:HG3	2:35:B:VAL:HG21	10	0.35	0.16	0.33
(1,4177)	1:147:A:MET:HB3	2:35:B:VAL:HG21	10	0.35	0.16	0.33
(1,4177)	1:147:A:MET:HE1	2:35:C:VAL:HG13	10	0.35	0.16	0.33
(1,4177)	1:147:A:MET:HE2	2:35:C:VAL:HG11	10	0.35	0.16	0.33
(1,4177)	1:147:A:MET:HG2	2:35:B:VAL:HG21	10	0.35	0.16	0.33
(1,4177)	1:147:A:MET:HE1	2:35:C:VAL:HG11	10	0.35	0.16	0.33
(1,4177)	1:147:A:MET:HG2	2:35:B:VAL:HG22	10	0.35	0.16	0.33
(1,4177)	1:147:A:MET:HE3	2:39:B:CYS:HB2	10	0.35	0.16	0.33
(1,3761)	2:20:C:VAL:HG22	2:20:C:VAL:HB	10	0.35	0.02	0.34
(1,3761)	2:51:C:VAL:HG12	2:51:C:VAL:HB	10	0.35	0.02	0.34
(1,3761)	2:20:C:VAL:HG23	2:20:C:VAL:HB	10	0.35	0.02	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3761)	2:20:C:VAL:HG11	2:20:C:VAL:HB	10	0.35	0.02	0.34
(1,3751)	2:20:C:VAL:HG22	2:20:C:VAL:HB	10	0.35	0.02	0.34
(1,3751)	2:51:C:VAL:HG12	2:51:C:VAL:HB	10	0.35	0.02	0.34
(1,3751)	2:20:C:VAL:HG23	2:20:C:VAL:HB	10	0.35	0.02	0.34
(1,2493)	2:54:C:ILE:HB	2:54:C:ILE:HG23	10	0.34	0.03	0.36
(1,2493)	2:54:C:ILE:HB	2:54:C:ILE:HG21	10	0.34	0.03	0.36
(1,2493)	2:54:C:ILE:HB	2:54:C:ILE:HG22	10	0.34	0.03	0.36
(1,783)	1:106:A:ILE:HG21	1:106:A:ILE:HB	10	0.34	0.03	0.34
(1,783)	1:106:A:ILE:HG23	1:106:A:ILE:HB	10	0.34	0.03	0.34
(1,783)	1:106:A:ILE:HG22	1:106:A:ILE:HB	10	0.34	0.03	0.34
(1,494)	1:98:A:ILE:HA	1:101:A:ILE:HG12	10	0.33	0.11	0.31
(1,172)	1:78:A:LEU:HD21	1:78:A:LEU:HG	10	0.33	0.04	0.33
(1,172)	1:78:A:LEU:HD23	1:78:A:LEU:HG	10	0.33	0.04	0.33
(1,683)	1:106:A:ILE:HG12	1:106:A:ILE:H	10	0.33	0.14	0.35
(1,4189)	1:124:A:LYS:H	2:38:C:ASP:H	10	0.33	0.06	0.32
(1,134)	1:125:A:VAL:HG22	1:125:A:VAL:HB	10	0.32	0.03	0.32
(1,134)	1:125:A:VAL:HG23	1:125:A:VAL:HB	10	0.32	0.03	0.32
(1,134)	1:125:A:VAL:HG21	1:125:A:VAL:HB	10	0.32	0.03	0.32
(1,2076)	2:55:B:LEU:HD12	2:55:B:LEU:HG	10	0.32	0.03	0.34
(1,2076)	2:55:B:LEU:HD13	2:55:B:LEU:HG	10	0.32	0.03	0.34
(1,2076)	2:55:B:LEU:HD11	2:55:B:LEU:HG	10	0.32	0.03	0.34
(1,2077)	2:55:C:LEU:HD12	2:55:C:LEU:HG	10	0.31	0.03	0.31
(1,2077)	2:55:C:LEU:HD11	2:55:C:LEU:HG	10	0.31	0.03	0.31
(1,2077)	2:55:C:LEU:HD13	2:55:C:LEU:HG	10	0.31	0.03	0.31
(1,955)	1:131:A:PHE:HB3	1:131:A:PHE:H	10	0.3	0.05	0.32
(1,138)	1:97:A:THR:HG23	1:97:A:THR:HB	10	0.3	0.02	0.3
(1,138)	1:97:A:THR:HG21	1:97:A:THR:HB	10	0.3	0.02	0.3
(1,1466)	1:117:A:ILE:HG23	1:117:A:ILE:HB	10	0.3	0.03	0.3
(1,1466)	1:117:A:ILE:HG22	1:117:A:ILE:HB	10	0.3	0.03	0.3
(1,1466)	1:117:A:ILE:HG21	1:117:A:ILE:HB	10	0.3	0.03	0.3
(1,1611)	1:81:A:ILE:HB	1:81:A:ILE:HG23	10	0.28	0.02	0.29
(1,1611)	1:81:A:ILE:HB	1:81:A:ILE:HG21	10	0.28	0.02	0.29
(1,1611)	1:81:A:ILE:HB	1:81:A:ILE:HG22	10	0.28	0.02	0.29
(1,1611)	1:144:A:ILE:HB	1:144:A:ILE:HG23	10	0.28	0.02	0.29
(1,1611)	1:144:A:ILE:HB	1:144:A:ILE:HG21	10	0.28	0.02	0.29
(1,1650)	1:74:A:VAL:HG22	1:74:A:VAL:HB	10	0.28	0.03	0.29
(1,1650)	1:74:A:VAL:HG23	1:74:A:VAL:HB	10	0.28	0.03	0.29
(1,1650)	1:137:A:VAL:HG22	1:137:A:VAL:HB	10	0.28	0.03	0.29
(1,1650)	1:137:A:VAL:HG23	1:137:A:VAL:HB	10	0.28	0.03	0.29
(1,722)	1:148:A:ILE:HA	1:148:A:ILE:HD11	10	0.28	0.06	0.27
(1,722)	1:148:A:ILE:HA	1:148:A:ILE:HD12	10	0.28	0.06	0.27
(1,722)	1:148:A:ILE:HA	1:148:A:ILE:HD13	10	0.28	0.06	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,66)	1:83:A:ALA:HB3	1:83:A:ALA:H	10	0.28	0.04	0.29
(1,66)	1:83:A:ALA:HB1	1:83:A:ALA:H	10	0.28	0.04	0.29
(1,3727)	2:25:C:ILE:HG21	2:25:C:ILE:HG12	10	0.27	0.1	0.28
(1,3727)	2:25:C:ILE:HG23	2:30:C:ALA:HB2	10	0.27	0.1	0.28
(1,3727)	2:25:C:ILE:HG23	2:25:C:ILE:HG12	10	0.27	0.1	0.28
(1,3727)	2:25:C:ILE:HG22	2:30:C:ALA:HB3	10	0.27	0.1	0.28
(1,3727)	2:25:C:ILE:HG21	2:30:C:ALA:HB2	10	0.27	0.1	0.28
(1,1716)	1:101:A:ILE:HG21	1:101:A:ILE:H	10	0.27	0.02	0.27
(1,1716)	1:101:A:ILE:HG22	1:101:A:ILE:H	10	0.27	0.02	0.27
(1,3083)	2:41:C:SER:H	2:41:C:SER:HB3	10	0.27	0.01	0.27
(1,2346)	2:44:B:PHE:HB2	2:46:B:PHE:HD1	10	0.26	0.09	0.25
(1,112)	1:77:A:THR:HG22	1:78:A:LEU:H	10	0.26	0.06	0.26
(1,112)	1:77:A:THR:HG21	1:78:A:LEU:H	10	0.26	0.06	0.26
(1,112)	1:77:A:THR:HG23	1:78:A:LEU:H	10	0.26	0.06	0.26
(1,779)	1:74:A:VAL:HG13	1:74:A:VAL:HB	10	0.25	0.03	0.24
(1,779)	1:74:A:VAL:HG11	1:74:A:VAL:HB	10	0.25	0.03	0.24
(1,1845)	2:13:C:VAL:HA	2:13:C:VAL:HG21	10	0.23	0.03	0.24
(1,1845)	2:13:C:VAL:HA	2:13:C:VAL:HG23	10	0.23	0.03	0.24
(1,1845)	2:13:C:VAL:HA	2:13:C:VAL:HG22	10	0.23	0.03	0.24
(1,2067)	2:55:C:LEU:HD22	2:55:C:LEU:HG	10	0.21	0.02	0.21
(1,2067)	2:55:C:LEU:HD21	2:55:C:LEU:HG	10	0.21	0.02	0.21
(1,1157)	1:152:A:LEU:HA	1:152:A:LEU:H	10	0.21	0.02	0.21
(1,1609)	1:114:A:ILE:HB	1:114:A:ILE:HG21	10	0.21	0.04	0.21
(1,1609)	1:114:A:ILE:HB	1:114:A:ILE:HG23	10	0.21	0.04	0.21
(1,1609)	1:114:A:ILE:HB	1:114:A:ILE:HG22	10	0.21	0.04	0.21
(1,2066)	2:55:B:LEU:HD23	2:55:B:LEU:HG	10	0.21	0.02	0.2
(1,2066)	2:55:B:LEU:HD22	2:55:B:LEU:HG	10	0.21	0.02	0.2
(1,1432)	1:117:A:ILE:HD12	1:117:A:ILE:HG13	10	0.2	0.05	0.2
(1,1432)	1:117:A:ILE:HD13	1:117:A:ILE:HG13	10	0.2	0.05	0.2
(1,1432)	1:117:A:ILE:HD11	1:117:A:ILE:HG13	10	0.2	0.05	0.2
(1,1844)	2:13:B:VAL:HA	2:13:B:VAL:HG23	10	0.2	0.03	0.21
(1,1844)	2:13:B:VAL:HA	2:13:B:VAL:HG22	10	0.2	0.03	0.21
(1,1844)	2:13:B:VAL:HA	2:13:B:VAL:HG21	10	0.2	0.03	0.21
(1,144)	1:140:A:ALA:HB3	1:140:A:ALA:HA	10	0.19	0.02	0.19
(1,144)	1:140:A:ALA:HB2	1:140:A:ALA:HA	10	0.19	0.02	0.19
(1,3558)	2:25:B:ILE:HD12	2:25:B:ILE:HG12	10	0.18	0.03	0.19
(1,3558)	2:25:B:ILE:HD13	2:25:B:ILE:HG12	10	0.18	0.03	0.19
(1,787)	1:120:A:LEU:HG	1:120:A:LEU:HD21	10	0.18	0.04	0.17
(1,787)	1:120:A:LEU:HG	1:120:A:LEU:HD23	10	0.18	0.04	0.17
(1,787)	1:120:A:LEU:HG	1:120:A:LEU:HD22	10	0.18	0.04	0.17
(1,2488)	2:68:B:ILE:HG21	2:68:B:ILE:HG13	10	0.18	0.04	0.17
(1,2488)	2:68:B:ILE:HG22	2:68:B:ILE:HG13	10	0.18	0.04	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2488)	2:68:B:ILE:HG23	2:68:B:ILE:HG13	10	0.18	0.04	0.17
(1,16)	1:98:A:ILE:HD13	1:98:A:ILE:HG12	10	0.16	0.03	0.16
(1,16)	1:98:A:ILE:HD12	1:98:A:ILE:HG12	10	0.16	0.03	0.16
(1,16)	1:98:A:ILE:HD11	1:98:A:ILE:HG12	10	0.16	0.03	0.16
(1,3050)	2:16:B:PHE:HB3	2:16:B:PHE:H	10	0.15	0.02	0.16
(1,1448)	1:78:A:LEU:HD13	1:90:A:HIS:HE1	9	2.77	0.8	2.89
(1,1448)	1:78:A:LEU:HD13	1:104:A:HIS:HE1	9	2.77	0.8	2.89
(1,63)	1:83:A:ALA:HB1	1:85:A:LYS:HE3	9	2.53	0.32	2.39
(1,1452)	1:78:A:LEU:HD21	1:90:A:HIS:HE1	9	2.33	1.24	2.8
(1,1347)	1:141:A:ASN:HD22	1:121:A:LEU:HD13	9	2.17	0.59	1.99
(1,1347)	1:141:A:ASN:HD22	1:121:A:LEU:HD12	9	2.17	0.59	1.99
(1,1172)	1:85:A:LYS:HE3	1:83:A:ALA:H	9	1.74	0.37	1.59
(1,3543)	2:51:C:VAL:HG23	2:13:C:VAL:HB	9	1.45	0.51	1.64
(1,3543)	2:51:C:VAL:HG21	2:13:C:VAL:HB	9	1.45	0.51	1.64
(1,3543)	2:51:C:VAL:HG22	2:13:C:VAL:HB	9	1.45	0.51	1.64
(1,3543)	2:51:C:VAL:HG22	2:49:C:GLU:HG3	9	1.45	0.51	1.64
(1,3543)	2:51:C:VAL:HG23	2:49:C:GLU:HG3	9	1.45	0.51	1.64
(1,786)	1:126:A:LEU:HD11	1:124:A:LYS:HD3	9	1.42	0.74	1.25
(1,786)	1:126:A:LEU:HD13	1:124:A:LYS:HD3	9	1.42	0.74	1.25
(1,786)	1:126:A:LEU:HD12	1:124:A:LYS:HD3	9	1.42	0.74	1.25
(1,1123)	1:87:A:SER:H	1:79:A:LYS:HD3	9	1.35	0.33	1.38
(1,2159)	2:13:C:VAL:HG23	2:48:C:ARG:HD3	9	1.28	0.41	1.53
(1,2159)	2:13:C:VAL:HG21	2:48:C:ARG:HD3	9	1.28	0.41	1.53
(1,778)	1:128:A:ASP:HB2	1:99:A:LEU:HD23	9	1.26	0.09	1.29
(1,778)	1:128:A:ASP:HB2	1:99:A:LEU:HD21	9	1.26	0.09	1.29
(1,2298)	2:19:B:ILE:HA	2:22:B:LYS:HD3	9	1.22	0.69	1.05
(1,735)	1:79:A:LYS:HD3	1:79:A:LYS:HA	9	1.08	0.18	1.16
(1,2695)	2:54:C:ILE:HG23	2:46:C:PHE:HB2	9	1.07	0.32	1.16
(1,2695)	2:54:C:ILE:HG21	2:46:C:PHE:HB2	9	1.07	0.32	1.16
(1,2695)	2:54:C:ILE:HG22	2:46:C:PHE:HB2	9	1.07	0.32	1.16
(1,1593)	1:142:A:SER:HB2	1:137:A:VAL:HB	9	1.03	0.22	1.03
(1,229)	1:118:A:LYS:HB2	1:118:A:LYS:HE3	9	1.02	0.47	0.93
(1,732)	1:81:A:ILE:HA	1:79:A:LYS:HD3	9	1.01	0.54	1.06
(1,898)	1:85:A:LYS:HB3	1:86:A:PHE:H	9	1.0	0.45	1.11
(1,1198)	1:113:A:HIS:H	1:116:A:GLU:HB3	9	1.0	0.57	0.76
(1,186)	1:120:A:LEU:HD22	1:120:A:LEU:H	9	0.98	0.64	0.62
(1,186)	1:120:A:LEU:HD23	1:120:A:LEU:H	9	0.98	0.64	0.62
(1,186)	1:120:A:LEU:HD21	1:120:A:LEU:H	9	0.98	0.64	0.62
(1,1809)	1:103:A:GLN:HE22	1:114:A:ILE:HG21	9	0.97	0.39	0.79
(1,1809)	1:103:A:GLN:HE22	1:99:A:LEU:HD11	9	0.97	0.39	0.79
(1,1809)	1:103:A:GLN:HE22	1:99:A:LEU:HD12	9	0.97	0.39	0.79
(1,1809)	1:103:A:GLN:HE22	1:114:A:ILE:HG23	9	0.97	0.39	0.79

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1594)	1:142:A:SER:HB2	1:121:A:LEU:HD13	9	0.97	0.26	0.85
(1,1594)	1:142:A:SER:HB2	1:74:A:VAL:HG21	9	0.97	0.26	0.85
(1,1594)	1:142:A:SER:HB2	1:76:A:LEU:HD13	9	0.97	0.26	0.85
(1,1594)	1:142:A:SER:HB2	1:121:A:LEU:HD12	9	0.97	0.26	0.85
(1,2614)	2:13:B:VAL:HG12	2:48:B:ARG:HG2	9	0.85	1.0	0.33
(1,2614)	2:13:B:VAL:HG13	2:48:B:ARG:HG2	9	0.85	1.0	0.33
(1,1803)	1:82:A:GLN:HE21	1:81:A:ILE:HG22	9	0.82	0.57	0.59
(1,3182)	2:12:B:ILE:HD11	2:9:B:ALA:H	9	0.81	0.5	0.74
(1,3182)	2:12:B:ILE:HD12	2:9:B:ALA:H	9	0.81	0.5	0.74
(1,3182)	2:12:B:ILE:HD13	2:9:B:ALA:H	9	0.81	0.5	0.74
(1,80)	1:148:A:ILE:HG22	1:112:A:SER:HA	9	0.81	0.19	0.77
(1,80)	1:148:A:ILE:HG23	1:112:A:SER:HA	9	0.81	0.19	0.77
(1,80)	1:148:A:ILE:HG21	1:112:A:SER:HA	9	0.81	0.19	0.77
(1,162)	1:78:A:LEU:HD23	1:92:A:PHE:HZ	9	0.79	0.57	0.65
(1,162)	1:78:A:LEU:HD21	1:92:A:PHE:HZ	9	0.79	0.57	0.65
(1,2060)	2:55:B:LEU:HD22	2:14:B:ASN:H	9	0.75	0.42	0.56
(1,2060)	2:55:B:LEU:HD21	2:14:B:ASN:H	9	0.75	0.42	0.56
(1,1435)	1:98:A:ILE:HG23	1:128:A:ASP:H	9	0.74	0.21	0.8
(1,1435)	1:98:A:ILE:HG22	1:128:A:ASP:H	9	0.74	0.21	0.8
(1,1801)	1:82:A:GLN:HE22	1:81:A:ILE:HG22	9	0.73	0.42	0.73
(1,1801)	1:82:A:GLN:HE22	1:81:A:ILE:HG21	9	0.73	0.42	0.73
(1,1801)	1:82:A:GLN:HE22	1:81:A:ILE:HD12	9	0.73	0.42	0.73
(1,2501)	2:25:C:ILE:HG22	2:20:C:VAL:HB	9	0.68	0.28	0.69
(1,2501)	2:25:C:ILE:HG21	2:20:C:VAL:HB	9	0.68	0.28	0.69
(1,2501)	2:25:C:ILE:HG23	2:20:C:VAL:HB	9	0.68	0.28	0.69
(1,535)	1:150:A:PRO:HA	1:116:A:GLU:HG3	9	0.66	0.33	0.53
(1,4051)	2:54:C:ILE:HB	2:50:C:ALA:H	9	0.65	0.12	0.72
(1,2113)	2:13:C:VAL:HG22	2:51:C:VAL:HB	9	0.64	0.93	0.37
(1,2113)	2:13:C:VAL:HG21	2:51:C:VAL:HB	9	0.64	0.93	0.37
(1,1455)	1:132:A:LEU:HD21	1:94:A:PRO:HA	9	0.63	0.27	0.52
(1,1455)	1:132:A:LEU:HD23	1:94:A:PRO:HA	9	0.63	0.27	0.52
(1,2193)	2:25:C:ILE:HD11	2:30:C:ALA:HA	9	0.62	0.19	0.58
(1,2964)	2:48:B:ARG:HB3	2:48:B:ARG:H	9	0.59	0.02	0.59
(1,2038)	2:5:B:LYS:HB3	2:44:B:PHE:HZ	9	0.59	0.33	0.55
(3,33)	1:149:A:LYS:H	1:116:A:GLU:O	9	0.58	0.25	0.66
(1,3575)	2:33:C:LEU:HB2	2:33:C:LEU:HD22	9	0.57	0.29	0.78
(1,3575)	2:33:C:LEU:HB2	2:33:C:LEU:HD21	9	0.57	0.29	0.78
(1,3575)	2:33:C:LEU:HD23	2:43:B:ALA:HB2	9	0.57	0.29	0.78
(1,3575)	2:33:C:LEU:HB2	2:33:C:LEU:HD23	9	0.57	0.29	0.78
(1,3575)	2:33:C:LEU:HD22	2:43:B:ALA:HB1	9	0.57	0.29	0.78
(1,1704)	1:121:A:LEU:H	1:121:A:LEU:HD12	9	0.57	0.05	0.57
(1,1704)	1:121:A:LEU:H	1:121:A:LEU:HD23	9	0.57	0.05	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1704)	1:121:A:LEU:H	1:121:A:LEU:HD22	9	0.57	0.05	0.57
(1,1704)	1:121:A:LEU:H	1:144:A:ILE:HG23	9	0.57	0.05	0.57
(1,3744)	2:40:B:ILE:HD11	2:36:C:ALA:HB3	9	0.57	0.14	0.53
(1,3744)	2:40:B:ILE:HD12	2:36:B:ALA:HB2	9	0.57	0.14	0.53
(1,3744)	2:40:B:ILE:HD12	2:36:C:ALA:HB1	9	0.57	0.14	0.53
(1,3744)	2:40:B:ILE:HD12	2:36:C:ALA:HB3	9	0.57	0.14	0.53
(1,3744)	2:40:B:ILE:HD13	2:36:B:ALA:HB2	9	0.57	0.14	0.53
(1,460)	1:126:A:LEU:HD11	1:120:A:LEU:HA	9	0.56	0.34	0.5
(1,460)	1:126:A:LEU:HD13	1:120:A:LEU:HA	9	0.56	0.34	0.5
(1,460)	1:126:A:LEU:HD12	1:120:A:LEU:HA	9	0.56	0.34	0.5
(1,3317)	2:26:C:SER:H	2:33:C:LEU:HD13	9	0.56	0.21	0.63
(1,3317)	2:26:C:SER:H	2:33:C:LEU:HD11	9	0.56	0.21	0.63
(1,3317)	2:26:C:SER:H	2:33:C:LEU:HD12	9	0.56	0.21	0.63
(1,1140)	1:82:A:GLN:HG2	1:82:A:GLN:H	9	0.55	0.21	0.53
(1,2541)	2:36:C:ALA:HB1	2:33:C:LEU:HD12	9	0.53	0.19	0.6
(1,1661)	1:149:A:LYS:HB3	1:149:A:LYS:HE3	9	0.52	0.24	0.45
(1,1661)	1:149:A:LYS:HE3	1:149:A:LYS:HD3	9	0.52	0.24	0.45
(1,113)	1:77:A:THR:HG22	1:88:A:ILE:H	9	0.51	0.19	0.53
(1,113)	1:77:A:THR:HG21	1:88:A:ILE:H	9	0.51	0.19	0.53
(1,113)	1:77:A:THR:HG23	1:88:A:ILE:H	9	0.51	0.19	0.53
(1,201)	1:144:A:ILE:HG23	1:120:A:LEU:H	9	0.51	0.28	0.43
(1,201)	1:144:A:ILE:HG22	1:120:A:LEU:H	9	0.51	0.28	0.43
(1,201)	1:144:A:ILE:HG21	1:120:A:LEU:H	9	0.51	0.28	0.43
(1,4099)	2:17:C:SER:H	2:12:C:ILE:HG23	9	0.51	0.09	0.48
(1,4099)	2:17:C:SER:H	2:12:C:ILE:HG22	9	0.51	0.09	0.48
(1,4099)	2:17:C:SER:H	2:12:C:ILE:HG21	9	0.51	0.09	0.48
(1,759)	1:114:A:ILE:HA	1:114:A:ILE:HG23	9	0.51	0.06	0.51
(1,759)	1:114:A:ILE:HA	1:114:A:ILE:HG22	9	0.51	0.06	0.51
(1,759)	1:114:A:ILE:HA	1:114:A:ILE:HG21	9	0.51	0.06	0.51
(1,1461)	1:120:A:LEU:HD22	1:145:A:THR:H	9	0.5	0.24	0.46
(1,1461)	1:126:A:LEU:HD21	1:145:A:THR:H	9	0.5	0.24	0.46
(1,1461)	1:120:A:LEU:HD23	1:145:A:THR:H	9	0.5	0.24	0.46
(1,1683)	1:77:A:THR:H	1:76:A:LEU:HD11	9	0.49	0.24	0.37
(1,1683)	1:77:A:THR:H	1:76:A:LEU:HD12	9	0.49	0.24	0.37
(1,1683)	1:77:A:THR:H	1:76:A:LEU:HD13	9	0.49	0.24	0.37
(1,1699)	1:98:A:ILE:HG23	1:128:A:ASP:H	9	0.47	0.21	0.53
(1,1699)	1:98:A:ILE:HG22	1:128:A:ASP:H	9	0.47	0.21	0.53
(1,1808)	1:99:A:LEU:HG	1:103:A:GLN:HE22	9	0.46	0.33	0.43
(1,1808)	1:103:A:GLN:HE22	1:114:A:ILE:HG13	9	0.46	0.33	0.43
(1,1787)	1:111:A:ALA:H	1:106:A:ILE:HG23	9	0.45	0.11	0.4
(1,1787)	1:111:A:ALA:H	1:106:A:ILE:HG22	9	0.45	0.11	0.4
(1,1787)	1:111:A:ALA:H	1:148:A:ILE:HD12	9	0.45	0.11	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1159)	1:152:A:LEU:HG	1:152:A:LEU:H	9	0.44	0.21	0.46
(1,3658)	2:51:B:VAL:HG23	2:46:B:PHE:HE2	9	0.41	0.3	0.34
(1,3658)	2:51:B:VAL:HG21	2:46:B:PHE:HE2	9	0.41	0.3	0.34
(1,3658)	2:51:B:VAL:HG22	2:46:B:PHE:HE2	9	0.41	0.3	0.34
(1,3320)	2:19:B:ILE:HG23	2:26:B:SER:H	9	0.39	0.12	0.34
(1,3320)	2:19:B:ILE:HG22	2:26:B:SER:H	9	0.39	0.12	0.34
(1,3320)	2:19:B:ILE:HG21	2:26:B:SER:H	9	0.39	0.12	0.34
(1,1428)	1:106:A:ILE:HD13	1:102:A:LYS:HB3	9	0.38	0.24	0.35
(1,1428)	1:106:A:ILE:HD12	1:102:A:LYS:HB3	9	0.38	0.24	0.35
(1,1428)	1:106:A:ILE:HD11	1:102:A:LYS:HB3	9	0.38	0.24	0.35
(3,139)	2:38:C:ASP:H	2:34:C:ASN:O	9	0.37	0.06	0.36
(1,1723)	1:102:A:LYS:H	1:117:A:ILE:HD11	9	0.33	0.11	0.34
(1,1723)	1:102:A:LYS:H	1:117:A:ILE:HD12	9	0.33	0.11	0.34
(1,1723)	1:114:A:ILE:HD12	1:102:A:LYS:H	9	0.33	0.11	0.34
(1,1723)	1:102:A:LYS:H	1:117:A:ILE:HD13	9	0.33	0.11	0.34
(1,1033)	1:106:A:ILE:HG13	1:106:A:ILE:H	9	0.31	0.1	0.3
(1,2183)	2:9:C:ALA:HA	2:40:C:ILE:HG23	9	0.31	0.11	0.26
(1,2183)	2:9:C:ALA:HA	2:40:C:ILE:HG22	9	0.31	0.11	0.26
(1,2183)	2:9:C:ALA:HA	2:40:C:ILE:HG21	9	0.31	0.11	0.26
(1,1132)	1:126:A:LEU:H	1:126:A:LEU:HB3	9	0.31	0.09	0.29
(3,140)	2:38:C:ASP:N	2:34:C:ASN:O	9	0.3	0.05	0.3
(1,1655)	1:81:A:ILE:HG12	1:81:A:ILE:HD13	9	0.27	0.03	0.28
(1,1655)	1:81:A:ILE:HG12	1:81:A:ILE:HD12	9	0.27	0.03	0.28
(1,3082)	2:41:B:SER:H	2:41:B:SER:HB3	9	0.27	0.01	0.28
(1,184)	1:130:A:LEU:HD21	1:130:A:LEU:H	9	0.27	0.09	0.28
(1,184)	1:130:A:LEU:HD23	1:130:A:LEU:H	9	0.27	0.09	0.28
(1,2347)	2:44:C:PHE:HB2	2:46:C:PHE:HD1	9	0.27	0.09	0.27
(1,3561)	2:25:C:ILE:HD13	2:25:C:ILE:HG13	9	0.22	0.04	0.22
(1,3561)	2:25:C:ILE:HD12	2:25:C:ILE:HG13	9	0.22	0.04	0.22
(1,809)	1:126:A:LEU:HB2	1:126:A:LEU:H	9	0.22	0.05	0.23
(1,2489)	2:68:C:ILE:HG21	2:68:C:ILE:HG13	9	0.19	0.03	0.19
(1,2489)	2:68:C:ILE:HG23	2:68:C:ILE:HG13	9	0.19	0.03	0.19
(1,2489)	2:68:C:ILE:HG22	2:68:C:ILE:HG13	9	0.19	0.03	0.19
(1,3559)	2:25:C:ILE:HD11	2:25:C:ILE:HG12	9	0.19	0.02	0.19
(1,3559)	2:25:C:ILE:HD13	2:25:C:ILE:HG12	9	0.19	0.02	0.19
(1,10)	1:120:A:LEU:HD12	1:120:A:LEU:HG	9	0.18	0.04	0.19
(1,10)	1:120:A:LEU:HD11	1:120:A:LEU:HG	9	0.18	0.04	0.19
(1,652)	1:146:A:VAL:HB	1:146:A:VAL:HG22	9	0.16	0.03	0.18
(1,652)	1:146:A:VAL:HB	1:146:A:VAL:HG23	9	0.16	0.03	0.18
(1,833)	1:105:A:LEU:HD11	1:105:A:LEU:HG	9	0.16	0.03	0.16
(1,833)	1:105:A:LEU:HD12	1:105:A:LEU:HG	9	0.16	0.03	0.16
(1,833)	1:105:A:LEU:HD13	1:105:A:LEU:HG	9	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3051)	2:16:C:PHE:HB3	2:16:C:PHE:H	9	0.15	0.02	0.16
(1,3717)	2:19:C:ILE:HG21	2:19:C:ILE:HG12	9	0.14	0.03	0.14
(1,3717)	2:19:C:ILE:HG23	2:19:C:ILE:HG12	9	0.14	0.03	0.14
(1,3717)	2:19:C:ILE:HG22	2:19:C:ILE:HG12	9	0.14	0.03	0.14
(1,93)	1:74:A:VAL:HG11	1:93:A:SER:HA	8	3.03	0.2	3.01
(1,95)	1:74:A:VAL:HG11	1:94:A:PRO:HD3	8	2.78	0.26	2.8
(1,95)	1:74:A:VAL:HG12	1:94:A:PRO:HD3	8	2.78	0.26	2.8
(1,2388)	2:20:B:VAL:HG21	2:34:B:ASN:HD22	8	2.47	1.54	3.08
(1,2388)	2:20:B:VAL:HG22	2:34:B:ASN:HD22	8	2.47	1.54	3.08
(1,2389)	2:20:C:VAL:HG21	2:34:C:ASN:HD22	8	1.98	1.6	1.5
(1,2389)	2:20:C:VAL:HG22	2:34:C:ASN:HD22	8	1.98	1.6	1.5
(1,2389)	2:20:C:VAL:HG23	2:34:C:ASN:HD22	8	1.98	1.6	1.5
(1,94)	1:74:A:VAL:HG11	1:94:A:PRO:HA	8	1.91	0.24	1.97
(1,8)	1:120:A:LEU:HD13	1:147:A:MET:HG3	8	1.57	0.59	1.78
(1,8)	1:120:A:LEU:HD12	1:147:A:MET:HG3	8	1.57	0.59	1.78
(1,1570)	1:139:A:PRO:HA	1:137:A:VAL:HG22	8	1.53	0.16	1.5
(1,1614)	1:150:A:PRO:HB2	1:152:A:LEU:HD12	8	1.51	0.66	1.6
(1,1614)	1:90:A:HIS:HB2	1:76:A:LEU:HD13	8	1.51	0.66	1.6
(1,1614)	1:150:A:PRO:HB2	1:148:A:ILE:HG21	8	1.51	0.66	1.6
(1,1614)	1:90:A:HIS:HB2	1:76:A:LEU:HD11	8	1.51	0.66	1.6
(1,56)	1:114:A:ILE:HD13	1:103:A:GLN:HE21	8	1.5	0.45	1.46
(1,56)	1:114:A:ILE:HD11	1:103:A:GLN:HE21	8	1.5	0.45	1.46
(1,56)	1:114:A:ILE:HD12	1:103:A:GLN:HE21	8	1.5	0.45	1.46
(1,1328)	1:100:A:GLN:HE21	1:99:A:LEU:HD11	8	1.31	0.63	1.42
(1,1557)	1:81:A:ILE:HA	1:85:A:LYS:HD3	8	1.25	0.4	1.25
(1,2299)	2:19:C:ILE:HA	2:22:C:LYS:HD3	8	1.11	0.59	0.96
(1,183)	1:99:A:LEU:HD11	1:100:A:GLN:HE22	8	0.98	0.55	0.78
(1,183)	1:99:A:LEU:HD12	1:100:A:GLN:HE22	8	0.98	0.55	0.78
(1,3929)	2:39:C:CYS:HB2	2:35:C:VAL:HB	8	0.95	0.4	0.92
(1,3929)	2:39:C:CYS:HB3	2:35:B:VAL:HB	8	0.95	0.4	0.92
(1,2147)	2:23:C:LYS:HE3	2:23:C:LYS:HG3	8	0.95	0.03	0.96
(1,3544)	2:51:B:VAL:HG23	2:48:B:ARG:HB3	8	0.88	0.4	0.96
(1,3544)	2:51:B:VAL:HG21	2:48:B:ARG:HB3	8	0.88	0.4	0.96
(1,2192)	2:25:B:ILE:HD12	2:30:B:ALA:HA	8	0.87	0.84	0.52
(1,2192)	2:25:B:ILE:HD13	2:30:B:ALA:HA	8	0.87	0.84	0.52
(1,2192)	2:25:B:ILE:HD11	2:30:B:ALA:HA	8	0.87	0.84	0.52
(1,3548)	2:55:B:LEU:HD11	2:12:B:ILE:HA	8	0.85	0.37	0.87
(1,3548)	2:55:B:LEU:HD11	2:8:B:ILE:HA	8	0.85	0.37	0.87
(1,3548)	2:55:B:LEU:HD12	2:8:B:ILE:HA	8	0.85	0.37	0.87
(1,35)	1:106:A:ILE:HD11	1:113:A:HIS:HA	8	0.84	0.24	0.8
(1,35)	1:106:A:ILE:HD13	1:113:A:HIS:HA	8	0.84	0.24	0.8
(1,35)	1:106:A:ILE:HD12	1:113:A:HIS:HA	8	0.84	0.24	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2500)	2:25:B:ILE:HG23	2:20:B:VAL:HB	8	0.8	0.49	1.01
(1,2500)	2:25:B:ILE:HG21	2:20:B:VAL:HB	8	0.8	0.49	1.01
(1,2594)	2:57:B:LYS:HB3	2:68:C:ILE:HG13	8	0.75	0.31	0.72
(1,1169)	1:125:A:VAL:HG21	1:125:A:VAL:H	8	0.7	0.03	0.71
(1,1169)	1:125:A:VAL:HG23	1:125:A:VAL:H	8	0.7	0.03	0.71
(1,1169)	1:125:A:VAL:HG22	1:125:A:VAL:H	8	0.7	0.03	0.71
(1,3850)	2:40:B:ILE:HG23	2:13:B:VAL:HB	8	0.68	0.33	0.77
(1,3850)	2:40:B:ILE:HG21	2:13:B:VAL:HB	8	0.68	0.33	0.77
(1,3850)	2:40:B:ILE:HG22	2:13:B:VAL:HB	8	0.68	0.33	0.77
(1,58)	1:114:A:ILE:HD11	1:99:A:LEU:HA	8	0.66	0.58	0.48
(1,58)	1:114:A:ILE:HD13	1:99:A:LEU:HA	8	0.66	0.58	0.48
(1,58)	1:114:A:ILE:HD12	1:99:A:LEU:HA	8	0.66	0.58	0.48
(1,177)	1:132:A:LEU:HD23	1:97:A:THR:HA	8	0.65	0.44	0.58
(1,177)	1:132:A:LEU:HD22	1:97:A:THR:HA	8	0.65	0.44	0.58
(1,147)	1:132:A:LEU:HD23	1:98:A:ILE:H	8	0.6	0.31	0.58
(1,147)	1:132:A:LEU:HD22	1:98:A:ILE:H	8	0.6	0.31	0.58
(1,2065)	2:55:C:LEU:HD21	2:51:C:VAL:HB	8	0.57	0.21	0.66
(1,2065)	2:55:C:LEU:HD23	2:51:C:VAL:HB	8	0.57	0.21	0.66
(1,2065)	2:55:C:LEU:HD22	2:51:C:VAL:HB	8	0.57	0.21	0.66
(1,791)	1:136:A:LYS:HG3	1:136:A:LYS:HE3	8	0.57	0.16	0.6
(1,2114)	2:13:B:VAL:HG22	2:48:B:ARG:HG2	8	0.56	0.49	0.32
(1,2114)	2:13:B:VAL:HG21	2:48:B:ARG:HG2	8	0.56	0.49	0.32
(1,2114)	2:13:B:VAL:HG23	2:48:B:ARG:HG2	8	0.56	0.49	0.32
(1,2965)	2:48:C:ARG:HB3	2:48:C:ARG:H	8	0.55	0.13	0.6
(1,3962)	2:36:B:ALA:HB1	2:40:C:ILE:HA	8	0.54	0.28	0.37
(1,3962)	2:36:B:ALA:HB3	2:40:C:ILE:HA	8	0.54	0.28	0.37
(1,3962)	2:36:B:ALA:HB2	2:40:C:ILE:HA	8	0.54	0.28	0.37
(1,2426)	2:68:B:ILE:HD13	2:60:C:PHE:HD2	8	0.51	0.36	0.46
(1,2426)	2:68:B:ILE:HD13	2:60:C:PHE:HD1	8	0.51	0.36	0.46
(1,2426)	2:68:B:ILE:HD12	2:60:C:PHE:HD1	8	0.51	0.36	0.46
(1,511)	1:139:A:PRO:HD2	1:138:A:THR:HB	8	0.51	0.26	0.5
(1,2043)	2:5:C:LYS:HD3	2:44:C:PHE:HZ	8	0.51	0.16	0.48
(1,3722)	2:25:B:ILE:HG23	2:5:C:LYS:HE3	8	0.5	0.2	0.5
(1,3722)	2:25:B:ILE:HG21	2:5:C:LYS:HE3	8	0.5	0.2	0.5
(1,3664)	2:33:B:LEU:HD22	2:16:B:PHE:HD1	8	0.47	0.22	0.52
(1,3664)	2:33:B:LEU:HD22	2:44:C:PHE:HZ	8	0.47	0.22	0.52
(1,3664)	2:33:B:LEU:HD23	2:16:B:PHE:HD1	8	0.47	0.22	0.52
(1,3664)	2:33:B:LEU:HD21	2:16:B:PHE:HD2	8	0.47	0.22	0.52
(1,3664)	2:33:B:LEU:HD23	2:44:C:PHE:HZ	8	0.47	0.22	0.52
(1,4098)	2:17:B:SER:H	2:12:B:ILE:HG23	8	0.46	0.19	0.53
(1,4098)	2:17:B:SER:H	2:12:B:ILE:HG21	8	0.46	0.19	0.53
(1,4098)	2:17:B:SER:H	2:12:B:ILE:HG22	8	0.46	0.19	0.53

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2630)	2:51:B:VAL:HB	2:55:B:LEU:HG	8	0.46	0.31	0.36
(1,3723)	2:25:C:ILE:HG22	2:5:B:LYS:HE3	8	0.46	0.28	0.43
(1,3723)	2:25:C:ILE:HG21	2:5:B:LYS:HE3	8	0.46	0.28	0.43
(1,3723)	2:25:C:ILE:HG23	2:5:B:LYS:HE3	8	0.46	0.28	0.43
(1,3477)	2:55:C:LEU:HD23	2:14:C:ASN:HD21	8	0.45	0.33	0.36
(1,3477)	2:55:C:LEU:HD21	2:14:C:ASN:HD21	8	0.45	0.33	0.36
(1,3316)	2:26:B:SER:H	2:33:B:LEU:HD12	8	0.45	0.16	0.4
(1,3316)	2:26:B:SER:H	2:33:B:LEU:HD13	8	0.45	0.16	0.4
(1,3316)	2:26:B:SER:H	2:33:B:LEU:HD11	8	0.45	0.16	0.4
(1,2)	1:120:A:LEU:HD13	1:120:A:LEU:H	8	0.45	0.2	0.45
(1,2)	1:120:A:LEU:HD11	1:120:A:LEU:H	8	0.45	0.2	0.45
(1,3693)	2:9:C:ALA:HA	2:46:C:PHE:HE1	8	0.45	0.16	0.46
(1,3693)	2:9:C:ALA:HA	2:16:B:PHE:HZ	8	0.45	0.16	0.46
(1,2790)	2:33:B:LEU:HD13	2:19:B:ILE:HB	8	0.43	0.11	0.48
(1,2790)	2:33:B:LEU:HD11	2:19:B:ILE:HB	8	0.43	0.11	0.48
(1,180)	1:132:A:LEU:HD11	1:96:A:ASP:HB2	8	0.42	0.21	0.34
(1,180)	1:132:A:LEU:HD12	1:96:A:ASP:HB2	8	0.42	0.21	0.34
(1,1707)	1:144:A:ILE:HG23	1:120:A:LEU:H	8	0.4	0.15	0.4
(1,1707)	1:120:A:LEU:H	1:119:A:LEU:HD12	8	0.4	0.15	0.4
(1,1707)	1:120:A:LEU:H	1:119:A:LEU:HD11	8	0.4	0.15	0.4
(1,1707)	1:144:A:ILE:HG21	1:120:A:LEU:H	8	0.4	0.15	0.4
(1,1707)	1:120:A:LEU:H	1:119:A:LEU:HD13	8	0.4	0.15	0.4
(1,1802)	1:82:A:GLN:HE21	1:82:A:GLN:HB3	8	0.39	0.12	0.41
(1,1802)	1:82:A:GLN:HE21	1:82:A:GLN:HB2	8	0.39	0.12	0.41
(1,3421)	2:51:C:VAL:H	2:54:C:ILE:HG12	8	0.38	0.22	0.34
(1,3704)	2:6:B:GLU:HA	2:46:B:PHE:HE1	8	0.37	0.19	0.42
(1,3704)	2:6:B:GLU:HA	2:44:B:PHE:HZ	8	0.37	0.19	0.42
(1,1060)	1:116:A:GLU:HG2	1:116:A:GLU:H	8	0.33	0.27	0.24
(1,638)	1:132:A:LEU:HB3	1:135:A:LEU:HD13	8	0.32	0.19	0.24
(1,638)	1:132:A:LEU:HB3	1:135:A:LEU:HD12	8	0.32	0.19	0.24
(1,3232)	2:72:B:ALA:H	2:72:B:ALA:HB2	8	0.3	0.1	0.26
(1,3232)	2:72:B:ALA:H	2:72:B:ALA:HB3	8	0.3	0.1	0.26
(1,1236)	1:99:A:LEU:HD13	1:99:A:LEU:H	8	0.25	0.07	0.22
(1,1236)	1:99:A:LEU:HD12	1:99:A:LEU:H	8	0.25	0.07	0.22
(1,1236)	1:99:A:LEU:HD11	1:99:A:LEU:H	8	0.25	0.07	0.22
(1,2405)	2:8:C:ILE:HG21	2:15:B:TYR:H	8	0.22	0.1	0.16
(1,2405)	2:8:C:ILE:HG23	2:15:B:TYR:H	8	0.22	0.1	0.16
(1,3560)	2:25:B:ILE:HD11	2:25:B:ILE:HG13	8	0.21	0.04	0.22
(1,3560)	2:25:B:ILE:HD12	2:25:B:ILE:HG13	8	0.21	0.04	0.22
(1,3560)	2:25:B:ILE:HD11	2:43:C:ALA:HB1	8	0.21	0.04	0.22
(1,3560)	2:25:B:ILE:HD11	2:43:C:ALA:HB3	8	0.21	0.04	0.22
(1,1855)	2:16:C:PHE:HB2	2:16:C:PHE:H	8	0.18	0.06	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3716)	2:19:B:ILE:HG22	2:19:B:ILE:HG12	8	0.14	0.02	0.14
(1,3716)	2:19:B:ILE:HG23	2:19:B:ILE:HG12	8	0.14	0.02	0.14
(1,3716)	2:19:B:ILE:HG21	2:19:B:ILE:HG12	8	0.14	0.02	0.14
(1,73)	1:88:A:ILE:HG23	1:90:A:HIS:HE1	7	2.31	1.65	1.97
(1,73)	1:88:A:ILE:HG22	1:90:A:HIS:HE1	7	2.31	1.65	1.97
(1,804)	1:121:A:LEU:HD21	1:141:A:ASN:HD21	7	1.78	1.04	1.47
(1,2615)	2:13:C:VAL:HG11	2:48:C:ARG:HG2	7	1.38	0.85	1.41
(1,2615)	2:13:C:VAL:HG12	2:48:C:ARG:HG2	7	1.38	0.85	1.41
(1,2615)	2:13:C:VAL:HG13	2:48:C:ARG:HG2	7	1.38	0.85	1.41
(1,1820)	1:129:A:ASN:HD21	1:130:A:LEU:HD21	7	1.37	0.65	1.14
(1,1820)	1:151:A:ASN:HD21	1:152:A:LEU:HD13	7	1.37	0.65	1.14
(1,1820)	1:129:A:ASN:HD21	1:99:A:LEU:HD12	7	1.37	0.65	1.14
(1,790)	1:126:A:LEU:HG	1:124:A:LYS:HE3	7	1.31	0.72	1.31
(1,571)	1:93:A:SER:HB3	1:96:A:ASP:HB3	7	1.3	0.21	1.22
(1,3731)	2:12:C:ILE:HD11	2:13:C:VAL:HG12	7	1.27	0.41	1.39
(1,3731)	2:12:C:ILE:HD13	2:13:C:VAL:HG12	7	1.27	0.41	1.39
(1,3731)	2:12:C:ILE:HD12	2:13:C:VAL:HG13	7	1.27	0.41	1.39
(1,3731)	2:12:C:ILE:HD11	2:13:C:VAL:HG11	7	1.27	0.41	1.39
(1,3545)	2:51:C:VAL:HG23	2:48:C:ARG:HB3	7	1.24	0.74	1.67
(1,3545)	2:51:C:VAL:HG22	2:48:C:ARG:HB3	7	1.24	0.74	1.67
(1,3545)	2:51:C:VAL:HG22	2:47:C:GLU:HB2	7	1.24	0.74	1.67
(1,3545)	2:51:C:VAL:HG23	2:47:C:GLU:HB2	7	1.24	0.74	1.67
(1,3928)	2:39:B:CYS:HB2	2:35:B:VAL:HB	7	1.2	0.29	1.34
(1,3928)	2:39:B:CYS:HB3	2:35:C:VAL:HB	7	1.2	0.29	1.34
(1,702)	1:122:A:LYS:HE3	1:122:A:LYS:H	7	1.16	0.41	1.13
(1,3684)	2:12:B:ILE:HD12	2:15:B:TYR:HD2	7	1.15	0.47	1.07
(1,3684)	2:12:B:ILE:HD11	2:15:C:TYR:HD2	7	1.15	0.47	1.07
(1,3684)	2:12:B:ILE:HD11	2:15:B:TYR:HD2	7	1.15	0.47	1.07
(1,3684)	2:12:B:ILE:HD12	2:15:C:TYR:HD1	7	1.15	0.47	1.07
(1,3684)	2:12:B:ILE:HD13	2:15:C:TYR:HD2	7	1.15	0.47	1.07
(1,1467)	1:145:A:THR:HG23	1:82:A:GLN:HE22	7	1.1	0.52	0.97
(1,1467)	1:145:A:THR:HG22	1:141:A:ASN:HD21	7	1.1	0.52	0.97
(1,1295)	1:129:A:ASN:H	1:97:A:THR:HB	7	1.04	0.58	0.98
(1,703)	1:122:A:LYS:HE3	1:141:A:ASN:HD22	7	1.03	0.85	0.81
(1,2042)	2:5:B:LYS:HD3	2:44:B:PHE:HZ	7	1.0	0.24	1.02
(1,85)	1:73:A:MET:HE2	1:73:A:MET:HA	7	0.97	0.18	0.95
(1,85)	1:73:A:MET:HE1	1:73:A:MET:HA	7	0.97	0.18	0.95
(1,4014)	2:60:B:PHE:HD2	2:68:C:ILE:HD11	7	0.92	0.54	0.71
(1,4014)	2:60:B:PHE:HD1	2:8:B:ILE:HD13	7	0.92	0.54	0.71
(1,4014)	2:60:B:PHE:HD1	2:68:C:ILE:HD12	7	0.92	0.54	0.71
(1,1670)	1:136:A:LYS:HA	1:136:A:LYS:HE3	7	0.91	0.4	0.86
(1,1670)	1:135:A:LEU:HA	1:124:A:LYS:HE3	7	0.91	0.4	0.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1545)	1:136:A:LYS:HA	1:136:A:LYS:HE3	7	0.9	0.4	0.85
(1,1545)	1:135:A:LEU:HA	1:124:A:LYS:HE3	7	0.9	0.4	0.85
(1,3557)	2:25:C:ILE:HD12	2:5:B:LYS:HD2	7	0.89	0.44	0.86
(1,116)	1:125:A:VAL:HG23	1:120:A:LEU:H	7	0.89	1.1	0.23
(1,116)	1:125:A:VAL:HG22	1:120:A:LEU:H	7	0.89	1.1	0.23
(1,3970)	2:8:B:ILE:HD12	2:60:C:PHE:HE1	7	0.88	0.71	0.55
(1,3970)	2:8:B:ILE:HD13	2:60:B:PHE:HE1	7	0.88	0.71	0.55
(1,3970)	2:8:B:ILE:HD13	2:60:C:PHE:HE1	7	0.88	0.71	0.55
(1,3970)	2:8:B:ILE:HD12	2:60:C:PHE:HE2	7	0.88	0.71	0.55
(1,3971)	2:8:C:ILE:HD12	2:60:B:PHE:HE1	7	0.83	0.49	0.85
(1,3971)	2:8:C:ILE:HD11	2:60:C:PHE:HE1	7	0.83	0.49	0.85
(1,3971)	2:8:C:ILE:HD11	2:60:B:PHE:HE1	7	0.83	0.49	0.85
(1,3971)	2:8:C:ILE:HD12	2:60:B:PHE:HE2	7	0.83	0.49	0.85
(1,3048)	2:50:B:ALA:H	2:13:B:VAL:HG12	7	0.77	0.44	0.66
(1,3048)	2:50:B:ALA:H	2:13:B:VAL:HG13	7	0.77	0.44	0.66
(1,2631)	2:51:C:VAL:HB	2:55:C:LEU:HG	7	0.76	1.08	0.33
(1,3818)	2:6:B:GLU:HB3	2:46:B:PHE:HD1	7	0.75	0.16	0.81
(1,3818)	2:6:B:GLU:HB3	2:46:B:PHE:HD2	7	0.75	0.16	0.81
(1,785)	1:122:A:LYS:HD3	1:121:A:LEU:HD12	7	0.75	0.4	0.68
(1,785)	1:122:A:LYS:HD3	1:121:A:LEU:HD11	7	0.75	0.4	0.68
(1,3549)	2:55:C:LEU:HD12	2:12:C:ILE:HA	7	0.74	0.24	0.73
(1,3549)	2:55:C:LEU:HD11	2:8:C:ILE:HA	7	0.74	0.24	0.73
(1,3549)	2:55:C:LEU:HD13	2:12:C:ILE:HA	7	0.74	0.24	0.73
(1,3549)	2:55:C:LEU:HD11	2:12:C:ILE:HA	7	0.74	0.24	0.73
(1,2595)	2:57:C:LYS:HB3	2:68:B:ILE:HG13	7	0.72	0.22	0.73
(1,2211)	2:22:C:LYS:HA	2:24:C:GLU:HB2	7	0.7	0.34	0.67
(1,3556)	2:25:B:ILE:HD13	2:5:C:LYS:HD2	7	0.7	0.27	0.55
(1,3556)	2:25:B:ILE:HD11	2:5:C:LYS:HD2	7	0.7	0.27	0.55
(1,3556)	2:25:B:ILE:HD12	2:5:C:LYS:HD2	7	0.7	0.27	0.55
(1,642)	1:97:A:THR:HG21	1:100:A:GLN:HG3	7	0.69	0.57	0.63
(1,642)	1:97:A:THR:HG22	1:100:A:GLN:HG3	7	0.69	0.57	0.63
(1,642)	1:97:A:THR:HG23	1:100:A:GLN:HG3	7	0.69	0.57	0.63
(1,1037)	1:107:A:SER:HB3	1:107:A:SER:H	7	0.69	0.04	0.7
(1,2693)	2:50:C:ALA:HB1	2:47:C:GLU:HB2	7	0.67	0.47	0.8
(1,2693)	2:50:C:ALA:HB3	2:47:C:GLU:HB2	7	0.67	0.47	0.8
(1,2693)	2:50:C:ALA:HB2	2:47:C:GLU:HB2	7	0.67	0.47	0.8
(1,2641)	2:33:C:LEU:HD13	2:20:C:VAL:HG13	7	0.65	0.44	0.53
(1,2641)	2:33:C:LEU:HD13	2:20:C:VAL:HG11	7	0.65	0.44	0.53
(1,2641)	2:33:C:LEU:HD11	2:20:C:VAL:HG12	7	0.65	0.44	0.53
(1,2641)	2:33:C:LEU:HD13	2:20:C:VAL:HG12	7	0.65	0.44	0.53
(1,1663)	1:85:A:LYS:HG2	1:85:A:LYS:HE3	7	0.64	0.16	0.66
(1,697)	1:79:A:LYS:HE3	1:79:A:LYS:HG3	7	0.64	0.3	0.69

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,55)	1:114:A:ILE:HD13	1:103:A:GLN:HE22	7	0.61	0.39	0.59
(1,55)	1:114:A:ILE:HD11	1:103:A:GLN:HE22	7	0.61	0.39	0.59
(1,55)	1:114:A:ILE:HD12	1:103:A:GLN:HE22	7	0.61	0.39	0.59
(1,2941)	2:44:C:PHE:HZ	2:33:B:LEU:HD23	7	0.59	0.36	0.44
(1,2941)	2:44:C:PHE:HZ	2:33:B:LEU:HD22	7	0.59	0.36	0.44
(1,2941)	2:44:C:PHE:HZ	2:33:B:LEU:HD21	7	0.59	0.36	0.44
(1,867)	1:145:A:THR:HG22	1:145:A:THR:H	7	0.57	0.26	0.54
(1,867)	1:145:A:THR:HG21	1:145:A:THR:H	7	0.57	0.26	0.54
(1,725)	1:148:A:ILE:HD13	1:80:A:LYS:HD3	7	0.56	0.42	0.45
(1,725)	1:148:A:ILE:HD12	1:80:A:LYS:HD3	7	0.56	0.42	0.45
(1,2309)	2:52:C:SER:HA	2:55:C:LEU:HD11	7	0.55	0.5	0.21
(1,2309)	2:52:C:SER:HA	2:55:C:LEU:HD13	7	0.55	0.5	0.21
(1,2309)	2:52:C:SER:HA	2:55:C:LEU:HD12	7	0.55	0.5	0.21
(1,3628)	2:18:B:SER:HB3	2:19:B:ILE:HD13	7	0.54	0.24	0.49
(1,3628)	2:18:B:SER:HB3	2:19:B:ILE:HD11	7	0.54	0.24	0.49
(1,3628)	2:18:B:SER:HB3	2:19:B:ILE:HD12	7	0.54	0.24	0.49
(1,3162)	2:6:B:GLU:HB2	2:7:B:GLU:H	7	0.54	0.13	0.6
(1,661)	1:76:A:LEU:HD23	1:76:A:LEU:HA	7	0.52	0.17	0.57
(1,3163)	2:6:C:GLU:HB2	2:7:C:GLU:H	7	0.46	0.11	0.51
(1,3476)	2:55:B:LEU:HD21	2:14:B:ASN:HD21	7	0.44	0.22	0.56
(1,1411)	1:116:A:GLU:HG3	1:151:A:ASN:H	7	0.44	0.16	0.43
(1,1450)	1:99:A:LEU:HD21	1:102:A:LYS:H	7	0.43	0.06	0.44
(1,1450)	1:99:A:LEU:HD22	1:102:A:LYS:H	7	0.43	0.06	0.44
(3,34)	1:149:A:LYS:N	1:116:A:GLU:O	7	0.42	0.16	0.4
(1,75)	1:98:A:ILE:HG22	1:128:A:ASP:HA	7	0.41	0.16	0.46
(1,75)	1:98:A:ILE:HG23	1:128:A:ASP:HA	7	0.41	0.16	0.46
(1,1793)	1:141:A:ASN:HB2	1:138:A:THR:H	7	0.4	0.13	0.38
(1,1793)	1:141:A:ASN:HB2	1:140:A:ALA:H	7	0.4	0.13	0.38
(1,2423)	2:25:C:ILE:HD12	2:44:B:PHE:HZ	7	0.4	0.25	0.25
(1,3321)	2:19:C:ILE:HG23	2:26:C:SER:H	7	0.39	0.15	0.37
(1,3321)	2:19:C:ILE:HG22	2:26:C:SER:H	7	0.39	0.15	0.37
(1,3321)	2:19:C:ILE:HG21	2:26:C:SER:H	7	0.39	0.15	0.37
(1,889)	1:130:A:LEU:HB3	1:130:A:LEU:H	7	0.35	0.14	0.33
(1,4176)	1:145:A:THR:HG21	2:35:C:VAL:HG13	7	0.35	0.14	0.31
(1,4176)	1:145:A:THR:HG21	2:35:C:VAL:HG11	7	0.35	0.14	0.31
(1,4176)	1:145:A:THR:OG1	2:35:C:VAL:HG22	7	0.35	0.14	0.31
(1,4176)	1:145:A:THR:OG1	2:35:C:VAL:HG21	7	0.35	0.14	0.31
(1,3963)	2:36:C:ALA:HB2	2:40:B:ILE:HA	7	0.31	0.19	0.23
(1,1266)	1:107:A:SER:H	1:106:A:ILE:HG21	7	0.31	0.11	0.29
(1,3139)	2:2:C:SER:H	2:3:C:ALA:H	7	0.3	0.12	0.3
(1,89)	1:101:A:ILE:HG21	1:119:A:LEU:HA	7	0.3	0.15	0.28
(1,89)	1:101:A:ILE:HG23	1:119:A:LEU:HA	7	0.3	0.15	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,89)	1:101:A:ILE:HG22	1:119:A:LEU:HA	7	0.3	0.15	0.28
(1,3233)	2:72:C:ALA:H	2:72:C:ALA:HB1	7	0.29	0.12	0.35
(1,3233)	2:72:C:ALA:H	2:72:C:ALA:HB2	7	0.29	0.12	0.35
(1,533)	1:114:A:ILE:HA	1:114:A:ILE:HG12	7	0.28	0.17	0.22
(1,3968)	2:25:B:ILE:HG23	2:32:B:SER:H	7	0.26	0.09	0.25
(1,3968)	2:25:B:ILE:HG22	2:44:C:PHE:HD1	7	0.26	0.09	0.25
(1,3968)	2:25:B:ILE:HG21	2:32:B:SER:H	7	0.26	0.09	0.25
(1,756)	1:146:A:VAL:HG21	1:119:A:LEU:HA	7	0.24	0.1	0.21
(1,756)	1:146:A:VAL:HG22	1:119:A:LEU:HA	7	0.24	0.1	0.21
(1,3726)	2:25:B:ILE:HG22	2:30:B:ALA:HB2	7	0.23	0.11	0.18
(1,3726)	2:25:B:ILE:HG23	2:30:B:ALA:HB1	7	0.23	0.11	0.18
(1,3726)	2:25:B:ILE:HG22	2:25:B:ILE:HG12	7	0.23	0.11	0.18
(1,261)	1:129:A:ASN:HB2	1:129:A:ASN:HD21	7	0.23	0.07	0.22
(1,1854)	2:16:B:PHE:HB2	2:16:B:PHE:H	7	0.17	0.04	0.18
(1,3011)	2:5:C:LYS:HB2	2:5:C:LYS:H	7	0.13	0.01	0.13
(1,1412)	1:151:A:ASN:HA	1:151:A:ASN:H	7	0.12	0.01	0.13
(1,3010)	2:5:B:LYS:HB2	2:5:B:LYS:H	7	0.12	0.0	0.12
(1,707)	1:122:A:LYS:HE3	1:143:A:THR:HG23	6	2.44	1.56	2.12
(1,707)	1:122:A:LYS:HE3	1:143:A:THR:HG21	6	2.44	1.56	2.12
(1,48)	1:88:A:ILE:HD12	1:90:A:HIS:HE1	6	2.27	0.93	1.84
(1,2786)	2:20:B:VAL:HG13	2:34:B:ASN:HD22	6	2.07	0.91	2.48
(1,2786)	2:20:B:VAL:HG12	2:34:B:ASN:HD22	6	2.07	0.91	2.48
(1,2786)	2:20:B:VAL:HG11	2:34:B:ASN:HD22	6	2.07	0.91	2.48
(1,3733)	2:12:C:ILE:HD13	2:40:C:ILE:HG22	6	1.41	0.31	1.48
(1,3733)	2:12:C:ILE:HD13	2:40:C:ILE:HD13	6	1.41	0.31	1.48
(1,3733)	2:12:C:ILE:HD13	2:40:C:ILE:HD12	6	1.41	0.31	1.48
(1,3733)	2:12:C:ILE:HD13	2:40:C:ILE:HG23	6	1.41	0.31	1.48
(1,3733)	2:12:C:ILE:HD11	2:40:C:ILE:HD11	6	1.41	0.31	1.48
(1,704)	1:122:A:LYS:HE3	1:141:A:ASN:HD21	6	1.15	0.85	0.82
(1,4015)	2:60:C:PHE:HD1	2:8:C:ILE:HD13	6	1.13	0.39	1.18
(1,4015)	2:60:C:PHE:HD1	2:8:C:ILE:HD11	6	1.13	0.39	1.18
(1,4015)	2:60:C:PHE:HD2	2:68:B:ILE:HD13	6	1.13	0.39	1.18
(1,4015)	2:60:C:PHE:HD1	2:68:B:ILE:HD12	6	1.13	0.39	1.18
(1,3730)	2:12:B:ILE:HD11	2:13:B:VAL:HG13	6	1.07	0.5	1.16
(1,3730)	2:12:B:ILE:HD11	2:13:B:VAL:HG11	6	1.07	0.5	1.16
(1,3730)	2:12:B:ILE:HD12	2:13:B:VAL:HG11	6	1.07	0.5	1.16
(1,3730)	2:12:B:ILE:HD13	2:13:B:VAL:HG13	6	1.07	0.5	1.16
(1,3100)	2:23:B:LYS:HG3	2:23:B:LYS:H	6	1.01	0.34	1.14
(1,2498)	2:25:B:ILE:HG23	2:20:B:VAL:HG12	6	0.98	0.38	1.11
(1,2498)	2:25:B:ILE:HG22	2:20:B:VAL:HG11	6	0.98	0.38	1.11
(1,2498)	2:25:B:ILE:HG23	2:20:B:VAL:HG13	6	0.98	0.38	1.11
(1,2498)	2:25:B:ILE:HG21	2:20:B:VAL:HG12	6	0.98	0.38	1.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2950)	2:60:B:PHE:HD1	2:54:B:ILE:HB	6	0.94	0.14	0.92
(1,2950)	2:60:B:PHE:HD2	2:54:B:ILE:HB	6	0.94	0.14	0.92
(1,2146)	2:23:B:LYS:HE3	2:23:B:LYS:HG3	6	0.8	0.21	0.92
(1,2179)	2:9:C:ALA:HA	2:12:C:ILE:HD13	6	0.8	0.22	0.86
(1,2179)	2:9:C:ALA:HA	2:12:C:ILE:HD11	6	0.8	0.22	0.86
(1,2427)	2:68:C:ILE:HD11	2:60:B:PHE:HD2	6	0.76	0.68	0.49
(1,2427)	2:68:C:ILE:HD13	2:60:B:PHE:HD2	6	0.76	0.68	0.49
(1,2427)	2:68:C:ILE:HD12	2:60:B:PHE:HD1	6	0.76	0.68	0.49
(1,3683)	2:12:C:ILE:HD13	2:16:B:PHE:HD1	6	0.74	0.53	0.48
(1,3683)	2:12:C:ILE:HD12	2:16:B:PHE:HD1	6	0.74	0.53	0.48
(1,3683)	2:12:C:ILE:HD12	2:16:C:PHE:HD1	6	0.74	0.53	0.48
(1,3819)	2:6:C:GLU:HB3	2:46:C:PHE:HD2	6	0.74	0.25	0.84
(1,3819)	2:6:C:GLU:HB3	2:46:C:PHE:HD1	6	0.74	0.25	0.84
(1,3819)	2:6:C:GLU:HB3	2:44:C:PHE:HZ	6	0.74	0.25	0.84
(1,3324)	2:27:B:GLU:HG3	2:27:B:GLU:H	6	0.68	0.28	0.77
(1,461)	1:96:A:ASP:HA	1:97:A:THR:HG22	6	0.68	0.31	0.64
(1,3659)	2:51:C:VAL:HG23	2:46:C:PHE:HE2	6	0.65	0.62	0.38
(1,3659)	2:51:C:VAL:HG22	2:46:C:PHE:HE2	6	0.65	0.62	0.38
(1,3659)	2:51:C:VAL:HG22	2:46:C:PHE:HD2	6	0.65	0.62	0.38
(1,1041)	1:108:A:GLU:HG3	1:108:A:GLU:H	6	0.64	0.36	0.71
(1,2951)	2:60:C:PHE:HD2	2:54:C:ILE:HB	6	0.6	0.28	0.62
(1,2951)	2:60:C:PHE:HD1	2:54:C:ILE:HB	6	0.6	0.28	0.62
(1,3629)	2:18:C:SER:HB3	2:19:C:ILE:HD13	6	0.6	0.33	0.59
(1,3629)	2:17:C:SER:HA	2:19:C:ILE:HG23	6	0.6	0.33	0.59
(1,3851)	2:40:C:ILE:HG23	2:13:C:VAL:HB	6	0.6	0.32	0.56
(1,3851)	2:40:C:ILE:HG21	2:13:C:VAL:HB	6	0.6	0.32	0.56
(1,3851)	2:40:C:ILE:HG22	2:13:C:VAL:HB	6	0.6	0.32	0.56
(1,655)	1:81:A:ILE:HG12	1:145:A:THR:HA	6	0.56	0.31	0.54
(1,531)	1:137:A:VAL:HA	1:138:A:THR:HG23	6	0.56	0.28	0.49
(1,531)	1:137:A:VAL:HA	1:138:A:THR:HG21	6	0.56	0.28	0.49
(1,2039)	2:5:C:LYS:HB3	2:44:C:PHE:HZ	6	0.52	0.23	0.46
(1,2409)	2:19:C:ILE:HG21	2:44:B:PHE:HZ	6	0.46	0.27	0.35
(1,2409)	2:19:C:ILE:HG23	2:44:B:PHE:HZ	6	0.46	0.27	0.35
(1,2409)	2:19:C:ILE:HG22	2:44:B:PHE:HZ	6	0.46	0.27	0.35
(1,2422)	2:25:B:ILE:HD13	2:44:C:PHE:HZ	6	0.45	0.24	0.45
(1,2422)	2:25:B:ILE:HD11	2:44:C:PHE:HZ	6	0.45	0.24	0.45
(1,2422)	2:25:B:ILE:HD12	2:44:C:PHE:HZ	6	0.45	0.24	0.45
(1,1419)	1:107:A:SER:HB3	1:108:A:GLU:H	6	0.44	0.09	0.44
(1,3705)	2:6:C:GLU:HA	2:46:C:PHE:HE1	6	0.44	0.12	0.4
(1,1133)	1:126:A:LEU:HD11	1:126:A:LEU:H	6	0.44	0.23	0.4
(1,1133)	1:126:A:LEU:HD13	1:126:A:LEU:H	6	0.44	0.23	0.4
(1,1133)	1:126:A:LEU:HD12	1:126:A:LEU:H	6	0.44	0.23	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,119)	1:97:A:THR:HG22	1:131:A:PHE:HD1	6	0.42	0.29	0.34
(1,119)	1:97:A:THR:HG22	1:131:A:PHE:HD2	6	0.42	0.29	0.34
(1,3665)	2:33:C:LEU:HD21	2:44:B:PHE:HZ	6	0.42	0.18	0.38
(1,3665)	2:33:C:LEU:HD22	2:16:C:PHE:HD1	6	0.42	0.18	0.38
(1,3665)	2:33:C:LEU:HD23	2:44:B:PHE:HZ	6	0.42	0.18	0.38
(1,3665)	2:33:C:LEU:HD22	2:44:B:PHE:HZ	6	0.42	0.18	0.38
(1,3186)	2:40:B:ILE:H	2:13:B:VAL:HG12	6	0.42	0.15	0.45
(1,3186)	2:40:B:ILE:H	2:13:B:VAL:HG11	6	0.42	0.15	0.45
(1,110)	1:126:A:LEU:HD11	1:125:A:VAL:HA	6	0.41	0.25	0.34
(1,110)	1:126:A:LEU:HD13	1:125:A:VAL:HA	6	0.41	0.25	0.34
(1,110)	1:126:A:LEU:HD12	1:125:A:VAL:HA	6	0.41	0.25	0.34
(1,749)	1:124:A:LYS:HG2	1:125:A:VAL:HA	6	0.4	0.27	0.34
(1,1071)	1:138:A:THR:H	1:138:A:THR:HG23	6	0.37	0.26	0.3
(1,1071)	1:138:A:THR:H	1:138:A:THR:HG21	6	0.37	0.26	0.3
(1,769)	1:132:A:LEU:HA	1:135:A:LEU:HD13	6	0.37	0.18	0.34
(1,949)	1:100:A:GLN:H	1:99:A:LEU:HD11	6	0.35	0.09	0.4
(1,949)	1:100:A:GLN:H	1:99:A:LEU:HD13	6	0.35	0.09	0.4
(1,3252)	2:21:B:GLU:HB3	2:21:B:GLU:H	6	0.35	0.14	0.34
(1,958)	1:121:A:LEU:H	1:126:A:LEU:HB3	6	0.33	0.24	0.22
(1,4008)	2:44:B:PHE:HZ	2:19:C:ILE:HG21	6	0.31	0.22	0.22
(1,4008)	2:44:B:PHE:HZ	2:19:C:ILE:HG23	6	0.31	0.22	0.22
(1,4008)	2:16:B:PHE:HZ	2:12:C:ILE:HG23	6	0.31	0.22	0.22
(1,4008)	2:44:B:PHE:HZ	2:19:C:ILE:HG22	6	0.31	0.22	0.22
(1,2599)	2:13:C:VAL:HG13	2:41:C:SER:HA	6	0.3	0.06	0.27
(1,2599)	2:13:C:VAL:HG11	2:41:C:SER:HA	6	0.3	0.06	0.27
(1,2599)	2:13:C:VAL:HG12	2:41:C:SER:HA	6	0.3	0.06	0.27
(1,1460)	1:120:A:LEU:HD22	1:125:A:VAL:HA	6	0.29	0.14	0.28
(1,1460)	1:132:A:LEU:HD13	1:132:A:LEU:HA	6	0.29	0.14	0.28
(1,3567)	2:19:C:ILE:HD12	2:5:B:LYS:HG2	6	0.29	0.05	0.3
(1,3567)	2:19:C:ILE:HD11	2:5:B:LYS:HG2	6	0.29	0.05	0.3
(1,437)	1:94:A:PRO:HD2	1:74:A:VAL:HG11	6	0.29	0.16	0.26
(1,3574)	2:33:B:LEU:HD23	2:43:C:ALA:HB1	6	0.28	0.25	0.19
(1,3574)	2:33:B:LEU:HD22	2:43:C:ALA:HB1	6	0.28	0.25	0.19
(1,3574)	2:33:B:LEU:HB2	2:33:B:LEU:HD23	6	0.28	0.25	0.19
(1,2962)	2:48:B:ARG:HG3	2:48:B:ARG:H	6	0.28	0.06	0.28
(1,3911)	2:12:C:ILE:HG13	2:11:C:LEU:H	6	0.28	0.04	0.28
(1,3230)	2:20:B:VAL:H	2:25:B:ILE:HG23	6	0.26	0.07	0.24
(1,3230)	2:20:B:VAL:H	2:25:B:ILE:HG21	6	0.26	0.07	0.24
(1,3253)	2:21:C:GLU:HB3	2:21:C:GLU:H	6	0.26	0.1	0.24
(1,1532)	1:151:A:ASN:HA	1:152:A:LEU:HG	6	0.26	0.1	0.24
(1,111)	1:126:A:LEU:HD12	1:124:A:LYS:HE2	6	0.25	0.08	0.22
(1,111)	1:126:A:LEU:HD11	1:124:A:LYS:HE2	6	0.25	0.08	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,111)	1:126:A:LEU:HD13	1:124:A:LYS:HE2	6	0.25	0.08	0.22
(1,182)	1:132:A:LEU:HD12	1:92:A:PHE:HA	6	0.23	0.07	0.24
(1,2475)	2:12:C:ILE:HG21	2:40:C:ILE:HD11	6	0.22	0.09	0.18
(1,2475)	2:12:C:ILE:HG21	2:40:C:ILE:HD13	6	0.22	0.09	0.18
(1,2475)	2:12:C:ILE:HG21	2:40:C:ILE:HD12	6	0.22	0.09	0.18
(1,2475)	2:12:C:ILE:HG23	2:40:C:ILE:HD12	6	0.22	0.09	0.18
(1,2475)	2:12:C:ILE:HG23	2:40:C:ILE:HD11	6	0.22	0.09	0.18
(1,3725)	2:25:C:ILE:HG23	2:19:C:ILE:HB	6	0.22	0.06	0.22
(1,3725)	2:25:C:ILE:HG21	2:19:C:ILE:HB	6	0.22	0.06	0.22
(1,3725)	2:25:C:ILE:HG22	2:19:C:ILE:HB	6	0.22	0.06	0.22
(1,1081)	1:140:A:ALA:HB1	1:141:A:ASN:H	6	0.21	0.07	0.18
(1,1081)	1:140:A:ALA:HB3	1:141:A:ASN:H	6	0.21	0.07	0.18
(1,3563)	2:8:C:ILE:HD13	2:11:C:LEU:HA	6	0.21	0.04	0.22
(1,3563)	2:8:C:ILE:HD12	2:9:C:ALA:HA	6	0.21	0.04	0.22
(1,3563)	2:8:C:ILE:HD11	2:9:C:ALA:HA	6	0.21	0.04	0.22
(1,209)	1:151:A:ASN:HB3	1:151:A:ASN:HD21	6	0.19	0.06	0.18
(1,761)	1:106:A:ILE:HA	1:106:A:ILE:HG22	6	0.18	0.05	0.18
(1,761)	1:106:A:ILE:HA	1:106:A:ILE:HG23	6	0.18	0.05	0.18
(1,2152)	2:48:B:ARG:HD3	2:48:B:ARG:HB3	6	0.18	0.05	0.16
(1,1573)	1:137:A:VAL:HA	1:137:A:VAL:HG23	6	0.16	0.04	0.14
(1,1573)	1:137:A:VAL:HA	1:137:A:VAL:HG21	6	0.16	0.04	0.14
(1,3018)	2:9:B:ALA:H	2:9:B:ALA:HB2	6	0.15	0.02	0.16
(1,3018)	2:9:B:ALA:H	2:9:B:ALA:HB3	6	0.15	0.02	0.16
(1,2787)	2:20:C:VAL:HG11	2:34:C:ASN:HD22	5	1.9	0.91	2.58
(1,3671)	2:3:C:ALA:HB3	2:60:B:PHE:HD1	5	1.61	0.74	1.48
(1,3671)	2:3:C:ALA:HB3	2:60:C:PHE:HD1	5	1.61	0.74	1.48
(1,3671)	2:3:C:ALA:HB3	2:60:B:PHE:HD2	5	1.61	0.74	1.48
(1,3101)	2:23:C:LYS:HG3	2:23:C:LYS:H	5	1.18	0.05	1.19
(1,3325)	2:27:C:GLU:HG3	2:27:C:GLU:H	5	0.98	0.28	0.89
(1,4183)	1:120:A:LEU:HD11	2:35:C:VAL:H	5	0.96	0.5	1.04
(1,4183)	1:120:A:LEU:HD12	2:35:B:VAL:H	5	0.96	0.5	1.04
(1,4183)	1:120:A:LEU:HD12	2:35:C:VAL:H	5	0.96	0.5	1.04
(1,4183)	1:120:A:LEU:HD13	2:35:B:VAL:H	5	0.96	0.5	1.04
(1,4090)	2:16:B:PHE:H	2:12:C:ILE:HD12	5	0.92	0.46	0.84
(1,4090)	2:16:B:PHE:H	2:12:C:ILE:HD13	5	0.92	0.46	0.84
(1,2115)	2:13:C:VAL:HG21	2:48:C:ARG:HG2	5	0.92	0.4	1.17
(1,2115)	2:13:C:VAL:HG23	2:48:C:ARG:HG2	5	0.92	0.4	1.17
(1,3889)	2:18:C:SER:HB3	2:22:C:LYS:HD3	5	0.9	0.72	0.7
(1,3889)	2:18:C:SER:HB3	2:22:C:LYS:HG2	5	0.9	0.72	0.7
(1,3888)	2:18:B:SER:HB3	2:22:B:LYS:HG2	5	0.83	0.61	0.63
(1,3888)	2:18:B:SER:HB3	2:22:B:LYS:HD3	5	0.83	0.61	0.63
(1,4086)	2:15:B:TYR:H	2:12:C:ILE:HD12	5	0.77	0.27	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4086)	2:15:B:TYR:H	2:12:C:ILE:HD13	5	0.77	0.27	0.6
(1,2559)	2:55:C:LEU:HD21	2:13:C:VAL:HG22	5	0.76	0.3	0.63
(1,2559)	2:55:C:LEU:HD22	2:13:C:VAL:HG23	5	0.76	0.3	0.63
(1,2559)	2:55:C:LEU:HD23	2:13:C:VAL:HG21	5	0.76	0.3	0.63
(1,2559)	2:55:C:LEU:HD21	2:13:C:VAL:HG23	5	0.76	0.3	0.63
(1,3739)	2:68:C:ILE:HD11	2:11:B:LEU:HD23	5	0.7	0.5	0.67
(1,3739)	2:68:C:ILE:HD12	2:11:B:LEU:HD23	5	0.7	0.5	0.67
(1,3739)	2:68:C:ILE:HD13	2:11:B:LEU:HD23	5	0.7	0.5	0.67
(1,695)	1:79:A:LYS:HE3	1:81:A:ILE:HB	5	0.7	0.21	0.75
(1,1632)	1:147:A:MET:HG3	1:120:A:LEU:HB2	5	0.7	0.21	0.71
(1,2692)	2:50:B:ALA:HB3	2:47:B:GLU:HB2	5	0.67	0.71	0.35
(1,2692)	2:50:B:ALA:HB1	2:47:B:GLU:HB2	5	0.67	0.71	0.35
(1,3831)	2:40:C:ILE:HD12	2:13:C:VAL:HB	5	0.67	0.42	0.53
(1,3831)	2:40:C:ILE:HD13	2:13:C:VAL:HB	5	0.67	0.42	0.53
(1,3831)	2:40:C:ILE:HD11	2:13:C:VAL:HB	5	0.67	0.42	0.53
(1,2210)	2:22:B:LYS:HA	2:24:B:GLU:HB2	5	0.63	0.16	0.7
(1,3738)	2:68:B:ILE:HD13	2:11:C:LEU:HD22	5	0.62	0.22	0.59
(1,3738)	2:68:B:ILE:HD13	2:11:C:LEU:HD21	5	0.62	0.22	0.59
(1,3738)	2:68:B:ILE:HD13	2:11:C:LEU:HD23	5	0.62	0.22	0.59
(1,2538)	2:12:B:ILE:HG23	2:12:B:ILE:HG13	5	0.62	0.05	0.64
(1,2538)	2:12:B:ILE:HG22	2:12:B:ILE:HG13	5	0.62	0.05	0.64
(1,2538)	2:12:B:ILE:HG21	2:12:B:ILE:HG13	5	0.62	0.05	0.64
(1,1810)	1:99:A:LEU:HG	1:103:A:GLN:HE21	5	0.56	0.67	0.23
(1,1810)	1:103:A:GLN:HE21	1:114:A:ILE:HG13	5	0.56	0.67	0.23
(1,3222)	2:17:B:SER:HB3	2:17:B:SER:H	5	0.56	0.01	0.56
(1,3223)	2:17:C:SER:HB3	2:17:C:SER:H	5	0.56	0.01	0.56
(1,734)	1:87:A:SER:HA	1:79:A:LYS:HD3	5	0.55	0.19	0.47
(1,1697)	1:90:A:HIS:H	1:76:A:LEU:HD11	5	0.55	0.18	0.57
(1,1697)	1:90:A:HIS:H	1:76:A:LEU:HD12	5	0.55	0.18	0.57
(1,1697)	1:78:A:LEU:HD11	1:90:A:HIS:H	5	0.55	0.18	0.57
(1,26)	1:144:A:ILE:HD13	1:121:A:LEU:H	5	0.54	0.41	0.52
(1,26)	1:144:A:ILE:HD12	1:121:A:LEU:H	5	0.54	0.41	0.52
(1,26)	1:144:A:ILE:HD11	1:121:A:LEU:H	5	0.54	0.41	0.52
(1,247)	1:103:A:GLN:HG2	1:100:A:GLN:HE22	5	0.53	0.25	0.59
(1,2408)	2:19:B:ILE:HG21	2:44:C:PHE:HZ	5	0.52	0.16	0.62
(1,2408)	2:19:B:ILE:HG23	2:44:C:PHE:HZ	5	0.52	0.16	0.62
(1,132)	1:138:A:THR:HG22	1:141:A:ASN:HB3	5	0.51	0.21	0.37
(1,132)	1:138:A:THR:HG23	1:141:A:ASN:HB3	5	0.51	0.21	0.37
(1,2044)	2:5:B:LYS:HD2	2:44:B:PHE:HZ	5	0.5	0.19	0.44
(1,3954)	2:5:B:LYS:HD3	2:19:C:ILE:HD11	5	0.49	0.27	0.49
(1,3954)	2:5:B:LYS:HD3	2:19:C:ILE:HG21	5	0.49	0.27	0.49
(1,3954)	2:5:B:LYS:HD3	2:19:C:ILE:HG23	5	0.49	0.27	0.49

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2563)	2:11:C:LEU:HD22	2:55:C:LEU:HD23	5	0.49	0.25	0.43
(1,2563)	2:11:C:LEU:HD23	2:55:C:LEU:HD23	5	0.49	0.25	0.43
(1,2563)	2:11:C:LEU:HD23	2:55:C:LEU:HD22	5	0.49	0.25	0.43
(1,2563)	2:11:C:LEU:HD21	2:55:C:LEU:HD22	5	0.49	0.25	0.43
(1,2563)	2:11:C:LEU:HD21	2:55:C:LEU:HD23	5	0.49	0.25	0.43
(1,3623)	2:40:C:ILE:HA	2:33:B:LEU:HG	5	0.47	0.2	0.58
(1,3623)	2:12:C:ILE:HA	2:13:C:VAL:HG11	5	0.47	0.2	0.58
(1,2472)	2:12:B:ILE:HG22	2:13:B:VAL:HG13	5	0.46	0.24	0.44
(1,2472)	2:12:B:ILE:HG21	2:13:B:VAL:HG13	5	0.46	0.24	0.44
(1,2472)	2:12:B:ILE:HG21	2:13:B:VAL:HG11	5	0.46	0.24	0.44
(1,2472)	2:12:B:ILE:HG23	2:13:B:VAL:HG12	5	0.46	0.24	0.44
(1,2472)	2:12:B:ILE:HG22	2:13:B:VAL:HG11	5	0.46	0.24	0.44
(1,3936)	2:13:B:VAL:HG22	2:48:B:ARG:HG3	5	0.44	0.14	0.44
(1,3936)	2:13:B:VAL:HG21	2:48:B:ARG:HG3	5	0.44	0.14	0.44
(1,3936)	2:13:B:VAL:HG23	2:48:B:ARG:HG3	5	0.44	0.14	0.44
(1,44)	1:88:A:ILE:HD13	1:78:A:LEU:HB3	5	0.44	0.18	0.45
(1,2829)	2:6:C:GLU:HG2	2:9:C:ALA:HB3	5	0.43	0.3	0.35
(1,5)	1:119:A:LEU:HD22	1:102:A:LYS:H	5	0.43	0.56	0.13
(1,5)	1:119:A:LEU:HD21	1:102:A:LYS:H	5	0.43	0.56	0.13
(1,5)	1:119:A:LEU:HD23	1:102:A:LYS:H	5	0.43	0.56	0.13
(1,3092)	2:13:B:VAL:HG12	2:41:B:SER:H	5	0.41	0.08	0.44
(1,3092)	2:13:B:VAL:HG11	2:41:B:SER:H	5	0.41	0.08	0.44
(1,3092)	2:13:B:VAL:HG13	2:41:B:SER:H	5	0.41	0.08	0.44
(1,3570)	2:13:B:VAL:HG22	2:48:B:ARG:HG3	5	0.4	0.15	0.4
(1,3570)	2:13:B:VAL:HG21	2:50:B:ALA:HB2	5	0.4	0.15	0.4
(1,3570)	2:13:B:VAL:HG23	2:48:B:ARG:HG3	5	0.4	0.15	0.4
(1,2836)	2:40:B:ILE:HB	2:13:B:VAL:HG12	5	0.39	0.1	0.42
(1,2836)	2:40:B:ILE:HB	2:13:B:VAL:HG11	5	0.39	0.1	0.42
(1,1350)	1:141:A:ASN:HB3	1:141:A:ASN:HD21	5	0.38	0.14	0.42
(1,1211)	1:81:A:ILE:H	1:82:A:GLN:HG2	5	0.37	0.22	0.46
(1,762)	1:119:A:LEU:HA	1:144:A:ILE:HG23	5	0.37	0.31	0.14
(1,2270)	2:20:B:VAL:HA	2:25:B:ILE:HG23	5	0.37	0.18	0.42
(1,2940)	2:44:B:PHE:HZ	2:33:C:LEU:HD21	5	0.36	0.14	0.4
(1,2940)	2:44:B:PHE:HZ	2:33:C:LEU:HD23	5	0.36	0.14	0.4
(1,2940)	2:44:B:PHE:HZ	2:33:C:LEU:HD22	5	0.36	0.14	0.4
(1,2702)	2:13:B:VAL:HA	2:40:B:ILE:HD13	5	0.35	0.18	0.3
(1,2702)	2:13:B:VAL:HA	2:40:B:ILE:HD11	5	0.35	0.18	0.3
(1,2880)	2:33:B:LEU:HD11	2:19:B:ILE:HD12	5	0.34	0.09	0.34
(1,1392)	1:144:A:ILE:HG12	1:144:A:ILE:H	5	0.34	0.16	0.27
(1,1736)	1:110:A:LYS:H	1:105:A:LEU:HB3	5	0.34	0.18	0.33
(1,1417)	1:73:A:MET:HB3	1:74:A:VAL:H	5	0.33	0.24	0.15
(1,158)	1:99:A:LEU:HD21	1:103:A:GLN:H	5	0.33	0.06	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,158)	1:99:A:LEU:HD22	1:103:A:GLN:H	5	0.33	0.06	0.34
(1,4009)	2:44:C:PHE:HZ	2:19:B:ILE:HG21	5	0.32	0.17	0.21
(1,4009)	2:16:C:PHE:HZ	2:12:B:ILE:HG22	5	0.32	0.17	0.21
(1,4009)	2:16:C:PHE:HZ	2:12:B:ILE:HG21	5	0.32	0.17	0.21
(1,4009)	2:44:C:PHE:HZ	2:19:B:ILE:HG23	5	0.32	0.17	0.21
(1,235)	1:118:A:LYS:HB3	1:118:A:LYS:HE3	5	0.31	0.09	0.29
(1,3724)	2:25:B:ILE:HG22	2:19:B:ILE:HB	5	0.31	0.12	0.3
(1,3724)	2:25:B:ILE:HG21	2:19:B:ILE:HB	5	0.31	0.12	0.3
(1,3724)	2:25:B:ILE:HG23	2:19:B:ILE:HB	5	0.31	0.12	0.3
(1,31)	1:106:A:ILE:HD13	1:112:A:SER:H	5	0.3	0.08	0.27
(1,31)	1:106:A:ILE:HD12	1:112:A:SER:H	5	0.3	0.08	0.27
(1,31)	1:106:A:ILE:HD11	1:112:A:SER:H	5	0.3	0.08	0.27
(1,2791)	2:33:C:LEU:HD12	2:19:C:ILE:HB	5	0.3	0.07	0.28
(1,2791)	2:33:C:LEU:HD13	2:19:C:ILE:HB	5	0.3	0.07	0.28
(1,3796)	2:8:B:ILE:HG21	2:9:B:ALA:HB2	5	0.3	0.11	0.27
(1,3796)	2:8:B:ILE:HG21	2:9:B:ALA:HB3	5	0.3	0.11	0.27
(1,3197)	2:14:C:ASN:H	2:48:C:ARG:HA	5	0.27	0.17	0.21
(1,2598)	2:13:B:VAL:HG13	2:41:B:SER:HA	5	0.25	0.1	0.2
(1,2598)	2:13:B:VAL:HG12	2:41:B:SER:HA	5	0.25	0.1	0.2
(1,418)	1:136:A:LYS:HG2	1:136:A:LYS:H	5	0.25	0.07	0.25
(1,2153)	2:48:C:ARG:HD3	2:48:C:ARG:HB3	5	0.22	0.06	0.23
(1,3174)	2:7:B:GLU:H	2:4:B:SER:HB3	5	0.2	0.11	0.15
(1,2404)	2:8:B:ILE:HG22	2:15:C:TYR:H	5	0.17	0.05	0.17
(1,2404)	2:8:B:ILE:HG21	2:15:C:TYR:H	5	0.17	0.05	0.17
(1,3019)	2:9:C:ALA:H	2:9:C:ALA:HB3	5	0.15	0.03	0.17
(1,3019)	2:9:C:ALA:H	2:9:C:ALA:HB1	5	0.15	0.03	0.17
(1,103)	1:143:A:THR:HG23	1:143:A:THR:HB	5	0.13	0.0	0.13
(1,103)	1:143:A:THR:HG21	1:143:A:THR:HB	5	0.13	0.0	0.13
(1,103)	1:143:A:THR:HG22	1:143:A:THR:HB	5	0.13	0.0	0.13
(3,18)	1:144:A:ILE:N	1:77:A:THR:O	5	0.12	0.01	0.11
(3,9)	1:86:A:PHE:H	1:80:A:LYS:O	5	0.12	0.01	0.12
(1,2072)	2:51:B:VAL:HG21	2:51:B:VAL:HB	5	0.11	0.01	0.12
(1,2072)	2:51:B:VAL:HG22	2:51:B:VAL:HB	5	0.11	0.01	0.12
(1,3670)	2:3:B:ALA:HB2	2:60:C:PHE:HD1	4	1.88	0.51	1.73
(1,3670)	2:3:B:ALA:HB3	2:60:B:PHE:HD1	4	1.88	0.51	1.73
(1,2891)	2:21:C:GLU:HA	2:23:C:LYS:HE3	4	1.52	0.23	1.58
(1,2890)	2:21:B:GLU:HA	2:23:B:LYS:HE3	4	1.51	0.5	1.66
(1,2698)	2:54:B:ILE:HG23	2:6:B:GLU:HG3	4	1.33	0.65	1.6
(1,2698)	2:54:B:ILE:HG22	2:6:B:GLU:HG3	4	1.33	0.65	1.6
(1,2699)	2:54:C:ILE:HG23	2:6:C:GLU:HG3	4	1.32	0.82	1.25
(1,2699)	2:54:C:ILE:HG21	2:6:C:GLU:HG3	4	1.32	0.82	1.25
(1,2699)	2:54:C:ILE:HG22	2:6:C:GLU:HG3	4	1.32	0.82	1.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3732)	2:12:B:ILE:HD11	2:40:B:ILE:HG21	4	1.18	0.15	1.16
(1,3732)	2:12:B:ILE:HD11	2:40:B:ILE:HG22	4	1.18	0.15	1.16
(1,3732)	2:12:B:ILE:HD13	2:40:B:ILE:HD12	4	1.18	0.15	1.16
(1,3732)	2:12:B:ILE:HD11	2:40:B:ILE:HD12	4	1.18	0.15	1.16
(1,4179)	1:147:A:MET:HE3	2:35:C:VAL:H	4	1.13	0.34	1.01
(1,4179)	1:147:A:MET:HE3	2:35:B:VAL:H	4	1.13	0.34	1.01
(1,4179)	1:147:A:MET:HE1	2:35:B:VAL:H	4	1.13	0.34	1.01
(1,117)	1:125:A:VAL:HG22	1:126:A:LEU:H	4	1.06	0.93	1.02
(1,1351)	1:141:A:ASN:HD21	1:121:A:LEU:HG	4	1.06	0.68	1.08
(1,2521)	2:51:C:VAL:HA	2:54:C:ILE:HD11	4	1.06	1.18	0.44
(1,3527)	2:6:C:GLU:HG2	2:46:C:PHE:HD1	4	0.85	0.89	0.42
(1,3527)	2:6:C:GLU:HG2	2:46:C:PHE:HD2	4	0.85	0.89	0.42
(1,610)	1:108:A:GLU:HG3	1:107:A:SER:HB3	4	0.78	0.51	0.73
(1,3133)	2:1:C:ASP:H	2:2:C:SER:H	4	0.75	0.03	0.73
(1,3)	1:120:A:LEU:HD13	1:119:A:LEU:H	4	0.74	0.38	0.89
(1,3)	1:120:A:LEU:HD11	1:119:A:LEU:H	4	0.74	0.38	0.89
(1,3)	1:120:A:LEU:HD12	1:119:A:LEU:H	4	0.74	0.38	0.89
(1,686)	1:122:A:LYS:HA	1:122:A:LYS:HD3	4	0.68	0.69	0.35
(1,2562)	2:11:B:LEU:HD22	2:55:B:LEU:HD21	4	0.65	0.21	0.6
(1,2562)	2:11:B:LEU:HD23	2:55:B:LEU:HD21	4	0.65	0.21	0.6
(1,156)	1:99:A:LEU:HD22	1:103:A:GLN:HE21	4	0.65	0.61	0.34
(1,156)	1:99:A:LEU:HD21	1:103:A:GLN:HE21	4	0.65	0.61	0.34
(1,2539)	2:12:C:ILE:HG22	2:12:C:ILE:HG13	4	0.64	0.03	0.64
(1,2539)	2:12:C:ILE:HG21	2:12:C:ILE:HG13	4	0.64	0.03	0.64
(1,2178)	2:9:B:ALA:HA	2:12:B:ILE:HD11	4	0.64	0.57	0.4
(1,2178)	2:9:B:ALA:HA	2:12:B:ILE:HD13	4	0.64	0.57	0.4
(1,4087)	2:15:C:TYR:H	2:12:B:ILE:HD13	4	0.64	0.02	0.64
(1,4087)	2:15:C:TYR:H	2:12:B:ILE:HD12	4	0.64	0.02	0.64
(1,4087)	2:15:C:TYR:H	2:12:B:ILE:HD11	4	0.64	0.02	0.64
(1,2954)	2:16:B:PHE:HZ	2:12:C:ILE:HD12	4	0.63	0.45	0.56
(1,2954)	2:16:B:PHE:HZ	2:12:C:ILE:HD11	4	0.63	0.45	0.56
(1,2954)	2:16:B:PHE:HZ	2:12:C:ILE:HD13	4	0.63	0.45	0.56
(1,3643)	2:68:C:ILE:HB	2:71:C:SER:H	4	0.54	0.23	0.56
(1,2357)	2:49:C:GLU:HG2	2:49:C:GLU:H	4	0.54	0.27	0.54
(1,2937)	2:6:C:GLU:HG2	2:44:C:PHE:HD1	4	0.54	0.26	0.54
(1,3642)	2:68:B:ILE:HB	2:71:B:SER:H	4	0.53	0.25	0.6
(1,2473)	2:12:C:ILE:HG23	2:13:C:VAL:HG12	4	0.52	0.31	0.52
(1,2473)	2:12:C:ILE:HG22	2:13:C:VAL:HG12	4	0.52	0.31	0.52
(1,2473)	2:12:C:ILE:HG23	2:13:C:VAL:HG13	4	0.52	0.31	0.52
(1,2473)	2:12:C:ILE:HG23	2:13:C:VAL:HG11	4	0.52	0.31	0.52
(1,1818)	1:99:A:LEU:HD23	1:129:A:ASN:HD22	4	0.5	0.28	0.48
(1,1818)	1:129:A:ASN:HD22	1:130:A:LEU:HD21	4	0.5	0.28	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3816)	2:6:B:GLU:HB2	2:46:B:PHE:HD1	4	0.5	0.15	0.52
(1,3816)	2:6:B:GLU:HB2	2:46:B:PHE:HD2	4	0.5	0.15	0.52
(1,3817)	2:6:C:GLU:HB2	2:46:C:PHE:HD1	4	0.5	0.35	0.35
(1,3817)	2:6:C:GLU:HB2	2:46:C:PHE:HD2	4	0.5	0.35	0.35
(1,3588)	2:5:B:LYS:HE2	2:19:C:ILE:HG21	4	0.5	0.1	0.5
(1,3588)	2:5:B:LYS:HE2	2:19:C:ILE:HG22	4	0.5	0.1	0.5
(1,3588)	2:5:B:LYS:HE2	2:19:C:ILE:HD11	4	0.5	0.1	0.5
(1,1662)	1:149:A:LYS:HG3	1:149:A:LYS:HE3	4	0.49	0.21	0.5
(1,2245)	2:55:C:LEU:HD23	2:11:C:LEU:HA	4	0.46	0.21	0.51
(1,2245)	2:55:C:LEU:HD21	2:11:C:LEU:HA	4	0.46	0.21	0.51
(1,2245)	2:55:C:LEU:HD22	2:11:C:LEU:HA	4	0.46	0.21	0.51
(1,1567)	1:143:A:THR:HB	1:144:A:ILE:HB	4	0.44	0.17	0.52
(1,1567)	1:145:A:THR:HB	1:144:A:ILE:HB	4	0.44	0.17	0.52
(1,3823)	2:40:C:ILE:HD12	2:36:C:ALA:HA	4	0.44	0.16	0.46
(1,3823)	2:40:C:ILE:HD11	2:36:C:ALA:HA	4	0.44	0.16	0.46
(1,1794)	1:138:A:THR:H	1:121:A:LEU:HD22	4	0.43	0.26	0.36
(1,1794)	1:138:A:THR:H	1:121:A:LEU:HD21	4	0.43	0.26	0.36
(1,1760)	1:152:A:LEU:HB3	1:153:A:GLU:H	4	0.4	0.25	0.34
(1,2691)	2:50:C:ALA:HB1	2:47:C:GLU:HB3	4	0.38	0.26	0.31
(1,2691)	2:50:C:ALA:HB3	2:47:C:GLU:HB3	4	0.38	0.26	0.31
(1,3593)	2:9:C:ALA:HA	2:12:C:ILE:HG21	4	0.37	0.14	0.42
(1,3593)	2:9:C:ALA:HA	2:12:C:ILE:HG23	4	0.37	0.14	0.42
(1,3550)	2:25:B:ILE:HD11	2:5:C:LYS:HE3	4	0.36	0.2	0.36
(1,3550)	2:25:B:ILE:HD13	2:5:C:LYS:HE3	4	0.36	0.2	0.36
(1,2520)	2:51:B:VAL:HA	2:54:B:ILE:HD12	4	0.36	0.15	0.34
(1,2520)	2:51:B:VAL:HA	2:54:B:ILE:HD11	4	0.36	0.15	0.34
(1,2520)	2:51:B:VAL:HA	2:54:B:ILE:HD13	4	0.36	0.15	0.34
(1,1528)	1:121:A:LEU:HA	1:122:A:LYS:HB3	4	0.35	0.23	0.24
(1,3551)	2:25:C:ILE:HD12	2:5:B:LYS:HE3	4	0.35	0.17	0.34
(1,2380)	2:55:B:LEU:HD12	2:60:B:PHE:HD2	4	0.34	0.14	0.34
(1,2380)	2:55:B:LEU:HD13	2:60:B:PHE:HD1	4	0.34	0.14	0.34
(1,155)	1:135:A:LEU:HD12	1:137:A:VAL:H	4	0.32	0.16	0.31
(1,155)	1:135:A:LEU:HD13	1:137:A:VAL:H	4	0.32	0.16	0.31
(1,2308)	2:52:B:SER:HA	2:55:B:LEU:HD11	4	0.31	0.25	0.18
(1,2308)	2:52:B:SER:HA	2:55:B:LEU:HD13	4	0.31	0.25	0.18
(1,4005)	2:44:C:PHE:HZ	2:25:B:ILE:HG22	4	0.31	0.05	0.33
(1,4005)	2:44:C:PHE:HZ	2:25:B:ILE:HG21	4	0.31	0.05	0.33
(1,4005)	2:46:C:PHE:HE2	2:54:C:ILE:HG21	4	0.31	0.05	0.33
(1,3138)	2:2:B:SER:H	2:3:B:ALA:H	4	0.28	0.1	0.27
(1,4004)	2:44:B:PHE:HZ	2:25:C:ILE:HG23	4	0.27	0.1	0.27
(1,4004)	2:44:B:PHE:HZ	2:25:C:ILE:HG22	4	0.27	0.1	0.27
(1,4004)	2:44:B:PHE:HZ	2:25:C:ILE:HG21	4	0.27	0.1	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4004)	2:46:B:PHE:HE2	2:54:B:ILE:HG23	4	0.27	0.1	0.27
(1,2186)	2:30:B:ALA:HA	2:20:B:VAL:HG12	4	0.27	0.04	0.28
(1,2186)	2:30:B:ALA:HA	2:20:B:VAL:HG13	4	0.27	0.04	0.28
(1,738)	1:115:A:SER:HA	1:114:A:ILE:HG13	4	0.25	0.18	0.17
(1,2810)	2:25:B:ILE:HA	2:33:B:LEU:HD12	4	0.25	0.12	0.2
(1,2810)	2:25:B:ILE:HA	2:33:B:LEU:HD13	4	0.25	0.12	0.2
(1,3175)	2:7:C:GLU:H	2:4:C:SER:HB3	4	0.25	0.12	0.22
(3,89)	2:38:B:ASP:H	2:34:B:ASN:O	4	0.24	0.13	0.18
(1,2784)	2:51:B:VAL:HG22	2:14:B:ASN:H	4	0.24	0.08	0.2
(1,4126)	2:19:B:ILE:HA	2:25:B:ILE:H	4	0.24	0.09	0.24
(1,3797)	2:8:C:ILE:HG23	2:9:C:ALA:HB1	4	0.22	0.09	0.2
(1,2356)	2:49:B:GLU:HG2	2:49:B:GLU:H	4	0.22	0.08	0.18
(1,2811)	2:25:C:ILE:HA	2:33:C:LEU:HD11	4	0.22	0.11	0.18
(1,2811)	2:25:C:ILE:HA	2:33:C:LEU:HD13	4	0.22	0.11	0.18
(1,2946)	2:44:B:PHE:HB2	2:46:B:PHE:HE1	4	0.22	0.08	0.22
(1,2946)	2:44:B:PHE:HB2	2:46:B:PHE:HE2	4	0.22	0.08	0.22
(1,3158)	2:42:B:GLU:HB3	2:42:B:GLU:H	4	0.22	0.04	0.23
(1,585)	1:91:A:ASP:HB3	1:92:A:PHE:HA	4	0.21	0.02	0.22
(1,2947)	2:44:C:PHE:HB2	2:46:C:PHE:HE1	4	0.21	0.03	0.2
(1,2947)	2:44:C:PHE:HB2	2:46:C:PHE:HE2	4	0.21	0.03	0.2
(1,281)	1:120:A:LEU:HB2	1:145:A:THR:HB	4	0.21	0.08	0.2
(1,2963)	2:48:C:ARG:HG3	2:48:C:ARG:H	4	0.21	0.06	0.22
(1,19)	1:98:A:ILE:HD13	1:132:A:LEU:HA	4	0.19	0.1	0.14
(1,3562)	2:8:B:ILE:HD11	2:11:C:LEU:HA	4	0.19	0.06	0.17
(1,3562)	2:8:B:ILE:HD11	2:9:B:ALA:HA	4	0.19	0.06	0.17
(1,3562)	2:8:B:ILE:HD12	2:11:B:LEU:HA	4	0.19	0.06	0.17
(1,547)	1:150:A:PRO:HD3	1:149:A:LYS:HA	4	0.19	0.05	0.18
(1,1070)	1:111:A:ALA:HB2	1:111:A:ALA:H	4	0.18	0.05	0.16
(1,1070)	1:111:A:ALA:HB3	1:111:A:ALA:H	4	0.18	0.05	0.16
(1,1789)	1:127:A:HIS:H	1:98:A:ILE:HG23	4	0.18	0.02	0.16
(1,1789)	1:126:A:LEU:HD11	1:127:A:HIS:H	4	0.18	0.02	0.16
(1,3891)	2:18:C:SER:HB3	2:19:C:ILE:HG12	4	0.18	0.04	0.18
(1,3891)	2:18:C:SER:HB3	2:22:C:LYS:HG3	4	0.18	0.04	0.18
(1,3154)	2:4:B:SER:HB3	2:6:B:GLU:H	4	0.16	0.04	0.17
(1,2549)	2:20:C:VAL:HG11	2:20:C:VAL:HB	4	0.11	0.01	0.11
(1,2549)	2:20:C:VAL:HG13	2:20:C:VAL:HB	4	0.11	0.01	0.11
(1,15)	1:98:A:ILE:HD13	1:98:A:ILE:HG13	4	0.11	0.01	0.11
(1,15)	1:98:A:ILE:HD12	1:98:A:ILE:HG13	4	0.11	0.01	0.11
(1,3525)	2:6:C:GLU:HG3	2:46:C:PHE:HD1	3	1.39	0.53	1.74
(1,3525)	2:6:C:GLU:HG3	2:46:C:PHE:HD2	3	1.39	0.53	1.74
(1,3682)	2:12:B:ILE:HD13	2:16:C:PHE:HD1	3	1.2	0.49	1.29
(1,3682)	2:12:B:ILE:HD12	2:16:C:PHE:HD1	3	1.2	0.49	1.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,53)	1:114:A:ILE:HD13	1:103:A:GLN:H	3	1.13	0.4	0.98
(1,53)	1:114:A:ILE:HD11	1:103:A:GLN:H	3	1.13	0.4	0.98
(1,2490)	2:54:B:ILE:HG21	2:7:B:GLU:HG2	3	1.08	0.23	1.03
(1,2721)	2:54:C:ILE:HD12	2:6:C:GLU:HG3	3	1.08	0.54	1.37
(1,2721)	2:54:C:ILE:HD13	2:6:C:GLU:HG3	3	1.08	0.54	1.37
(1,2721)	2:54:C:ILE:HD11	2:6:C:GLU:HG3	3	1.08	0.54	1.37
(1,2720)	2:54:B:ILE:HD12	2:6:B:GLU:HG3	3	1.06	0.2	0.98
(1,51)	1:88:A:ILE:HD12	1:92:A:PHE:HZ	3	1.04	0.76	0.92
(1,51)	1:88:A:ILE:HD13	1:92:A:PHE:HZ	3	1.04	0.76	0.92
(1,2491)	2:54:C:ILE:HG22	2:7:C:GLU:HG2	3	0.87	0.29	0.8
(1,2491)	2:54:C:ILE:HG23	2:7:C:GLU:HG2	3	0.87	0.29	0.8
(1,673)	1:81:A:ILE:HG13	1:145:A:THR:HA	3	0.85	0.96	0.19
(1,231)	1:149:A:LYS:HB3	1:149:A:LYS:HE3	3	0.84	0.69	0.57
(1,3132)	2:1:B:ASP:H	2:2:B:SER:H	3	0.81	0.06	0.84
(1,1656)	1:124:A:LYS:HD3	1:121:A:LEU:HD22	3	0.8	0.18	0.9
(1,1656)	1:124:A:LYS:HD3	1:121:A:LEU:HD23	3	0.8	0.18	0.9
(1,709)	1:122:A:LYS:HE3	1:141:A:ASN:HA	3	0.79	0.38	0.66
(1,1758)	1:83:A:ALA:H	1:85:A:LYS:HG2	3	0.75	0.52	0.46
(1,3571)	2:13:C:VAL:HG21	2:48:C:ARG:HG3	3	0.73	0.04	0.71
(1,1399)	1:80:A:LYS:HE3	1:148:A:ILE:H	3	0.69	0.44	0.74
(1,3932)	2:18:B:SER:HB3	2:22:B:LYS:HE3	3	0.69	0.37	0.63
(1,3932)	2:18:B:SER:HB3	2:15:B:TYR:HB3	3	0.69	0.37	0.63
(1,3937)	2:51:C:VAL:HG22	2:55:C:LEU:HG	3	0.67	0.09	0.72
(1,3937)	2:13:C:VAL:HG21	2:48:C:ARG:HG3	3	0.67	0.09	0.72
(1,3983)	2:15:C:TYR:HD2	2:12:B:ILE:HD13	3	0.66	0.36	0.88
(1,3983)	2:15:C:TYR:HD2	2:12:B:ILE:HD11	3	0.66	0.36	0.88
(1,3983)	2:15:C:TYR:HD2	2:12:B:ILE:HD12	3	0.66	0.36	0.88
(1,2012)	2:47:B:GLU:HG3	2:47:B:GLU:H	3	0.64	0.15	0.66
(1,2775)	2:71:C:SER:HB3	2:68:C:ILE:H	3	0.63	0.29	0.79
(1,4091)	2:16:C:PHE:H	2:12:B:ILE:HD13	3	0.62	0.18	0.6
(1,4091)	2:16:C:PHE:H	2:12:B:ILE:HD12	3	0.62	0.18	0.6
(1,795)	1:80:A:LYS:HE3	1:86:A:PHE:HZ	3	0.55	0.47	0.29
(1,1440)	1:74:A:VAL:HG11	1:137:A:VAL:H	3	0.55	0.15	0.46
(1,1440)	1:74:A:VAL:HG12	1:137:A:VAL:H	3	0.55	0.15	0.46
(1,1440)	1:74:A:VAL:HG11	1:96:A:ASP:H	3	0.55	0.15	0.46
(1,3147)	2:6:C:GLU:H	2:6:C:GLU:HB3	3	0.55	0.0	0.55
(1,3023)	2:48:C:ARG:HG2	2:48:C:ARG:H	3	0.55	0.18	0.65
(1,3146)	2:6:B:GLU:H	2:6:B:GLU:HB3	3	0.55	0.01	0.55
(1,2013)	2:47:C:GLU:HG3	2:47:C:GLU:H	3	0.55	0.35	0.43
(1,1622)	1:128:A:ASP:HB2	1:99:A:LEU:HG	3	0.52	0.01	0.52
(1,3015)	2:5:C:LYS:HG2	2:5:C:LYS:H	3	0.5	0.25	0.37
(1,3045)	2:47:C:GLU:HB2	2:50:C:ALA:H	3	0.44	0.42	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,719)	1:148:A:ILE:HD12	1:112:A:SER:H	3	0.43	0.17	0.41
(1,28)	1:144:A:ILE:HD11	1:121:A:LEU:HA	3	0.41	0.21	0.29
(1,897)	1:85:A:LYS:HB2	1:86:A:PHE:H	3	0.4	0.02	0.4
(1,3803)	2:3:C:ALA:HB1	2:7:C:GLU:H	3	0.4	0.21	0.34
(1,3939)	2:33:C:LEU:HD11	2:5:B:LYS:HE3	3	0.4	0.11	0.35
(1,3939)	2:33:C:LEU:HD11	2:40:B:ILE:HA	3	0.4	0.11	0.35
(1,1733)	1:129:A:ASN:H	1:97:A:THR:HG21	3	0.39	0.23	0.34
(1,1733)	1:129:A:ASN:H	1:97:A:THR:HG23	3	0.39	0.23	0.34
(1,3955)	2:5:C:LYS:HD3	2:19:B:ILE:HD11	3	0.37	0.12	0.45
(1,3955)	2:5:C:LYS:HD3	2:19:B:ILE:HG23	3	0.37	0.12	0.45
(1,3955)	2:5:C:LYS:HD3	2:19:B:ILE:HD13	3	0.37	0.12	0.45
(1,4057)	2:17:C:SER:HA	2:18:C:SER:H	3	0.36	0.0	0.36
(1,1680)	1:145:A:THR:H	1:121:A:LEU:HG	3	0.35	0.07	0.39
(1,1680)	1:145:A:THR:H	1:79:A:LYS:HB2	3	0.35	0.07	0.39
(1,724)	1:148:A:ILE:HD13	1:80:A:LYS:HE3	3	0.34	0.15	0.32
(1,3566)	2:19:B:ILE:HD11	2:5:C:LYS:HG2	3	0.34	0.1	0.32
(1,3566)	2:19:B:ILE:HD13	2:5:C:LYS:HG2	3	0.34	0.1	0.32
(1,2070)	2:51:B:VAL:HG22	2:14:B:ASN:HA	3	0.34	0.12	0.42
(1,3196)	2:14:B:ASN:H	2:48:B:ARG:HA	3	0.34	0.26	0.18
(1,4056)	2:17:B:SER:HA	2:18:B:SER:H	3	0.33	0.02	0.34
(1,2226)	2:5:B:LYS:HA	2:8:B:ILE:HG13	3	0.33	0.05	0.35
(1,3231)	2:20:C:VAL:H	2:25:C:ILE:HG22	3	0.33	0.1	0.35
(1,2271)	2:20:C:VAL:HA	2:25:C:ILE:HG21	3	0.32	0.13	0.39
(1,2271)	2:20:C:VAL:HA	2:25:C:ILE:HG22	3	0.32	0.13	0.39
(1,1465)	1:117:A:ILE:HG22	1:102:A:LYS:HB3	3	0.31	0.13	0.26
(1,1465)	1:117:A:ILE:HG23	1:102:A:LYS:HB3	3	0.31	0.13	0.26
(1,1479)	1:82:A:GLN:HG3	1:82:A:GLN:H	3	0.3	0.14	0.3
(1,3589)	2:5:C:LYS:HE2	2:19:B:ILE:HD11	3	0.3	0.14	0.24
(1,3589)	2:5:C:LYS:HE2	2:19:B:ILE:HG21	3	0.3	0.14	0.24
(1,265)	1:114:A:ILE:HG12	1:103:A:GLN:HE22	3	0.28	0.08	0.32
(1,2227)	2:5:C:LYS:HA	2:8:C:ILE:HG13	3	0.27	0.12	0.29
(1,3071)	2:40:C:ILE:HG13	2:40:C:ILE:H	3	0.26	0.2	0.12
(1,3153)	2:6:C:GLU:HG3	2:6:C:GLU:H	3	0.25	0.03	0.24
(1,2690)	2:50:B:ALA:HB3	2:47:B:GLU:HB3	3	0.25	0.21	0.11
(1,2690)	2:50:B:ALA:HB1	2:47:B:GLU:HB3	3	0.25	0.21	0.11
(1,2881)	2:33:C:LEU:HD12	2:19:C:ILE:HD11	3	0.25	0.07	0.24
(1,2881)	2:33:C:LEU:HD11	2:19:C:ILE:HD11	3	0.25	0.07	0.24
(1,154)	1:135:A:LEU:HD12	1:136:A:LYS:H	3	0.24	0.15	0.14
(1,1766)	1:135:A:LEU:H	1:126:A:LEU:HD12	3	0.24	0.04	0.26
(1,513)	1:145:A:THR:HB	1:120:A:LEU:HD23	3	0.23	0.03	0.22
(1,513)	1:145:A:THR:HB	1:120:A:LEU:HD22	3	0.23	0.03	0.22
(1,181)	1:132:A:LEU:HD12	1:92:A:PHE:HB2	3	0.22	0.12	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,181)	1:132:A:LEU:HD13	1:92:A:PHE:HB2	3	0.22	0.12	0.15
(1,1179)	1:82:A:GLN:H	1:80:A:LYS:HD2	3	0.22	0.09	0.2
(1,2555)	2:20:C:VAL:HG13	2:30:C:ALA:HB3	3	0.22	0.07	0.24
(1,2555)	2:20:C:VAL:HG11	2:30:C:ALA:HB3	3	0.22	0.07	0.24
(1,2474)	2:12:B:ILE:HG22	2:40:B:ILE:HD13	3	0.2	0.09	0.14
(1,2474)	2:12:B:ILE:HG21	2:40:B:ILE:HD13	3	0.2	0.09	0.14
(1,760)	1:106:A:ILE:HG21	1:107:A:SER:HA	3	0.19	0.04	0.17
(1,625)	1:101:A:ILE:HB	1:98:A:ILE:HG21	3	0.18	0.06	0.16
(1,625)	1:101:A:ILE:HB	1:98:A:ILE:HG22	3	0.18	0.06	0.16
(1,1893)	2:23:C:LYS:HA	2:23:C:LYS:HG3	3	0.17	0.04	0.16
(1,2821)	2:5:C:LYS:HE2	2:24:B:GLU:HB3	3	0.15	0.02	0.14
(1,1892)	2:23:B:LYS:HA	2:23:B:LYS:HG3	3	0.15	0.03	0.16
(1,1616)	1:83:A:ALA:HB2	1:84:A:PRO:HB2	3	0.15	0.03	0.16
(1,1616)	1:83:A:ALA:HB1	1:84:A:PRO:HB2	3	0.15	0.03	0.16
(1,2464)	2:71:B:SER:HB3	2:71:B:SER:H	3	0.14	0.0	0.14
(1,2556)	2:35:B:VAL:HG12	2:36:B:ALA:HB1	3	0.14	0.03	0.14
(1,2556)	2:35:B:VAL:HG11	2:36:B:ALA:HB1	3	0.14	0.03	0.14
(1,1550)	1:85:A:LYS:HA	1:85:A:LYS:HG2	3	0.14	0.04	0.11
(1,1550)	1:85:A:LYS:HA	1:85:A:LYS:HG3	3	0.14	0.04	0.11
(1,2820)	2:5:B:LYS:HE2	2:24:C:GLU:HB3	3	0.14	0.02	0.13
(1,2465)	2:71:C:SER:HB3	2:71:C:SER:H	3	0.13	0.03	0.12
(1,3026)	2:55:B:LEU:HB2	2:56:B:GLY:H	3	0.12	0.0	0.12
(1,2548)	2:20:B:VAL:HG12	2:20:B:VAL:HB	3	0.12	0.01	0.11
(1,2548)	2:20:B:VAL:HG11	2:20:B:VAL:HB	3	0.12	0.01	0.11
(1,2261)	2:51:C:VAL:HG23	2:51:C:VAL:HA	3	0.11	0.01	0.11
(1,2261)	2:51:C:VAL:HG22	2:51:C:VAL:HA	3	0.11	0.01	0.11
(1,1186)	1:135:A:LEU:HB2	1:135:A:LEU:H	3	0.11	0.01	0.11
(1,2259)	2:51:C:VAL:HA	2:54:C:ILE:HB	2	1.78	1.66	1.78
(1,2084)	2:25:B:ILE:HD13	2:25:B:ILE:HG22	2	1.33	0.59	1.33
(1,137)	1:125:A:VAL:HG22	1:127:A:HIS:HA	2	1.31	0.86	1.31
(1,137)	1:125:A:VAL:HG23	1:127:A:HIS:HA	2	1.31	0.86	1.31
(1,559)	1:115:A:SER:HA	1:114:A:ILE:HG22	2	1.26	1.14	1.26
(1,559)	1:115:A:SER:HA	1:114:A:ILE:HG21	2	1.26	1.14	1.26
(1,142)	1:140:A:ALA:HB3	1:141:A:ASN:HD22	2	1.19	0.61	1.19
(1,4109)	2:21:C:GLU:H	2:22:C:LYS:HG3	2	1.18	0.08	1.18
(1,3149)	2:5:C:LYS:HG3	2:6:C:GLU:H	2	1.12	0.2	1.12
(1,3151)	2:5:C:LYS:HG2	2:6:C:GLU:H	2	1.12	0.1	1.12
(1,803)	1:99:A:LEU:HG	1:103:A:GLN:HE21	2	1.02	0.11	1.02
(1,728)	1:99:A:LEU:HG	1:103:A:GLN:HE22	2	1.01	0.32	1.01
(1,3933)	2:18:C:SER:HB3	2:22:C:LYS:HE3	2	0.9	0.17	0.9
(1,3933)	2:18:C:SER:HB3	2:15:C:TYR:HB3	2	0.9	0.17	0.9
(1,3259)	2:22:C:LYS:HG3	2:22:C:LYS:H	2	0.9	0.29	0.9

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1346)	1:141:A:ASN:HD22	1:138:A:THR:HG22	2	0.82	0.25	0.82
(1,1346)	1:141:A:ASN:HD22	1:138:A:THR:HG23	2	0.82	0.25	0.82
(1,1068)	1:119:A:LEU:HD23	1:119:A:LEU:H	2	0.77	0.42	0.77
(1,1068)	1:119:A:LEU:HD22	1:119:A:LEU:H	2	0.77	0.42	0.77
(1,1175)	1:153:A:GLU:H	1:152:A:LEU:HD21	2	0.77	0.09	0.77
(1,1175)	1:153:A:GLU:H	1:152:A:LEU:HD23	2	0.77	0.09	0.77
(1,2713)	2:54:C:ILE:HD11	2:51:C:VAL:H	2	0.72	0.49	0.72
(1,139)	1:125:A:VAL:HG23	1:125:A:VAL:HA	2	0.68	0.44	0.68
(1,139)	1:125:A:VAL:HG22	1:125:A:VAL:HA	2	0.68	0.44	0.68
(1,3322)	2:25:B:ILE:HG12	2:26:B:SER:H	2	0.67	0.31	0.67
(1,1829)	1:147:A:MET:H	1:146:A:VAL:HG21	2	0.65	0.5	0.65
(1,1829)	1:147:A:MET:H	1:119:A:LEU:HD11	2	0.65	0.5	0.65
(1,2244)	2:55:B:LEU:HD22	2:11:B:LEU:HA	2	0.64	0.29	0.64
(1,2381)	2:55:C:LEU:HD13	2:60:C:PHE:HD2	2	0.6	0.42	0.6
(1,2381)	2:55:C:LEU:HD12	2:60:C:PHE:HD1	2	0.6	0.42	0.6
(1,372)	1:151:A:ASN:HA	1:151:A:ASN:HD21	2	0.59	0.05	0.59
(1,262)	1:80:A:LYS:HD3	1:86:A:PHE:HZ	2	0.58	0.44	0.58
(1,1265)	1:107:A:SER:H	1:108:A:GLU:HG3	2	0.57	0.36	0.57
(1,2558)	2:55:B:LEU:HD22	2:13:B:VAL:HG21	2	0.57	0.4	0.57
(1,3044)	2:47:B:GLU:HB2	2:50:B:ALA:H	2	0.54	0.28	0.54
(1,3801)	2:8:C:ILE:HG23	2:16:B:PHE:HD1	2	0.53	0.21	0.53
(1,3982)	2:15:B:TYR:HD2	2:12:C:ILE:HD11	2	0.53	0.41	0.53
(1,3982)	2:15:B:TYR:HD2	2:12:C:ILE:HD12	2	0.53	0.41	0.53
(1,4108)	2:21:B:GLU:H	2:22:B:LYS:HG3	2	0.53	0.13	0.53
(1,2955)	2:16:C:PHE:HZ	2:12:B:ILE:HD13	2	0.46	0.24	0.46
(1,2955)	2:16:C:PHE:HZ	2:12:B:ILE:HD12	2	0.46	0.24	0.46
(1,33)	1:106:A:ILE:HD12	1:113:A:HIS:HB3	2	0.46	0.16	0.46
(1,33)	1:106:A:ILE:HD11	1:113:A:HIS:HB3	2	0.46	0.16	0.46
(1,90)	1:101:A:ILE:HG21	1:78:A:LEU:HA	2	0.45	0.04	0.45
(1,90)	1:101:A:ILE:HG22	1:78:A:LEU:HA	2	0.45	0.04	0.45
(1,1603)	1:141:A:ASN:HB2	1:121:A:LEU:HD13	2	0.42	0.32	0.42
(1,1603)	1:141:A:ASN:HB2	1:121:A:LEU:HD12	2	0.42	0.32	0.42
(1,2100)	2:19:B:ILE:HD12	2:24:B:GLU:HG3	2	0.41	0.0	0.41
(1,2978)	2:25:B:ILE:HD12	2:30:B:ALA:H	2	0.4	0.22	0.4
(1,1167)	1:124:A:LYS:HG2	1:125:A:VAL:H	2	0.4	0.18	0.4
(1,358)	1:95:A:SER:HB2	1:131:A:PHE:HD2	2	0.4	0.05	0.4
(1,358)	1:95:A:SER:HB2	1:131:A:PHE:HD1	2	0.4	0.05	0.4
(1,3290)	2:19:B:ILE:HG22	2:25:B:ILE:H	2	0.39	0.04	0.39
(1,2651)	2:8:C:ILE:HG21	2:19:B:ILE:HG12	2	0.37	0.0	0.37
(1,1739)	1:118:A:LYS:H	1:118:A:LYS:HB3	2	0.35	0.0	0.35
(1,3564)	2:19:B:ILE:HB	2:19:B:ILE:HD11	2	0.35	0.01	0.35
(1,1139)	1:82:A:GLN:HG3	1:82:A:GLN:H	2	0.34	0.09	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2646)	2:55:B:LEU:HD13	2:11:B:LEU:HD23	2	0.34	0.1	0.34
(1,2715)	2:54:C:ILE:HD12	2:47:C:GLU:H	2	0.34	0.04	0.34
(1,2650)	2:8:B:ILE:HG22	2:19:C:ILE:HG12	2	0.33	0.07	0.33
(1,3890)	2:18:B:SER:HB3	2:19:B:ILE:HG12	2	0.33	0.1	0.33
(1,29)	1:144:A:ILE:HD11	1:144:A:ILE:HA	2	0.32	0.14	0.32
(1,4012)	2:44:B:PHE:HZ	2:5:B:LYS:HE2	2	0.32	0.21	0.32
(1,440)	1:83:A:ALA:HA	1:85:A:LYS:HE3	2	0.32	0.06	0.32
(1,1813)	1:141:A:ASN:HD22	1:122:A:LYS:HG2	2	0.31	0.19	0.31
(1,3616)	2:12:B:ILE:HA	2:12:C:ILE:HD13	2	0.31	0.02	0.31
(1,3616)	2:12:B:ILE:HA	2:12:C:ILE:HD12	2	0.31	0.02	0.31
(1,1761)	1:82:A:GLN:H	1:80:A:LYS:HD2	2	0.3	0.1	0.3
(1,868)	1:144:A:ILE:HG22	1:145:A:THR:H	2	0.28	0.08	0.28
(1,868)	1:144:A:ILE:HG23	1:145:A:THR:H	2	0.28	0.08	0.28
(1,4153)	2:54:C:ILE:H	2:55:C:LEU:HD11	2	0.28	0.14	0.28
(1,4153)	2:54:C:ILE:H	2:55:C:LEU:HD13	2	0.28	0.14	0.28
(1,2936)	2:6:B:GLU:HG2	2:44:B:PHE:HD1	2	0.27	0.04	0.27
(1,766)	1:76:A:LEU:HA	1:76:A:LEU:HD12	2	0.26	0.16	0.26
(1,148)	1:132:A:LEU:HD22	1:92:A:PHE:HD2	2	0.26	0.13	0.26
(1,148)	1:132:A:LEU:HD21	1:92:A:PHE:HD2	2	0.26	0.13	0.26
(1,3164)	2:7:B:GLU:H	2:7:B:GLU:HG3	2	0.26	0.03	0.26
(1,114)	1:77:A:THR:HG23	1:79:A:LYS:H	2	0.25	0.05	0.25
(3,90)	2:38:B:ASP:N	2:34:B:ASN:O	2	0.25	0.12	0.25
(1,751)	1:149:A:LYS:HG2	1:149:A:LYS:HE3	2	0.24	0.13	0.24
(1,1319)	1:82:A:GLN:HG3	1:82:A:GLN:HE21	2	0.24	0.0	0.24
(1,3592)	2:9:B:ALA:HA	2:12:B:ILE:HG23	2	0.23	0.11	0.23
(1,3592)	2:9:B:ALA:HA	2:12:B:ILE:HG21	2	0.23	0.11	0.23
(1,624)	1:141:A:ASN:HB3	1:121:A:LEU:HD13	2	0.23	0.02	0.23
(1,2712)	2:54:B:ILE:HD12	2:51:B:VAL:H	2	0.23	0.01	0.23
(1,2712)	2:54:B:ILE:HD11	2:51:B:VAL:H	2	0.23	0.01	0.23
(1,414)	1:118:A:LYS:HG2	1:118:A:LYS:H	2	0.22	0.08	0.22
(1,2585)	2:49:C:GLU:HG3	2:49:C:GLU:HA	2	0.22	0.04	0.22
(1,2652)	2:8:B:ILE:HG23	2:3:B:ALA:HB3	2	0.22	0.12	0.22
(1,2652)	2:8:B:ILE:HG22	2:3:B:ALA:HB1	2	0.22	0.12	0.22
(1,3014)	2:5:B:LYS:HG2	2:5:B:LYS:H	2	0.22	0.05	0.22
(1,3152)	2:6:B:GLU:HG3	2:6:B:GLU:H	2	0.22	0.06	0.22
(1,27)	1:144:A:ILE:HD12	1:143:A:THR:H	2	0.22	0.03	0.22
(1,27)	1:144:A:ILE:HD11	1:143:A:THR:H	2	0.22	0.03	0.22
(1,4161)	2:38:C:ASP:H	2:40:C:ILE:HD12	2	0.22	0.03	0.22
(1,1792)	1:141:A:ASN:HB3	1:138:A:THR:H	2	0.22	0.06	0.22
(1,1200)	1:113:A:HIS:H	1:106:A:ILE:HD13	2	0.22	0.07	0.22
(1,506)	1:112:A:SER:HA	1:106:A:ILE:HD11	2	0.2	0.02	0.2
(1,506)	1:112:A:SER:HA	1:106:A:ILE:HD13	2	0.2	0.02	0.2

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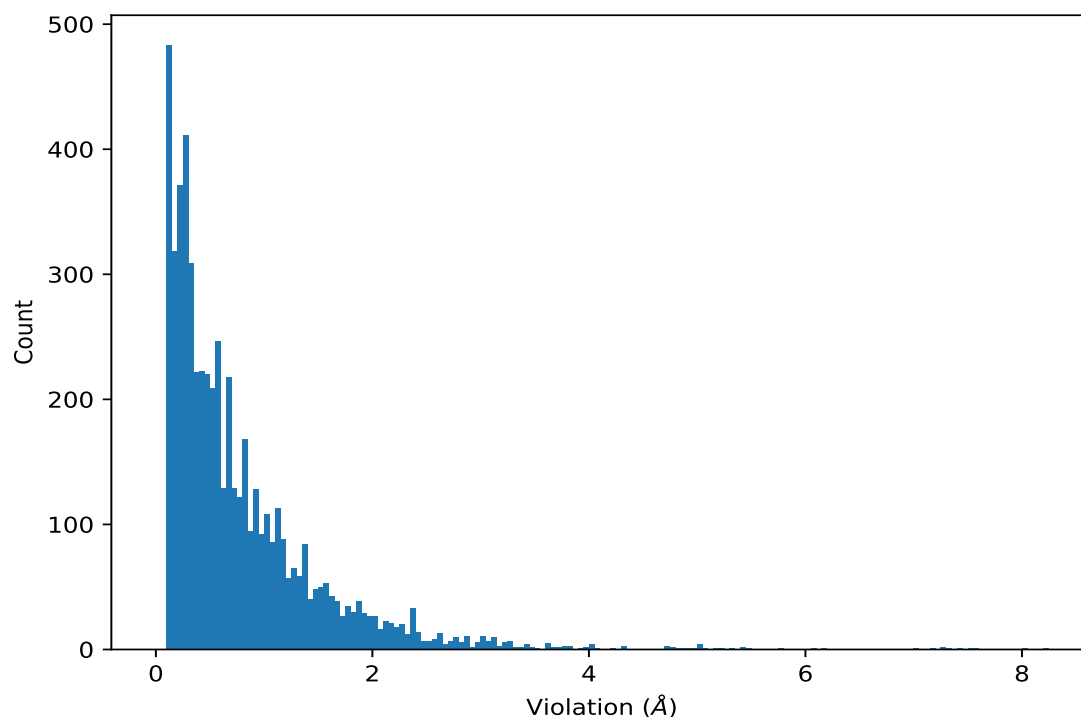
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2258)	2:51:B:VAL:HA	2:54:B:ILE:HB	2	0.2	0.02	0.2
(1,768)	1:76:A:LEU:HD13	1:132:A:LEU:HA	2	0.2	0.09	0.2
(1,1427)	1:106:A:ILE:HD12	1:104:A:HIS:H	2	0.2	0.09	0.2
(1,1427)	1:106:A:ILE:HD11	1:104:A:HIS:H	2	0.2	0.09	0.2
(1,1624)	1:132:A:LEU:HD11	1:93:A:SER:HA	2	0.2	0.08	0.2
(1,2512)	2:54:B:ILE:HD12	2:54:B:ILE:HG22	2	0.2	0.02	0.2
(1,1745)	1:82:A:GLN:H	1:81:A:ILE:HG22	2	0.2	0.04	0.2
(1,3355)	2:37:C:MET:H	2:40:C:ILE:HD13	2	0.19	0.05	0.19
(1,3355)	2:37:C:MET:H	2:40:C:ILE:HD11	2	0.19	0.05	0.19
(1,1719)	1:95:A:SER:HB3	1:95:A:SER:H	2	0.18	0.02	0.18
(1,1719)	1:93:A:SER:HB3	1:95:A:SER:H	2	0.18	0.02	0.18
(1,1606)	1:130:A:LEU:HB2	1:130:A:LEU:HD21	2	0.18	0.03	0.18
(1,1606)	1:152:A:LEU:HB2	1:152:A:LEU:HD12	2	0.18	0.03	0.18
(1,3714)	2:19:B:ILE:HG22	2:24:B:GLU:HB3	2	0.18	0.04	0.18
(1,3714)	2:19:B:ILE:HG23	2:24:B:GLU:HB3	2	0.18	0.04	0.18
(1,4160)	2:38:B:ASP:H	2:40:B:ILE:HD13	2	0.17	0.06	0.17
(1,3800)	2:8:B:ILE:HG23	2:16:C:PHE:HD1	2	0.17	0.04	0.17
(1,3800)	2:8:B:ILE:HG22	2:16:C:PHE:HD1	2	0.17	0.04	0.17
(1,3910)	2:12:B:ILE:HG13	2:11:B:LEU:H	2	0.17	0.02	0.17
(1,3605)	2:34:C:ASN:HA	2:20:C:VAL:HG11	2	0.16	0.02	0.16
(1,1438)	1:101:A:ILE:HG23	1:78:A:LEU:HB3	2	0.15	0.02	0.15
(1,61)	1:117:A:ILE:HD12	1:112:A:SER:H	2	0.15	0.0	0.15
(1,2497)	2:25:C:ILE:HG22	2:24:C:GLU:HB2	2	0.15	0.03	0.15
(1,193)	1:117:A:ILE:HG22	1:118:A:LYS:H	2	0.14	0.04	0.14
(1,193)	1:117:A:ILE:HG23	1:118:A:LYS:H	2	0.14	0.04	0.14
(1,2085)	2:25:C:ILE:HD11	2:25:C:ILE:HG21	2	0.14	0.02	0.14
(1,2085)	2:25:C:ILE:HD11	2:25:C:ILE:HG22	2	0.14	0.02	0.14
(1,2187)	2:30:C:ALA:HA	2:20:C:VAL:HG13	2	0.14	0.02	0.14
(1,2876)	2:13:B:VAL:HB	2:14:B:ASN:HA	2	0.14	0.02	0.14
(1,487)	1:139:A:PRO:HD2	1:138:A:THR:HA	2	0.13	0.02	0.13
(1,2863)	2:37:C:MET:HA	2:37:C:MET:HG2	2	0.13	0.01	0.13
(1,188)	1:101:A:ILE:HG13	1:101:A:ILE:HG23	2	0.12	0.01	0.12
(1,2496)	2:25:B:ILE:HG23	2:24:B:GLU:HB2	2	0.12	0.01	0.12
(1,2496)	2:25:B:ILE:HG21	2:24:B:GLU:HB2	2	0.12	0.01	0.12
(1,2479)	2:19:C:ILE:HB	2:19:C:ILE:HG21	2	0.11	0.0	0.11
(1,2479)	2:19:C:ILE:HB	2:19:C:ILE:HG22	2	0.11	0.0	0.11
(1,1968)	2:34:B:ASN:HB3	2:34:B:ASN:HD21	2	0.11	0.0	0.11
(1,2111)	2:13:C:VAL:HG21	2:13:C:VAL:HB	2	0.11	0.0	0.11
(1,2111)	2:13:C:VAL:HG23	2:13:C:VAL:HB	2	0.11	0.0	0.11
(1,3059)	2:26:C:SER:HB2	2:26:C:SER:H	2	0.11	0.0	0.11
(1,2166)	2:44:B:PHE:HB3	2:44:B:PHE:HB2	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)
(1,4172)	1:122:A:LYS:C	2:35:B:VAL:HG12	10	8.24
(1,4172)	1:122:A:LYS:C	2:35:B:VAL:HG11	1	8.03
(1,4172)	1:122:A:LYS:C	2:35:B:VAL:HG13	8	7.56
(1,4172)	1:122:A:LYS:C	2:35:B:VAL:HG11	4	7.53
(1,4172)	1:122:A:LYS:C	2:35:B:VAL:HG13	9	7.41
(1,4172)	1:122:A:LYS:H	2:35:B:VAL:HG13	3	7.33
(1,4172)	1:122:A:LYS:C	2:35:B:VAL:HG11	7	7.3
(1,4172)	1:122:A:LYS:C	2:35:B:VAL:HG11	6	7.25
(1,4172)	1:122:A:LYS:C	2:35:B:VAL:HG13	2	7.17
(1,135)	1:125:A:VAL:HG22	1:118:A:LYS:HE3	5	7.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4174)	1:124:A:LYS:C	2:35:B:VAL:HG11	10	6.15
(1,4174)	1:124:A:LYS:O	2:35:B:VAL:HG13	1	6.08
(1,4172)	1:122:A:LYS:HD2	2:39:B:CYS:SG	5	5.78
(1,4173)	1:123:A:GLY:HA2	2:35:B:VAL:HG11	1	5.46
(1,707)	1:122:A:LYS:HE3	1:143:A:THR:HG23	9	5.43
(1,4174)	1:124:A:LYS:C	2:35:B:VAL:HG13	6	5.4
(1,4174)	1:124:A:LYS:O	2:35:B:VAL:HG13	9	5.32
(1,4174)	1:124:A:LYS:O	2:35:B:VAL:HG13	3	5.23
(1,4173)	1:123:A:GLY:O	2:35:B:VAL:HG12	10	5.19
(1,73)	1:88:A:ILE:HG22	1:90:A:HIS:HE1	9	5.1
(1,4174)	1:124:A:LYS:O	2:35:B:VAL:HG13	7	5.05
(1,4174)	1:124:A:LYS:O	2:35:B:VAL:HG13	4	5.02
(1,4174)	1:124:A:LYS:O	2:35:B:VAL:HG12	8	5.02
(1,4174)	1:124:A:LYS:O	2:35:B:VAL:HG13	5	5.01
(1,708)	1:122:A:LYS:HE3	1:121:A:LEU:HD11	9	4.98
(1,4173)	1:123:A:GLY:O	2:35:B:VAL:HG13	5	4.9
(1,708)	1:122:A:LYS:HE3	1:121:A:LEU:HD12	2	4.88
(1,4174)	1:124:A:LYS:C	2:35:B:VAL:HG12	2	4.82
(1,2617)	2:51:C:VAL:HG22	2:46:C:PHE:HZ	9	4.77
(1,708)	1:122:A:LYS:HE3	1:121:A:LEU:HD12	1	4.76
(1,4173)	1:123:A:GLY:O	2:35:B:VAL:HG13	3	4.74
(1,4173)	1:123:A:GLY:O	2:35:B:VAL:HG13	9	4.72
(1,1660)	1:124:A:LYS:HE2	1:135:A:LEU:HD21	5	4.71
(1,4173)	1:123:A:GLY:O	2:35:B:VAL:HG11	7	4.35
(1,4173)	1:123:A:GLY:O	2:35:B:VAL:HG11	4	4.34
(1,4173)	1:123:A:GLY:O	2:35:B:VAL:HG13	8	4.32
(1,708)	1:122:A:LYS:HE3	1:121:A:LEU:HD12	4	4.22
(1,2389)	2:20:C:VAL:HG21	2:34:C:ASN:HD22	9	4.09
(1,4173)	1:123:A:GLY:O	2:35:B:VAL:HG13	6	4.04
(1,2389)	2:20:C:VAL:HG23	2:34:C:ASN:HD22	4	4.04
(1,2388)	2:20:B:VAL:HG22	2:34:B:ASN:HD22	3	4.03
(1,2388)	2:20:B:VAL:HG22	2:34:B:ASN:HD22	8	4.02
(1,1452)	1:78:A:LEU:HD21	1:90:A:HIS:HE1	9	3.99
(1,4173)	1:123:A:GLY:O	2:35:B:VAL:HG13	2	3.97
(1,708)	1:122:A:LYS:HE3	1:121:A:LEU:HD12	7	3.92
(1,708)	1:122:A:LYS:HE3	1:121:A:LEU:HD12	8	3.84
(1,73)	1:88:A:ILE:HG22	1:90:A:HIS:HE1	4	3.84
(1,708)	1:122:A:LYS:HE3	1:121:A:LEU:HD13	6	3.81
(1,804)	1:121:A:LEU:HD21	1:141:A:ASN:HD21	5	3.78
(1,2388)	2:20:B:VAL:HG22	2:34:B:ASN:HD22	4	3.77
(1,1448)	1:78:A:LEU:HD13	1:90:A:HIS:HE1	3	3.76
(1,1448)	1:78:A:LEU:HD13	1:104:A:HIS:HE1	6	3.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,135)	1:125:A:VAL:HG21	1:118:A:LYS:HE3	8	3.7
(1,1629)	1:105:A:LEU:HD11	1:104:A:HIS:HE1	3	3.67
(1,1452)	1:78:A:LEU:HD21	1:90:A:HIS:HE1	4	3.66
(1,2389)	2:20:C:VAL:HG21	2:34:C:ASN:HD22	5	3.65
(1,1660)	1:125:A:VAL:HG21	1:118:A:LYS:HE3	8	3.64
(1,2388)	2:20:B:VAL:HG22	2:34:B:ASN:HD22	7	3.63
(1,698)	1:79:A:LYS:HE3	1:81:A:ILE:HG23	2	3.63
(1,48)	1:88:A:ILE:HD12	1:90:A:HIS:HE1	9	3.61
(1,1629)	1:105:A:LEU:HD11	1:104:A:HIS:HE1	8	3.53
(1,48)	1:88:A:ILE:HD12	1:90:A:HIS:HE1	4	3.49
(1,1457)	1:120:A:LEU:HD22	1:118:A:LYS:HE3	5	3.48
(1,2259)	2:51:C:VAL:HA	2:54:C:ILE:HB	9	3.44
(1,1448)	1:78:A:LEU:HD13	1:104:A:HIS:HE1	9	3.44
(1,792)	1:134:A:ASP:HB2	1:130:A:LEU:HD21	8	3.44
(1,2616)	2:51:B:VAL:HG21	2:46:B:PHE:HZ	2	3.42
(1,2631)	2:51:C:VAL:HB	2:55:C:LEU:HG	9	3.39
(1,792)	1:134:A:ASP:HB2	1:130:A:LEU:HD22	7	3.38
(1,1629)	1:105:A:LEU:HD11	1:104:A:HIS:HE1	6	3.33
(1,93)	1:74:A:VAL:HG11	1:93:A:SER:HA	3	3.33
(1,2614)	2:13:B:VAL:HG12	2:48:B:ARG:HG2	9	3.29
(1,1629)	1:105:A:LEU:HD11	1:104:A:HIS:HE1	10	3.28
(1,95)	1:74:A:VAL:HG12	1:94:A:PRO:HD3	10	3.28
(1,792)	1:134:A:ASP:HB2	1:130:A:LEU:HD22	9	3.27
(1,93)	1:74:A:VAL:HG11	1:93:A:SER:HA	4	3.26
(1,2113)	2:13:C:VAL:HG21	2:51:C:VAL:HB	9	3.25
(1,1347)	1:141:A:ASN:HD22	1:121:A:LEU:HD12	4	3.25
(1,1629)	1:105:A:LEU:HD11	1:90:A:HIS:HE1	7	3.24
(1,705)	1:122:A:LYS:HE3	1:122:A:LYS:HB3	2	3.24
(1,2642)	2:25:B:ILE:HD13	2:20:B:VAL:HG11	2	3.23
(1,2545)	2:51:C:VAL:HG12	2:55:C:LEU:HG	9	3.23
(1,157)	1:99:A:LEU:HD22	1:103:A:GLN:HE22	8	3.23
(1,116)	1:125:A:VAL:HG23	1:120:A:LEU:H	1	3.23
(1,179)	1:120:A:LEU:HD23	1:147:A:MET:HG3	9	3.18
(1,1457)	1:120:A:LEU:HD21	1:118:A:LYS:HE3	10	3.16
(1,73)	1:88:A:ILE:HG22	1:90:A:HIS:HE1	10	3.16
(1,792)	1:134:A:ASP:HB2	1:130:A:LEU:HD23	5	3.15
(1,93)	1:74:A:VAL:HG11	1:93:A:SER:HA	10	3.15
(1,792)	1:134:A:ASP:HB2	1:130:A:LEU:HD22	10	3.14
(1,93)	1:74:A:VAL:HG11	1:93:A:SER:HA	9	3.13
(1,13)	1:119:A:LEU:HD21	1:98:A:ILE:HA	5	3.12
(1,2247)	2:11:C:LEU:HA	2:12:C:ILE:HD11	1	3.11
(1,2246)	2:11:B:LEU:HA	2:12:B:ILE:HD11	7	3.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1448)	1:78:A:LEU:HD13	1:104:A:HIS:HE1	8	3.11
(1,1629)	1:105:A:LEU:HD11	1:104:A:HIS:HE1	9	3.1
(1,792)	1:134:A:ASP:HB2	1:130:A:LEU:HD22	3	3.1
(1,2521)	2:51:C:VAL:HA	2:54:C:ILE:HD11	9	3.09
(1,786)	1:126:A:LEU:HD11	1:124:A:LYS:HD3	1	3.09
(1,2247)	2:11:C:LEU:HA	2:12:C:ILE:HD11	5	3.08
(1,1356)	1:151:A:ASN:HA	1:151:A:ASN:HD22	9	3.08
(1,1347)	1:141:A:ASN:HD22	1:121:A:LEU:HD13	7	3.08
(1,2246)	2:11:B:LEU:HA	2:12:B:ILE:HD13	4	3.06
(1,63)	1:83:A:ALA:HB1	1:85:A:LYS:HE3	1	3.06
(1,2089)	2:8:C:ILE:HD11	2:19:B:ILE:HG12	9	3.05
(1,703)	1:122:A:LYS:HE3	1:141:A:ASN:HD22	2	3.05
(1,3719)	2:54:C:ILE:HG23	2:13:C:VAL:HG22	9	3.03
(1,2246)	2:11:B:LEU:HA	2:12:B:ILE:HD11	9	3.02
(1,1353)	1:121:A:LEU:HD12	1:141:A:ASN:HD21	5	3.02
(1,792)	1:134:A:ASP:HB2	1:130:A:LEU:HD22	6	3.02
(1,2246)	2:11:B:LEU:HA	2:12:B:ILE:HD12	6	3.01
(1,157)	1:99:A:LEU:HD21	1:103:A:GLN:HE22	5	3.01
(1,57)	1:81:A:ILE:HD11	1:145:A:THR:HB	3	3.01
(1,1353)	1:121:A:LEU:HD13	1:141:A:ASN:HD21	4	3.0
(1,63)	1:83:A:ALA:HB1	1:85:A:LYS:HE3	4	3.0
(1,2247)	2:11:C:LEU:HA	2:12:C:ILE:HD13	10	2.99
(1,2071)	2:51:C:VAL:HG22	2:14:C:ASN:HA	9	2.98
(1,1629)	1:105:A:LEU:HD11	1:104:A:HIS:HE1	4	2.97
(1,1457)	1:120:A:LEU:HD22	1:118:A:LYS:HE3	8	2.96
(1,707)	1:122:A:LYS:HE3	1:143:A:THR:HG21	4	2.96
(1,704)	1:122:A:LYS:HE3	1:141:A:ASN:HD21	2	2.95
(1,2192)	2:25:B:ILE:HD12	2:30:B:ALA:HA	2	2.92
(1,57)	1:81:A:ILE:HD12	1:145:A:THR:HB	5	2.92
(1,1452)	1:78:A:LEU:HD21	1:90:A:HIS:HE1	8	2.9
(1,3671)	2:3:C:ALA:HB3	2:60:C:PHE:HD1	4	2.89
(1,1448)	1:78:A:LEU:HD13	1:90:A:HIS:HE1	10	2.89
(1,93)	1:74:A:VAL:HG11	1:93:A:SER:HA	7	2.89
(1,2247)	2:11:C:LEU:HA	2:12:C:ILE:HD12	4	2.88
(1,95)	1:74:A:VAL:HG11	1:94:A:PRO:HD3	9	2.87
(1,93)	1:74:A:VAL:HG11	1:93:A:SER:HA	6	2.87
(1,93)	1:74:A:VAL:HG11	1:93:A:SER:HA	8	2.87
(1,135)	1:125:A:VAL:HG21	1:118:A:LYS:HE3	1	2.86
(1,2616)	2:51:B:VAL:HG23	2:46:B:PHE:HZ	4	2.85
(1,95)	1:74:A:VAL:HG12	1:94:A:PRO:HD3	8	2.85
(1,1448)	1:78:A:LEU:HD13	1:104:A:HIS:HE1	4	2.83
(1,804)	1:121:A:LEU:HD21	1:141:A:ASN:HD21	4	2.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2786)	2:20:B:VAL:HG12	2:34:B:ASN:HD22	3	2.82
(1,1452)	1:78:A:LEU:HD21	1:90:A:HIS:HE1	3	2.82
(1,95)	1:74:A:VAL:HG12	1:94:A:PRO:HD3	3	2.82
(1,82)	1:148:A:ILE:HG21	1:150:A:PRO:HD2	7	2.81
(1,1452)	1:78:A:LEU:HD21	1:90:A:HIS:HE1	10	2.8
(1,1660)	1:125:A:VAL:HG21	1:118:A:LYS:HE3	1	2.79
(1,63)	1:83:A:ALA:HB1	1:85:A:LYS:HE3	7	2.79
(1,57)	1:81:A:ILE:HD12	1:145:A:THR:HB	6	2.79
(1,698)	1:79:A:LYS:HE3	1:81:A:ILE:HG21	7	2.78
(1,95)	1:74:A:VAL:HG11	1:94:A:PRO:HD3	1	2.78
(1,95)	1:74:A:VAL:HG11	1:94:A:PRO:HD3	4	2.78
(1,1452)	1:78:A:LEU:HD21	1:90:A:HIS:HE1	6	2.76
(1,834)	1:85:A:LYS:HE3	1:82:A:GLN:HA	4	2.75
(1,93)	1:74:A:VAL:HG11	1:93:A:SER:HA	1	2.75
(1,3780)	2:13:B:VAL:HG23	2:16:B:PHE:HE2	6	2.74
(1,82)	1:148:A:ILE:HG21	1:150:A:PRO:HD2	10	2.73
(1,2629)	2:37:C:MET:HB3	2:17:C:SER:HB3	1	2.71
(1,2628)	2:37:B:MET:HB3	2:17:B:SER:HB3	5	2.71
(1,2089)	2:8:C:ILE:HD11	2:19:B:ILE:HG12	5	2.71
(1,664)	1:119:A:LEU:HD12	1:146:A:VAL:HA	5	2.71
(1,720)	1:148:A:ILE:HD12	1:86:A:PHE:HZ	10	2.7
(1,2785)	2:51:C:VAL:HG22	2:14:C:ASN:H	9	2.69
(1,3670)	2:3:B:ALA:HB3	2:60:B:PHE:HD1	4	2.68
(1,792)	1:134:A:ASP:HB2	1:130:A:LEU:HD22	2	2.68
(1,2786)	2:20:B:VAL:HG12	2:34:B:ASN:HD22	7	2.67
(1,2786)	2:20:B:VAL:HG12	2:34:B:ASN:HD22	8	2.65
(1,705)	1:122:A:LYS:HE3	1:122:A:LYS:HB3	5	2.65
(1,3780)	2:13:B:VAL:HG23	2:16:B:PHE:HE2	7	2.64
(1,3737)	2:54:C:ILE:HD13	2:13:C:VAL:HG22	9	2.64
(1,2642)	2:25:B:ILE:HD11	2:20:B:VAL:HG11	10	2.63
(1,1457)	1:120:A:LEU:HD22	1:118:A:LYS:HE3	1	2.62
(1,2642)	2:25:B:ILE:HD12	2:20:B:VAL:HG12	1	2.61
(1,2629)	2:37:C:MET:HB3	2:17:C:SER:HB3	5	2.61
(1,2615)	2:13:C:VAL:HG13	2:48:C:ARG:HG2	10	2.61
(1,2534)	2:36:B:ALA:HB3	2:40:C:ILE:HG13	2	2.61
(1,705)	1:122:A:LYS:HE3	1:122:A:LYS:HB3	6	2.61
(1,2787)	2:20:C:VAL:HG11	2:34:C:ASN:HD22	9	2.6
(1,707)	1:122:A:LYS:HE3	1:143:A:THR:HG23	1	2.6
(1,2787)	2:20:C:VAL:HG11	2:34:C:ASN:HD22	4	2.59
(1,2616)	2:51:B:VAL:HG21	2:46:B:PHE:HZ	7	2.59
(1,2088)	2:8:B:ILE:HD13	2:19:C:ILE:HG12	5	2.59
(1,1629)	1:105:A:LEU:HD11	1:90:A:HIS:HE1	1	2.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	1:148:A:ILE:HG23	1:150:A:PRO:HD2	5	2.59
(1,2787)	2:20:C:VAL:HG11	2:34:C:ASN:HD22	5	2.58
(1,792)	1:134:A:ASP:HB2	1:130:A:LEU:HD22	4	2.57
(1,2617)	2:51:C:VAL:HG23	2:46:C:PHE:HZ	10	2.56
(1,2388)	2:20:B:VAL:HG22	2:34:B:ASN:HD22	6	2.54
(1,2088)	2:8:B:ILE:HD12	2:19:C:ILE:HG12	4	2.52
(1,1141)	1:82:A:GLN:H	1:80:A:LYS:HG2	10	2.52
(1,705)	1:122:A:LYS:HE3	1:122:A:LYS:HB3	4	2.51
(1,95)	1:74:A:VAL:HG12	1:94:A:PRO:HD3	6	2.51
(1,82)	1:148:A:ILE:HG23	1:150:A:PRO:HD2	4	2.5
(1,82)	1:148:A:ILE:HG21	1:150:A:PRO:HD2	9	2.5
(1,3741)	2:25:C:ILE:HD12	2:19:C:ILE:HD11	5	2.49
(1,705)	1:122:A:LYS:HE3	1:122:A:LYS:HB3	7	2.49
(1,8)	1:120:A:LEU:HD13	1:147:A:MET:HG3	9	2.49
(1,1614)	1:150:A:PRO:HB2	1:148:A:ILE:HG21	3	2.48
(1,63)	1:83:A:ALA:HB1	1:85:A:LYS:HE3	8	2.48
(1,82)	1:148:A:ILE:HG21	1:150:A:PRO:HD2	1	2.47
(1,157)	1:99:A:LEU:HD22	1:103:A:GLN:HE22	3	2.45
(1,2697)	2:54:C:ILE:HG21	2:51:C:VAL:HA	9	2.44
(1,1820)	1:129:A:ASN:HD21	1:130:A:LEU:HD21	10	2.44
(1,1172)	1:85:A:LYS:HE3	1:83:A:ALA:H	4	2.44
(1,860)	1:80:A:LYS:H	1:79:A:LYS:HD3	10	2.44
(1,57)	1:81:A:ILE:HD12	1:145:A:THR:HB	1	2.44
(1,2616)	2:51:B:VAL:HG21	2:46:B:PHE:HZ	8	2.43
(1,2088)	2:8:B:ILE:HD12	2:19:C:ILE:HG12	10	2.43
(1,1141)	1:82:A:GLN:H	1:80:A:LYS:HG2	3	2.43
(1,3934)	2:55:B:LEU:HD12	2:7:B:GLU:HG2	6	2.42
(1,2616)	2:51:B:VAL:HG23	2:46:B:PHE:HZ	10	2.42
(1,705)	1:122:A:LYS:HE3	1:122:A:LYS:HB3	1	2.42
(1,3780)	2:13:B:VAL:HG22	2:16:C:PHE:HE1	3	2.41
(1,3736)	2:54:B:ILE:HD11	2:13:B:VAL:HG23	4	2.41
(1,705)	1:122:A:LYS:HE3	1:122:A:LYS:HB3	8	2.41
(1,3193)	2:51:C:VAL:HG11	2:14:C:ASN:H	9	2.4
(1,2643)	2:25:C:ILE:HD11	2:20:C:VAL:HG13	1	2.4
(1,2616)	2:51:B:VAL:HG21	2:46:B:PHE:HZ	6	2.4
(1,1141)	1:82:A:GLN:H	1:80:A:LYS:HG2	4	2.4
(1,860)	1:80:A:LYS:H	1:79:A:LYS:HD3	8	2.4
(1,2643)	2:25:C:ILE:HD11	2:20:C:VAL:HG13	10	2.39
(1,2628)	2:37:B:MET:HB3	2:17:B:SER:HB3	9	2.39
(1,2246)	2:11:B:LEU:HA	2:12:B:ILE:HD12	8	2.39
(1,559)	1:115:A:SER:HA	1:114:A:ILE:HG22	1	2.39
(1,82)	1:148:A:ILE:HG21	1:150:A:PRO:HD2	6	2.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:83:A:ALA:HB1	1:85:A:LYS:HE3	6	2.39
(1,25)	1:144:A:ILE:HD12	1:120:A:LEU:H	7	2.39
(1,3527)	2:6:C:GLU:HG2	2:46:C:PHE:HD1	6	2.38
(1,2616)	2:51:B:VAL:HG23	2:46:B:PHE:HZ	1	2.38
(1,736)	1:114:A:ILE:HG12	1:102:A:LYS:HB3	1	2.38
(1,179)	1:120:A:LEU:HD23	1:147:A:MET:HG3	7	2.38
(1,82)	1:148:A:ILE:HG21	1:150:A:PRO:HD2	3	2.38
(1,63)	1:83:A:ALA:HB1	1:85:A:LYS:HE3	9	2.38
(1,2629)	2:37:C:MET:HB3	2:17:C:SER:HB3	9	2.37
(1,2629)	2:37:C:MET:HB3	2:17:C:SER:HB3	10	2.37
(1,2617)	2:51:C:VAL:HG23	2:46:C:PHE:HZ	3	2.37
(1,2617)	2:51:C:VAL:HG22	2:46:C:PHE:HZ	4	2.37
(1,2553)	2:35:C:VAL:HG12	2:37:C:MET:HB3	2	2.37
(1,1141)	1:82:A:GLN:H	1:80:A:LYS:HG2	6	2.37
(1,860)	1:80:A:LYS:H	1:79:A:LYS:HD3	7	2.37
(1,2699)	2:54:C:ILE:HG21	2:6:C:GLU:HG3	2	2.36
(1,1141)	1:82:A:GLN:H	1:80:A:LYS:HG2	8	2.36
(1,700)	1:79:A:LYS:HE3	1:81:A:ILE:HA	7	2.36
(1,3781)	2:13:C:VAL:HG22	2:16:C:PHE:HE2	1	2.35
(1,1629)	1:105:A:LEU:HD12	1:90:A:HIS:HE1	5	2.35
(1,1328)	1:100:A:GLN:HE21	1:99:A:LEU:HD11	6	2.35
(1,860)	1:80:A:LYS:H	1:79:A:LYS:HD3	2	2.35
(1,700)	1:79:A:LYS:HE3	1:81:A:ILE:HA	2	2.35
(1,860)	1:80:A:LYS:H	1:79:A:LYS:HD3	3	2.34
(1,708)	1:122:A:LYS:HE3	1:121:A:LEU:HD12	10	2.34
(1,3576)	2:33:B:LEU:HD22	2:19:B:ILE:HG23	2	2.33
(1,2617)	2:51:C:VAL:HG23	2:46:C:PHE:HZ	7	2.33
(1,95)	1:74:A:VAL:HG11	1:94:A:PRO:HD3	7	2.33
(1,2786)	2:20:B:VAL:HG11	2:34:B:ASN:HD22	4	2.32
(1,2158)	2:13:B:VAL:HG22	2:48:B:ARG:HD3	5	2.32
(1,860)	1:80:A:LYS:H	1:79:A:LYS:HD3	5	2.32
(1,792)	1:134:A:ASP:HB2	1:130:A:LEU:HD22	1	2.32
(1,3576)	2:33:B:LEU:HD21	2:19:B:ILE:HG22	4	2.31
(1,2552)	2:35:B:VAL:HG12	2:37:B:MET:HB3	4	2.31
(1,56)	1:114:A:ILE:HD11	1:103:A:GLN:HE21	8	2.31
(1,3576)	2:33:B:LEU:HD21	2:12:B:ILE:HG23	6	2.3
(1,3542)	2:51:B:VAL:HG21	2:49:B:GLU:HG3	2	2.3
(1,1141)	1:82:A:GLN:H	1:80:A:LYS:HG2	7	2.3
(1,698)	1:79:A:LYS:HE3	1:81:A:ILE:HG21	8	2.3
(1,63)	1:83:A:ALA:HB1	1:85:A:LYS:HE3	3	2.3
(1,157)	1:99:A:LEU:HD21	1:103:A:GLN:HE22	1	2.29
(1,2628)	2:37:B:MET:HB3	2:17:B:SER:HB3	1	2.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,860)	1:80:A:LYS:H	1:79:A:LYS:HD3	4	2.28
(1,57)	1:81:A:ILE:HD13	1:145:A:THR:HB	4	2.28
(1,3577)	2:33:C:LEU:HD23	2:19:C:ILE:HG23	7	2.27
(1,3576)	2:33:B:LEU:HD22	2:19:B:ILE:HG23	3	2.27
(1,1155)	1:137:A:VAL:H	1:137:A:VAL:HG23	5	2.27
(1,3970)	2:8:B:ILE:HD12	2:60:C:PHE:HE2	9	2.26
(1,2615)	2:13:C:VAL:HG11	2:48:C:ARG:HG2	3	2.26
(1,790)	1:126:A:LEU:HG	1:124:A:LYS:HE3	5	2.26
(1,3780)	2:13:B:VAL:HG21	2:16:B:PHE:HE2	1	2.25
(1,2645)	2:20:C:VAL:HG12	2:33:C:LEU:HD21	1	2.25
(1,2427)	2:68:C:ILE:HD11	2:60:B:PHE:HD2	2	2.25
(1,179)	1:120:A:LEU:HD22	1:147:A:MET:HG3	5	2.25
(1,157)	1:99:A:LEU:HD21	1:103:A:GLN:HE22	9	2.25
(1,2644)	2:20:B:VAL:HG11	2:33:B:LEU:HD22	1	2.24
(1,834)	1:85:A:LYS:HE3	1:82:A:GLN:HA	1	2.24
(1,3737)	2:54:C:ILE:HD12	2:13:C:VAL:HG23	5	2.23
(1,3737)	2:54:C:ILE:HD11	2:13:C:VAL:HG21	8	2.23
(1,2644)	2:20:B:VAL:HG11	2:33:B:LEU:HD22	10	2.23
(1,3934)	2:55:B:LEU:HD12	2:7:B:GLU:HG2	8	2.22
(1,3780)	2:13:B:VAL:HG23	2:16:B:PHE:HE1	8	2.22
(1,1347)	1:141:A:ASN:HD22	1:121:A:LEU:HD12	5	2.22
(1,179)	1:120:A:LEU:HD21	1:147:A:MET:HG3	8	2.22
(1,94)	1:74:A:VAL:HG11	1:94:A:PRO:HA	3	2.22
(1,82)	1:148:A:ILE:HG22	1:150:A:PRO:HD2	2	2.22
(1,3934)	2:55:B:LEU:HD12	2:7:B:GLU:HG2	2	2.21
(1,3576)	2:33:B:LEU:HD21	2:12:B:ILE:HG23	8	2.21
(1,1338)	1:99:A:LEU:HD11	1:103:A:GLN:HE21	8	2.21
(1,673)	1:81:A:ILE:HG13	1:145:A:THR:HA	2	2.21
(1,186)	1:120:A:LEU:HD23	1:120:A:LEU:H	10	2.21
(1,176)	1:132:A:LEU:HD21	1:96:A:ASP:HB2	2	2.21
(1,3741)	2:19:C:ILE:HD12	2:8:B:ILE:HG22	10	2.2
(1,3889)	2:18:C:SER:HB3	2:22:C:LYS:HD3	7	2.19
(1,3737)	2:54:C:ILE:HD11	2:13:C:VAL:HG21	2	2.19
(1,25)	1:144:A:ILE:HD12	1:120:A:LEU:H	6	2.19
(1,3577)	2:33:C:LEU:HD21	2:12:C:ILE:HG22	10	2.18
(1,2089)	2:8:C:ILE:HD11	2:19:B:ILE:HG12	1	2.18
(1,179)	1:120:A:LEU:HD21	1:147:A:MET:HG3	4	2.18
(1,179)	1:120:A:LEU:HD23	1:147:A:MET:HG3	6	2.18
(1,3781)	2:13:C:VAL:HG23	2:16:B:PHE:HE1	6	2.17
(1,860)	1:80:A:LYS:H	1:79:A:LYS:HD3	9	2.17
(1,135)	1:125:A:VAL:HG22	1:118:A:LYS:HE3	3	2.17
(1,63)	1:83:A:ALA:HB1	1:85:A:LYS:HE3	5	2.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4182)	1:120:A:LEU:HD22	2:38:B:ASP:H	6	2.16
(1,3576)	2:33:B:LEU:HD21	2:19:B:ILE:HG23	7	2.16
(1,1446)	1:97:A:THR:HG23	1:96:A:ASP:HB3	6	2.16
(1,1353)	1:121:A:LEU:HD13	1:141:A:ASN:HD21	7	2.16
(1,1172)	1:85:A:LYS:HE3	1:83:A:ALA:H	1	2.16
(1,137)	1:125:A:VAL:HG23	1:127:A:HIS:HA	5	2.16
(1,63)	1:83:A:ALA:HB1	1:85:A:LYS:HE3	10	2.16
(1,3737)	2:54:C:ILE:HD11	2:13:C:VAL:HG23	1	2.15
(1,2616)	2:51:B:VAL:HG22	2:46:B:PHE:HZ	3	2.15
(1,94)	1:74:A:VAL:HG11	1:94:A:PRO:HA	4	2.15
(1,2642)	2:25:B:ILE:HD12	2:20:B:VAL:HG13	4	2.14
(1,2617)	2:51:C:VAL:HG22	2:46:C:PHE:HZ	6	2.14
(1,2553)	2:35:C:VAL:HG12	2:37:C:MET:HB3	6	2.14
(1,1141)	1:82:A:GLN:H	1:80:A:LYS:HG2	1	2.14
(1,183)	1:99:A:LEU:HD11	1:100:A:GLN:HE22	6	2.14
(1,3737)	2:54:C:ILE:HD11	2:13:C:VAL:HG21	3	2.13
(1,2639)	2:35:C:VAL:HG22	2:37:C:MET:HB3	2	2.13
(1,2616)	2:51:B:VAL:HG23	2:46:B:PHE:HZ	5	2.13
(1,2553)	2:35:C:VAL:HG11	2:37:C:MET:HB3	4	2.13
(1,1347)	1:141:A:ASN:HD22	1:121:A:LEU:HD13	10	2.13
(1,3545)	2:51:C:VAL:HG23	2:47:C:GLU:HB2	10	2.12
(1,3182)	2:12:B:ILE:HD13	2:9:B:ALA:H	5	2.12
(1,1295)	1:129:A:ASN:H	1:97:A:THR:HB	5	2.12
(1,3781)	2:13:C:VAL:HG23	2:16:C:PHE:HE2	10	2.11
(1,2088)	2:8:B:ILE:HD11	2:19:C:ILE:HG12	9	2.11
(1,3935)	2:55:C:LEU:HD13	2:7:C:GLU:HG2	2	2.1
(1,3741)	2:25:C:ILE:HD12	2:19:C:ILE:HD11	9	2.1
(1,3736)	2:54:B:ILE:HD13	2:13:B:VAL:HG22	5	2.1
(1,3577)	2:33:C:LEU:HD23	2:19:C:ILE:HG23	3	2.1
(1,2642)	2:25:B:ILE:HD12	2:20:B:VAL:HG12	9	2.1
(1,1660)	1:125:A:VAL:HG22	1:118:A:LYS:HE3	3	2.1
(1,1446)	1:97:A:THR:HG22	1:96:A:ASP:HB3	8	2.1
(1,117)	1:125:A:VAL:HG22	1:126:A:LEU:H	5	2.1
(1,4052)	2:55:B:LEU:HD22	2:8:B:ILE:H	8	2.09
(1,3542)	2:51:B:VAL:HG21	2:13:B:VAL:HB	4	2.09
(1,2299)	2:19:C:ILE:HA	2:22:C:LYS:HD3	1	2.09
(1,1614)	1:90:A:HIS:HB2	1:76:A:LEU:HD11	7	2.09
(1,1446)	1:97:A:THR:HG22	1:96:A:ASP:HB3	1	2.09
(1,3737)	2:54:C:ILE:HD11	2:13:C:VAL:HG21	10	2.08
(1,2692)	2:50:B:ALA:HB1	2:47:B:GLU:HB2	4	2.08
(1,2063)	2:55:C:LEU:HD21	2:14:C:ASN:HB2	10	2.08
(1,94)	1:74:A:VAL:HG11	1:94:A:PRO:HA	7	2.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,57)	1:81:A:ILE:HD12	1:145:A:THR:HB	2	2.07
(1,3577)	2:33:C:LEU:HD23	2:19:C:ILE:HG23	6	2.06
(1,2628)	2:37:B:MET:HB3	2:17:B:SER:HB3	10	2.06
(1,2298)	2:19:B:ILE:HA	2:22:B:LYS:HD3	10	2.06
(1,834)	1:85:A:LYS:HE3	1:82:A:GLN:HA	10	2.06
(1,698)	1:79:A:LYS:HE3	1:81:A:ILE:HG21	4	2.06
(1,58)	1:114:A:ILE:HD11	1:99:A:LEU:HA	1	2.06
(1,2645)	2:20:C:VAL:HG12	2:33:C:LEU:HD21	10	2.05
(1,2629)	2:37:C:MET:HB3	2:17:C:SER:HB3	4	2.05
(1,157)	1:99:A:LEU:HD22	1:103:A:GLN:HE22	6	2.05
(1,2890)	2:21:B:GLU:HA	2:23:B:LYS:HE3	10	2.04
(1,2617)	2:51:C:VAL:HG23	2:46:C:PHE:HZ	5	2.04
(1,2553)	2:35:C:VAL:HG12	2:37:C:MET:HB3	3	2.04
(1,1803)	1:82:A:GLN:HE21	1:81:A:ILE:HG22	5	2.04
(1,4052)	2:55:B:LEU:HD22	2:8:B:ILE:H	2	2.03
(1,3780)	2:13:B:VAL:HG22	2:16:B:PHE:HE2	4	2.03
(1,3737)	2:54:C:ILE:HD11	2:13:C:VAL:HG21	6	2.03
(1,3736)	2:54:B:ILE:HD13	2:13:B:VAL:HG21	1	2.03
(1,3659)	2:51:C:VAL:HG22	2:46:C:PHE:HD2	9	2.03
(1,3576)	2:33:B:LEU:HD23	2:19:B:ILE:HG21	10	2.03
(1,2642)	2:25:B:ILE:HD12	2:20:B:VAL:HG12	5	2.03
(1,51)	1:88:A:ILE:HD12	1:92:A:PHE:HZ	2	2.03
(1,2644)	2:20:B:VAL:HG12	2:33:B:LEU:HD23	4	2.02
(1,2639)	2:35:C:VAL:HG22	2:37:C:MET:HB3	4	2.02
(1,2628)	2:37:B:MET:HB3	2:17:B:SER:HB3	4	2.02
(1,786)	1:126:A:LEU:HD11	1:124:A:LYS:HD3	8	2.02
(1,3888)	2:18:B:SER:HB3	2:22:B:LYS:HG2	1	2.01
(1,2298)	2:19:B:ILE:HA	2:22:B:LYS:HD3	9	2.01
(1,1820)	1:151:A:ASN:HD21	1:152:A:LEU:HD13	5	2.01
(1,56)	1:114:A:ILE:HD11	1:103:A:GLN:HE21	3	2.01
(1,4052)	2:55:B:LEU:HD22	2:8:B:ILE:H	6	2.0
(1,2882)	2:13:B:VAL:HG13	2:41:B:SER:HB3	7	2.0
(1,2642)	2:25:B:ILE:HD13	2:20:B:VAL:HG11	8	2.0
(1,176)	1:132:A:LEU:HD22	1:96:A:ASP:HB2	5	2.0
(1,3670)	2:3:B:ALA:HB2	2:60:C:PHE:HD1	5	1.99
(1,3577)	2:33:C:LEU:HD21	2:19:C:ILE:HG21	1	1.99
(1,2639)	2:35:C:VAL:HG22	2:37:C:MET:HB3	6	1.99
(1,1347)	1:141:A:ASN:HD22	1:121:A:LEU:HD13	1	1.99
(1,3543)	2:51:C:VAL:HG23	2:13:C:VAL:HB	7	1.98
(1,2643)	2:25:C:ILE:HD11	2:20:C:VAL:HG13	8	1.98
(1,94)	1:74:A:VAL:HG11	1:94:A:PRO:HA	10	1.98
(1,57)	1:81:A:ILE:HD11	1:145:A:THR:HB	8	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3736)	2:54:B:ILE:HD13	2:13:B:VAL:HG21	7	1.97
(1,3736)	2:54:B:ILE:HD13	2:13:B:VAL:HG22	10	1.97
(1,3312)	2:26:B:SER:H	2:44:C:PHE:HD1	7	1.97
(1,2389)	2:20:C:VAL:HG22	2:34:C:ASN:HD22	7	1.97
(1,2062)	2:55:B:LEU:HD22	2:14:B:ASN:HB2	1	1.97
(1,1347)	1:141:A:ASN:HD22	1:121:A:LEU:HD13	8	1.97
(1,790)	1:126:A:LEU:HG	1:124:A:LYS:HE3	2	1.97
(1,708)	1:122:A:LYS:HE3	1:121:A:LEU:HD13	3	1.97
(1,702)	1:122:A:LYS:HE3	1:122:A:LYS:H	9	1.97
(1,73)	1:88:A:ILE:HG22	1:90:A:HIS:HE1	8	1.97
(1,3934)	2:55:B:LEU:HD13	2:7:B:GLU:HG2	5	1.96
(1,3740)	2:19:B:ILE:HD12	2:8:C:ILE:HG21	9	1.96
(1,3313)	2:26:C:SER:H	2:44:B:PHE:HD1	3	1.96
(1,2298)	2:19:B:ILE:HA	2:22:B:LYS:HD3	1	1.96
(1,1467)	1:145:A:THR:HG22	1:141:A:ASN:HD21	10	1.96
(1,1446)	1:97:A:THR:HG22	1:96:A:ASP:HB3	9	1.96
(1,834)	1:85:A:LYS:HE3	1:82:A:GLN:HA	7	1.96
(1,790)	1:126:A:LEU:HG	1:124:A:LYS:HE3	6	1.96
(1,94)	1:74:A:VAL:HG11	1:94:A:PRO:HA	9	1.96
(1,4052)	2:55:B:LEU:HD21	2:8:B:ILE:H	7	1.95
(1,3736)	2:54:B:ILE:HD12	2:13:B:VAL:HG23	2	1.95
(1,3684)	2:12:B:ILE:HD12	2:15:C:TYR:HD1	6	1.95
(1,2063)	2:55:C:LEU:HD22	2:14:C:ASN:HB2	4	1.95
(1,1809)	1:103:A:GLN:HE22	1:114:A:ILE:HG23	8	1.95
(1,1347)	1:141:A:ASN:HD22	1:121:A:LEU:HD13	6	1.95
(1,82)	1:148:A:ILE:HG21	1:150:A:PRO:HD2	8	1.95
(1,3781)	2:13:C:VAL:HG23	2:16:C:PHE:HE2	3	1.94
(1,2546)	2:20:B:VAL:HG21	2:30:B:ALA:HB3	10	1.93
(1,1172)	1:85:A:LYS:HE3	1:83:A:ALA:H	7	1.93
(1,1123)	1:87:A:SER:H	1:79:A:LYS:HD3	8	1.93
(1,698)	1:79:A:LYS:HE3	1:81:A:ILE:HG21	10	1.93
(1,642)	1:97:A:THR:HG21	1:100:A:GLN:HG3	2	1.93
(1,52)	1:81:A:ILE:HD11	1:81:A:ILE:H	3	1.93
(1,4181)	1:120:A:LEU:HD12	2:31:B:ASP:H	4	1.92
(1,3736)	2:54:B:ILE:HD13	2:13:B:VAL:HG22	9	1.92
(1,3576)	2:33:B:LEU:HD22	2:19:B:ILE:HG21	1	1.92
(1,2084)	2:25:B:ILE:HD13	2:25:B:ILE:HG22	2	1.92
(1,1423)	1:119:A:LEU:HD22	1:117:A:ILE:HB	5	1.92
(1,8)	1:120:A:LEU:HD12	1:147:A:MET:HG3	6	1.92
(1,3874)	2:15:B:TYR:HA	2:12:C:ILE:HD13	9	1.91
(1,3577)	2:33:C:LEU:HD22	2:19:C:ILE:HG21	5	1.91
(1,3542)	2:51:B:VAL:HG22	2:13:B:VAL:HB	7	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2643)	2:25:C:ILE:HD11	2:20:C:VAL:HG13	9	1.91
(1,1614)	1:150:A:PRO:HB2	1:152:A:LEU:HD12	6	1.91
(1,1448)	1:78:A:LEU:HD13	1:90:A:HIS:HE1	7	1.91
(1,860)	1:80:A:LYS:H	1:79:A:LYS:HD3	1	1.91
(1,705)	1:122:A:LYS:HE3	1:122:A:LYS:HB3	9	1.91
(1,48)	1:88:A:ILE:HD12	1:90:A:HIS:HE1	10	1.91
(1,3737)	2:54:C:ILE:HD12	2:13:C:VAL:HG21	4	1.9
(1,3543)	2:51:C:VAL:HG23	2:13:C:VAL:HB	1	1.9
(1,2644)	2:20:B:VAL:HG11	2:33:B:LEU:HD22	9	1.9
(1,2089)	2:8:C:ILE:HD11	2:19:B:ILE:HG12	4	1.9
(1,2089)	2:8:C:ILE:HD11	2:19:B:ILE:HG12	10	1.9
(1,1446)	1:97:A:THR:HG22	1:96:A:ASP:HB3	2	1.9
(1,1446)	1:97:A:THR:HG21	1:100:A:GLN:HG3	5	1.9
(1,150)	1:78:A:LEU:HD11	1:92:A:PHE:HZ	2	1.9
(1,4182)	1:120:A:LEU:HD23	2:38:C:ASP:H	1	1.89
(1,4053)	2:55:C:LEU:HD21	2:8:C:ILE:H	8	1.89
(1,3740)	2:19:B:ILE:HD12	2:8:C:ILE:HG21	1	1.89
(1,2639)	2:35:C:VAL:HG22	2:37:C:MET:HB3	3	1.89
(1,2638)	2:35:B:VAL:HG21	2:37:B:MET:HB3	4	1.89
(1,1810)	1:99:A:LEU:HG	1:103:A:GLN:HE21	8	1.89
(1,1351)	1:141:A:ASN:HD21	1:121:A:LEU:HG	5	1.89
(1,1198)	1:113:A:HIS:H	1:116:A:GLU:HB3	9	1.89
(1,736)	1:114:A:ILE:HG12	1:102:A:LYS:HB3	3	1.89
(1,3736)	2:54:B:ILE:HD13	2:13:B:VAL:HG21	6	1.88
(1,2698)	2:54:B:ILE:HG22	2:6:B:GLU:HG3	6	1.88
(1,229)	1:118:A:LYS:HB2	1:118:A:LYS:HE3	5	1.88
(1,150)	1:78:A:LEU:HD13	1:92:A:PHE:HZ	5	1.88
(1,117)	1:125:A:VAL:HG22	1:126:A:LEU:H	1	1.88
(1,3780)	2:13:B:VAL:HG23	2:16:B:PHE:HE2	2	1.87
(1,3545)	2:51:C:VAL:HG22	2:47:C:GLU:HB2	9	1.87
(1,2699)	2:54:C:ILE:HG22	2:6:C:GLU:HG3	4	1.87
(1,2644)	2:20:B:VAL:HG13	2:33:B:LEU:HD21	6	1.87
(1,2643)	2:25:C:ILE:HD11	2:20:C:VAL:HG13	4	1.87
(1,1328)	1:100:A:GLN:HE21	1:99:A:LEU:HD11	4	1.87
(1,834)	1:85:A:LYS:HE3	1:82:A:GLN:HA	3	1.87
(1,8)	1:120:A:LEU:HD12	1:147:A:MET:HG3	7	1.87
(1,2299)	2:19:C:ILE:HA	2:22:C:LYS:HD3	10	1.86
(1,2088)	2:8:B:ILE:HD11	2:19:C:ILE:HG12	1	1.86
(1,686)	1:122:A:LYS:HA	1:122:A:LYS:HD3	9	1.86
(1,662)	1:119:A:LEU:HA	1:119:A:LEU:HD13	5	1.86
(1,52)	1:81:A:ILE:HD13	1:81:A:ILE:H	4	1.86
(1,3781)	2:13:C:VAL:HG23	2:16:B:PHE:HE1	4	1.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3737)	2:54:C:ILE:HD11	2:13:C:VAL:HG21	7	1.85
(1,2615)	2:13:C:VAL:HG11	2:48:C:ARG:HG2	8	1.85
(1,52)	1:81:A:ILE:HD12	1:81:A:ILE:H	5	1.85
(1,3781)	2:13:C:VAL:HG23	2:16:C:PHE:HE2	2	1.84
(1,3572)	2:33:B:LEU:HD23	2:19:B:ILE:HB	4	1.84
(1,3545)	2:51:C:VAL:HG23	2:48:C:ARG:HB3	3	1.84
(1,2546)	2:20:B:VAL:HG21	2:30:B:ALA:HB3	5	1.84
(1,135)	1:125:A:VAL:HG22	1:118:A:LYS:HE3	7	1.84
(1,4182)	1:120:A:LEU:HD21	2:31:B:ASP:H	5	1.83
(1,3781)	2:13:C:VAL:HG23	2:16:C:PHE:HE2	7	1.83
(1,3627)	2:41:C:SER:HB3	2:9:C:ALA:HB3	4	1.83
(1,3576)	2:33:B:LEU:HD23	2:19:B:ILE:HG21	5	1.83
(1,3572)	2:33:B:LEU:HD21	2:19:B:ILE:HB	6	1.83
(1,179)	1:120:A:LEU:HD23	1:147:A:MET:HG3	3	1.83
(1,135)	1:125:A:VAL:HG22	1:118:A:LYS:HE3	9	1.83
(1,3572)	2:33:B:LEU:HD21	2:19:B:ILE:HB	2	1.82
(1,2883)	2:13:C:VAL:HG12	2:41:C:SER:HB3	4	1.82
(1,2614)	2:13:B:VAL:HG12	2:48:B:ARG:HG2	5	1.82
(1,1356)	1:151:A:ASN:HA	1:151:A:ASN:HD22	10	1.82
(1,732)	1:81:A:ILE:HA	1:79:A:LYS:HD3	7	1.82
(1,3671)	2:3:C:ALA:HB3	2:60:B:PHE:HD1	1	1.81
(1,2799)	2:48:C:ARG:HA	2:51:C:VAL:HG11	9	1.81
(1,2617)	2:51:C:VAL:HG23	2:46:C:PHE:HZ	8	1.81
(1,2546)	2:20:B:VAL:HG21	2:30:B:ALA:HB3	9	1.81
(1,2063)	2:55:C:LEU:HD21	2:14:C:ASN:HB2	5	1.81
(1,8)	1:120:A:LEU:HD12	1:147:A:MET:HG3	8	1.81
(1,4053)	2:55:C:LEU:HD23	2:8:C:ILE:H	2	1.8
(1,2786)	2:20:B:VAL:HG12	2:34:B:ASN:HD22	6	1.8
(1,2698)	2:54:B:ILE:HG23	2:6:B:GLU:HG3	10	1.8
(1,2158)	2:13:B:VAL:HG21	2:48:B:ARG:HD3	6	1.8
(1,1457)	1:120:A:LEU:HD21	1:118:A:LYS:HE3	9	1.8
(1,1172)	1:85:A:LYS:HE3	1:83:A:ALA:H	10	1.8
(1,142)	1:140:A:ALA:HB3	1:141:A:ASN:HD22	2	1.8
(1,3781)	2:13:C:VAL:HG22	2:16:C:PHE:HE2	9	1.79
(1,3740)	2:19:B:ILE:HD13	2:8:C:ILE:HG21	7	1.79
(1,3525)	2:6:C:GLU:HG3	2:46:C:PHE:HD2	6	1.79
(1,2757)	2:7:C:GLU:HA	2:55:C:LEU:HD21	9	1.79
(1,1651)	1:88:A:ILE:HG22	1:89:A:GLU:HG3	2	1.79
(1,1570)	1:139:A:PRO:HA	1:137:A:VAL:HG22	10	1.79
(1,1356)	1:151:A:ASN:HA	1:151:A:ASN:HD22	3	1.79
(1,571)	1:93:A:SER:HB3	1:96:A:ASP:HB3	7	1.79
(1,231)	1:149:A:LYS:HB3	1:149:A:LYS:HE3	8	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:74:A:VAL:HG11	1:94:A:PRO:HA	1	1.79
(1,3626)	2:41:B:SER:HB3	2:9:B:ALA:HB1	3	1.78
(1,2617)	2:51:C:VAL:HG23	2:46:C:PHE:HZ	2	1.78
(1,2553)	2:35:C:VAL:HG12	2:37:C:MET:HB3	1	1.78
(1,2298)	2:19:B:ILE:HA	2:22:B:LYS:HD3	4	1.78
(1,1660)	1:125:A:VAL:HG22	1:118:A:LYS:HE3	7	1.78
(1,1356)	1:151:A:ASN:HA	1:151:A:ASN:HD22	6	1.78
(1,834)	1:85:A:LYS:HE3	1:82:A:GLN:HA	9	1.78
(1,48)	1:88:A:ILE:HD12	1:90:A:HIS:HE1	3	1.78
(1,4053)	2:55:C:LEU:HD23	2:8:C:ILE:H	3	1.77
(1,2159)	2:13:C:VAL:HG21	2:48:C:ARG:HD3	10	1.77
(1,1660)	1:125:A:VAL:HG22	1:118:A:LYS:HE3	9	1.77
(1,4182)	1:120:A:LEU:HD23	2:38:B:ASP:H	9	1.76
(1,3971)	2:8:C:ILE:HD12	2:60:B:PHE:HE2	9	1.76
(1,3733)	2:12:C:ILE:HD13	2:40:C:ILE:HD13	6	1.76
(1,3682)	2:12:B:ILE:HD12	2:16:C:PHE:HD1	10	1.76
(1,3627)	2:41:C:SER:HB3	2:9:C:ALA:HB2	7	1.76
(1,2891)	2:21:C:GLU:HA	2:23:C:LYS:HE3	9	1.76
(1,1338)	1:99:A:LEU:HD13	1:103:A:GLN:HE21	5	1.76
(1,8)	1:120:A:LEU:HD12	1:147:A:MET:HG3	4	1.76
(1,3780)	2:13:B:VAL:HG21	2:16:B:PHE:HE2	10	1.75
(1,3741)	2:19:C:ILE:HD12	2:8:B:ILE:HG22	6	1.75
(1,3621)	2:40:C:ILE:HA	2:36:B:ALA:HB3	2	1.75
(1,2617)	2:51:C:VAL:HG23	2:46:C:PHE:HZ	1	1.75
(1,116)	1:125:A:VAL:HG22	1:120:A:LEU:H	5	1.75
(1,52)	1:81:A:ILE:HD12	1:81:A:ILE:H	10	1.75
(1,3740)	2:25:B:ILE:HD13	2:19:B:ILE:HD11	5	1.74
(1,3543)	2:51:C:VAL:HG21	2:13:C:VAL:HB	8	1.74
(1,3525)	2:6:C:GLU:HG3	2:46:C:PHE:HD1	2	1.74
(1,2883)	2:13:C:VAL:HG11	2:41:C:SER:HB3	7	1.74
(1,2616)	2:51:B:VAL:HG23	2:46:B:PHE:HZ	9	1.74
(1,2387)	2:51:C:VAL:HG11	2:46:C:PHE:HE2	9	1.74
(1,1570)	1:139:A:PRO:HA	1:137:A:VAL:HG22	4	1.74
(1,1557)	1:81:A:ILE:HA	1:85:A:LYS:HD3	10	1.74
(1,1198)	1:113:A:HIS:H	1:116:A:GLU:HB3	4	1.74
(1,700)	1:79:A:LYS:HE3	1:81:A:ILE:HA	10	1.74
(1,162)	1:78:A:LEU:HD21	1:92:A:PHE:HZ	2	1.74
(1,3573)	2:33:C:LEU:HD21	2:19:C:ILE:HB	10	1.73
(1,1614)	1:150:A:PRO:HB2	1:152:A:LEU:HD12	1	1.73
(1,157)	1:99:A:LEU:HD22	1:103:A:GLN:HE22	7	1.73
(1,898)	1:85:A:LYS:HB3	1:86:A:PHE:H	8	1.72
(1,177)	1:132:A:LEU:HD23	1:97:A:THR:HA	5	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,162)	1:78:A:LEU:HD23	1:92:A:PHE:HZ	5	1.72
(1,4183)	1:120:A:LEU:HD13	2:35:B:VAL:H	10	1.71
(1,4180)	1:147:A:MET:HE3	2:38:B:ASP:H	2	1.71
(1,3572)	2:33:B:LEU:HD22	2:19:B:ILE:HB	10	1.71
(1,3542)	2:51:B:VAL:HG22	2:13:B:VAL:HB	6	1.71
(1,2645)	2:20:C:VAL:HG12	2:33:C:LEU:HD22	4	1.71
(1,2127)	2:54:C:ILE:HB	2:13:C:VAL:HG22	9	1.71
(1,2064)	2:55:B:LEU:HD22	2:51:B:VAL:HB	1	1.71
(1,2060)	2:55:B:LEU:HD22	2:14:B:ASN:H	1	1.71
(1,1651)	1:88:A:ILE:HG23	1:78:A:LEU:HB3	9	1.71
(1,834)	1:85:A:LYS:HE3	1:82:A:GLN:HA	2	1.71
(1,4182)	1:120:A:LEU:HD22	2:31:B:ASP:H	3	1.7
(1,4181)	1:120:A:LEU:HD11	2:31:B:ASP:H	2	1.7
(1,4090)	2:16:B:PHE:H	2:12:C:ILE:HD13	9	1.7
(1,3733)	2:12:C:ILE:HD11	2:40:C:ILE:HD11	9	1.7
(1,2088)	2:8:B:ILE:HD12	2:19:C:ILE:HG12	3	1.7
(1,1448)	1:78:A:LEU:HD13	1:90:A:HIS:HE1	1	1.7
(1,1123)	1:87:A:SER:H	1:79:A:LYS:HD3	3	1.7
(1,229)	1:118:A:LYS:HB2	1:118:A:LYS:HE3	8	1.7
(1,157)	1:99:A:LEU:HD23	1:103:A:GLN:HE22	4	1.7
(1,156)	1:99:A:LEU:HD22	1:103:A:GLN:HE21	8	1.7
(1,4179)	1:147:A:MET:HE1	2:35:B:VAL:H	5	1.69
(1,3573)	2:33:C:LEU:HD21	2:19:C:ILE:HB	1	1.69
(1,3573)	2:33:C:LEU:HD22	2:19:C:ILE:HB	4	1.69
(1,3543)	2:51:C:VAL:HG23	2:13:C:VAL:HB	4	1.69
(1,1328)	1:100:A:GLN:HE21	1:99:A:LEU:HD11	8	1.69
(1,700)	1:79:A:LYS:HE3	1:81:A:ILE:HA	8	1.69
(1,3780)	2:13:B:VAL:HG21	2:16:B:PHE:HE2	9	1.68
(1,3741)	2:19:C:ILE:HD12	2:8:B:ILE:HG22	7	1.68
(1,3718)	2:54:B:ILE:HG21	2:13:B:VAL:HG22	4	1.68
(1,3626)	2:41:B:SER:HB3	2:9:B:ALA:HB3	5	1.68
(1,3626)	2:41:B:SER:HB3	2:43:B:ALA:HB2	7	1.68
(1,2890)	2:21:B:GLU:HA	2:23:B:LYS:HE3	5	1.68
(1,2159)	2:13:C:VAL:HG21	2:48:C:ARG:HD3	8	1.68
(1,2089)	2:8:C:ILE:HD13	2:19:B:ILE:HG12	6	1.68
(1,53)	1:114:A:ILE:HD13	1:103:A:GLN:H	1	1.68
(1,4053)	2:55:C:LEU:HD23	2:8:C:ILE:H	7	1.67
(1,3736)	2:54:B:ILE:HD13	2:13:B:VAL:HG23	3	1.67
(1,3730)	2:12:B:ILE:HD11	2:13:B:VAL:HG13	5	1.67
(1,3572)	2:33:B:LEU:HD21	2:19:B:ILE:HB	3	1.67
(1,3545)	2:51:C:VAL:HG23	2:48:C:ARG:HB3	8	1.67
(1,2534)	2:36:B:ALA:HB1	2:40:C:ILE:HG13	4	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1021)	1:103:A:GLN:HG3	1:103:A:GLN:H	5	1.67
(1,3874)	2:15:B:TYR:HA	2:12:C:ILE:HD12	6	1.66
(1,3572)	2:33:B:LEU:HD21	2:19:B:ILE:HB	7	1.66
(1,2891)	2:21:C:GLU:HA	2:23:C:LYS:HE3	10	1.66
(1,2547)	2:20:C:VAL:HG22	2:30:C:ALA:HB3	7	1.66
(1,1820)	1:129:A:ASN:HD21	1:130:A:LEU:HD21	2	1.66
(1,1557)	1:81:A:ILE:HA	1:85:A:LYS:HD3	4	1.66
(1,52)	1:81:A:ILE:HD12	1:81:A:ILE:H	1	1.66
(1,3745)	2:40:C:ILE:HD11	2:36:C:ALA:HB3	7	1.65
(1,3573)	2:33:C:LEU:HD22	2:19:C:ILE:HB	6	1.65
(1,2890)	2:21:B:GLU:HA	2:23:B:LYS:HE3	1	1.65
(1,2547)	2:20:C:VAL:HG23	2:30:C:ALA:HB1	4	1.65
(1,1651)	1:88:A:ILE:HG21	1:89:A:GLU:HG3	4	1.65
(1,1356)	1:151:A:ASN:HA	1:151:A:ASN:HD22	4	1.65
(1,135)	1:125:A:VAL:HG21	1:118:A:LYS:HE3	10	1.65
(1,4187)	1:81:A:ILE:HG23	2:39:B:CYS:H	4	1.64
(1,4187)	1:81:A:ILE:HG23	2:39:B:CYS:H	8	1.64
(1,3736)	2:54:B:ILE:HD13	2:13:B:VAL:HG21	8	1.64
(1,3543)	2:51:C:VAL:HG21	2:13:C:VAL:HB	3	1.64
(1,2082)	2:25:B:ILE:HD13	2:19:B:ILE:HG23	2	1.64
(1,834)	1:85:A:LYS:HE3	1:82:A:GLN:HA	6	1.64
(1,707)	1:122:A:LYS:HE3	1:143:A:THR:HG21	6	1.64
(1,4053)	2:55:C:LEU:HD11	2:50:C:ALA:H	9	1.63
(1,4014)	2:60:B:PHE:HD1	2:8:B:ILE:HD13	10	1.63
(1,1347)	1:141:A:ASN:HD22	1:121:A:LEU:HD13	3	1.63
(1,732)	1:81:A:ILE:HA	1:79:A:LYS:HD3	2	1.63
(1,157)	1:99:A:LEU:HD22	1:103:A:GLN:HE22	10	1.63
(1,150)	1:78:A:LEU:HD13	1:92:A:PHE:HZ	6	1.63
(1,56)	1:114:A:ILE:HD11	1:103:A:GLN:HE21	9	1.63
(1,4187)	1:81:A:ILE:HG21	2:39:B:CYS:H	2	1.62
(1,2547)	2:20:C:VAL:HG21	2:30:C:ALA:HB3	5	1.62
(1,2547)	2:20:C:VAL:HG21	2:30:C:ALA:HB3	10	1.62
(1,1651)	1:88:A:ILE:HG21	1:89:A:GLU:HG3	5	1.62
(1,1434)	1:83:A:ALA:HB2	1:84:A:PRO:HG2	3	1.62
(1,1356)	1:151:A:ASN:HA	1:151:A:ASN:HD22	7	1.62
(1,1198)	1:113:A:HIS:H	1:116:A:GLU:HB3	7	1.62
(1,720)	1:148:A:ILE:HD13	1:86:A:PHE:HZ	9	1.62
(1,630)	1:78:A:LEU:HB2	1:146:A:VAL:HG22	2	1.62
(1,4081)	2:13:C:VAL:H	2:41:C:SER:HA	7	1.61
(1,3557)	2:25:C:ILE:HD12	2:5:B:LYS:HD2	4	1.61
(1,2644)	2:20:B:VAL:HG13	2:33:B:LEU:HD21	8	1.61
(1,2178)	2:9:B:ALA:HA	2:12:B:ILE:HD13	5	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2061)	2:55:C:LEU:HD21	2:14:C:ASN:H	10	1.61
(1,1570)	1:139:A:PRO:HA	1:137:A:VAL:HG22	6	1.61
(1,786)	1:126:A:LEU:HD11	1:124:A:LYS:HD3	6	1.61
(1,3731)	2:12:C:ILE:HD13	2:13:C:VAL:HG12	6	1.6
(1,3683)	2:12:C:ILE:HD12	2:16:C:PHE:HD1	9	1.6
(1,3621)	2:40:C:ILE:HA	2:36:B:ALA:HB2	4	1.6
(1,2547)	2:20:C:VAL:HG22	2:30:C:ALA:HB3	8	1.6
(1,2546)	2:20:B:VAL:HG22	2:30:B:ALA:HB3	4	1.6
(1,717)	1:120:A:LEU:HG	1:125:A:VAL:HA	1	1.6
(1,4187)	1:81:A:ILE:HG22	2:39:B:CYS:H	9	1.59
(1,4180)	1:147:A:MET:HE1	2:38:C:ASP:H	3	1.59
(1,4053)	2:55:C:LEU:HD23	2:8:C:ILE:H	6	1.59
(1,4015)	2:60:C:PHE:HD1	2:8:C:ILE:HD13	1	1.59
(1,3621)	2:40:C:ILE:HA	2:36:B:ALA:HB1	7	1.59
(1,2644)	2:20:B:VAL:HG13	2:33:B:LEU:HD21	7	1.59
(1,2088)	2:8:B:ILE:HD12	2:19:C:ILE:HG12	8	1.59
(1,1660)	1:125:A:VAL:HG21	1:118:A:LYS:HE3	10	1.59
(1,1172)	1:85:A:LYS:HE3	1:83:A:ALA:H	9	1.59
(1,707)	1:122:A:LYS:HE3	1:143:A:THR:HG21	8	1.59
(1,135)	1:125:A:VAL:HG21	1:118:A:LYS:HE3	4	1.59
(1,135)	1:125:A:VAL:HG22	1:118:A:LYS:HE3	6	1.59
(1,3740)	2:19:B:ILE:HD13	2:8:C:ILE:HG21	8	1.58
(1,3739)	2:68:C:ILE:HD11	2:11:B:LEU:HD23	2	1.58
(1,3733)	2:12:C:ILE:HD13	2:40:C:ILE:HG23	8	1.58
(1,3626)	2:41:B:SER:HB3	2:9:B:ALA:HB1	4	1.58
(1,2643)	2:25:C:ILE:HD11	2:20:C:VAL:HG13	5	1.58
(1,2309)	2:52:C:SER:HA	2:55:C:LEU:HD13	9	1.58
(1,1557)	1:81:A:ILE:HA	1:85:A:LYS:HD3	3	1.58
(1,1449)	1:78:A:LEU:HD12	1:90:A:HIS:H	2	1.58
(1,1448)	1:78:A:LEU:HD13	1:90:A:HIS:HE1	5	1.58
(1,52)	1:81:A:ILE:HD12	1:81:A:ILE:H	7	1.58
(1,52)	1:81:A:ILE:HD11	1:81:A:ILE:H	8	1.58
(1,2883)	2:13:C:VAL:HG11	2:41:C:SER:HB3	3	1.57
(1,2159)	2:13:C:VAL:HG23	2:48:C:ARG:HD3	5	1.57
(1,1328)	1:100:A:GLN:HE21	1:99:A:LEU:HD11	7	1.57
(1,1172)	1:85:A:LYS:HE3	1:83:A:ALA:H	3	1.57
(1,804)	1:121:A:LEU:HD21	1:141:A:ASN:HD21	6	1.57
(1,786)	1:126:A:LEU:HD11	1:124:A:LYS:HD3	2	1.57
(1,700)	1:79:A:LYS:HE3	1:81:A:ILE:HA	4	1.57
(1,52)	1:81:A:ILE:HD12	1:81:A:ILE:H	9	1.57
(1,48)	1:88:A:ILE:HD12	1:90:A:HIS:HE1	8	1.57
(1,3577)	2:33:C:LEU:HD23	2:19:C:ILE:HG21	4	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3554)	2:25:B:ILE:HD13	2:19:B:ILE:HB	4	1.56
(1,2695)	2:54:C:ILE:HG21	2:46:C:PHE:HB2	2	1.56
(1,2643)	2:25:C:ILE:HD11	2:20:C:VAL:HG13	6	1.56
(1,2546)	2:20:B:VAL:HG21	2:30:B:ALA:HB3	1	1.56
(1,1593)	1:142:A:SER:HB2	1:137:A:VAL:HB	9	1.56
(1,1449)	1:78:A:LEU:HD11	1:90:A:HIS:H	7	1.56
(1,1446)	1:97:A:THR:HG22	1:96:A:ASP:HB3	7	1.56
(1,1356)	1:151:A:ASN:HA	1:151:A:ASN:HD22	2	1.56
(1,785)	1:122:A:LYS:HD3	1:121:A:LEU:HD12	10	1.56
(1,57)	1:81:A:ILE:HD12	1:145:A:THR:HB	9	1.56
(1,4181)	1:120:A:LEU:HD12	2:31:B:ASP:H	3	1.55
(1,3935)	2:55:C:LEU:HD11	2:7:C:GLU:HG2	9	1.55
(1,3731)	2:12:C:ILE:HD13	2:13:C:VAL:HG12	7	1.55
(1,3572)	2:33:B:LEU:HD21	2:19:B:ILE:HB	8	1.55
(1,3553)	2:25:C:ILE:HD12	2:24:C:GLU:HB3	5	1.55
(1,3543)	2:51:C:VAL:HG22	2:13:C:VAL:HB	6	1.55
(1,3049)	2:50:C:ALA:H	2:13:C:VAL:HG13	1	1.55
(1,2089)	2:8:C:ILE:HD13	2:19:B:ILE:HG12	8	1.55
(1,94)	1:74:A:VAL:HG11	1:94:A:PRO:HA	6	1.55
(1,5)	1:119:A:LEU:HD22	1:102:A:LYS:H	5	1.55
(1,4014)	2:60:B:PHE:HD1	2:68:C:ILE:HD12	9	1.54
(1,3781)	2:13:C:VAL:HG22	2:16:C:PHE:HE2	5	1.54
(1,3741)	2:25:C:ILE:HD12	2:19:C:ILE:HD11	1	1.54
(1,3740)	2:19:B:ILE:HD13	2:8:C:ILE:HG23	3	1.54
(1,3673)	2:12:C:ILE:HG23	2:11:C:LEU:H	4	1.54
(1,3576)	2:33:B:LEU:HD23	2:19:B:ILE:HG21	9	1.54
(1,2721)	2:54:C:ILE:HD11	2:6:C:GLU:HG3	4	1.54
(1,2158)	2:13:B:VAL:HG22	2:48:B:ARG:HD3	10	1.54
(1,2063)	2:55:C:LEU:HD23	2:14:C:ASN:HB2	6	1.54
(1,186)	1:120:A:LEU:HD22	1:120:A:LEU:H	1	1.54
(1,185)	1:130:A:LEU:HD22	1:131:A:PHE:H	2	1.54
(1,150)	1:78:A:LEU:HD13	1:92:A:PHE:HZ	7	1.54
(1,94)	1:74:A:VAL:HG11	1:94:A:PRO:HA	8	1.54
(1,3935)	2:55:C:LEU:HD12	2:7:C:GLU:HG2	7	1.53
(1,3626)	2:41:B:SER:HB3	2:9:B:ALA:HB3	9	1.53
(1,3555)	2:25:C:ILE:HD12	2:19:C:ILE:HB	7	1.53
(1,3552)	2:25:B:ILE:HD13	2:24:B:GLU:HB3	9	1.53
(1,3542)	2:51:B:VAL:HG21	2:13:B:VAL:HB	8	1.53
(1,2643)	2:25:C:ILE:HD11	2:20:C:VAL:HG13	7	1.53
(1,2640)	2:33:B:LEU:HD11	2:20:B:VAL:HG11	10	1.53
(1,2159)	2:13:C:VAL:HG21	2:48:C:ARG:HD3	3	1.53
(1,2159)	2:13:C:VAL:HG23	2:48:C:ARG:HD3	9	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1660)	1:125:A:VAL:HG21	1:118:A:LYS:HE3	4	1.53
(1,1660)	1:125:A:VAL:HG22	1:118:A:LYS:HE3	6	1.53
(1,1570)	1:139:A:PRO:HA	1:137:A:VAL:HG22	9	1.53
(1,1356)	1:151:A:ASN:HA	1:151:A:ASN:HD22	8	1.53
(1,1172)	1:85:A:LYS:HE3	1:83:A:ALA:H	6	1.53
(1,732)	1:81:A:ILE:HA	1:79:A:LYS:HD3	4	1.53
(1,4181)	1:120:A:LEU:HD11	2:38:C:ASP:H	7	1.52
(1,4052)	2:55:B:LEU:HD21	2:8:B:ILE:H	3	1.52
(1,3935)	2:55:C:LEU:HD12	2:7:C:GLU:HG2	3	1.52
(1,3740)	2:19:B:ILE:HD12	2:8:C:ILE:HG21	10	1.52
(1,3684)	2:12:B:ILE:HD12	2:15:C:TYR:HD1	7	1.52
(1,2158)	2:13:B:VAL:HG21	2:48:B:ARG:HD3	2	1.52
(1,2082)	2:25:B:ILE:HD11	2:19:B:ILE:HG23	3	1.52
(1,1351)	1:141:A:ASN:HD21	1:121:A:LEU:HG	4	1.52
(1,4182)	1:120:A:LEU:HD23	2:38:B:ASP:H	8	1.51
(1,2114)	2:13:B:VAL:HG23	2:48:B:ARG:HG2	9	1.51
(1,1651)	1:88:A:ILE:HG23	1:78:A:LEU:HB3	8	1.51
(1,1172)	1:85:A:LYS:HE3	1:83:A:ALA:H	8	1.51
(1,630)	1:78:A:LEU:HB2	1:146:A:VAL:HG22	4	1.51
(1,57)	1:81:A:ILE:HD12	1:145:A:THR:HB	7	1.51
(1,25)	1:144:A:ILE:HD12	1:120:A:LEU:H	10	1.51
(1,3741)	2:19:C:ILE:HD12	2:8:B:ILE:HG22	3	1.5
(1,2891)	2:21:C:GLU:HA	2:23:C:LYS:HE3	1	1.5
(1,1670)	1:136:A:LYS:HA	1:136:A:LYS:HE3	2	1.5
(1,1123)	1:87:A:SER:H	1:79:A:LYS:HD3	1	1.5
(1,698)	1:79:A:LYS:HE3	1:81:A:ILE:HG21	3	1.5
(1,630)	1:78:A:LEU:HB2	1:146:A:VAL:HG22	6	1.5
(1,25)	1:144:A:ILE:HD11	1:120:A:LEU:H	2	1.5
(1,4187)	1:81:A:ILE:HG23	2:39:B:CYS:H	3	1.49
(1,3935)	2:55:C:LEU:HD12	2:7:C:GLU:HG2	8	1.49
(1,3831)	2:40:C:ILE:HD13	2:13:C:VAL:HB	2	1.49
(1,3627)	2:41:C:SER:HB3	2:9:C:ALA:HB2	5	1.49
(1,2243)	2:11:C:LEU:HA	2:54:C:ILE:HB	9	1.49
(1,1467)	1:145:A:THR:HG23	1:82:A:GLN:HE22	7	1.49
(1,1434)	1:83:A:ALA:HB2	1:84:A:PRO:HG2	5	1.49
(1,1353)	1:121:A:LEU:HD13	1:141:A:ASN:HD21	1	1.49
(1,610)	1:108:A:GLU:HG3	1:107:A:SER:HB3	3	1.49
(1,3935)	2:55:C:LEU:HD13	2:7:C:GLU:HG2	6	1.48
(1,3673)	2:12:C:ILE:HG22	2:11:C:LEU:H	1	1.48
(1,3671)	2:3:C:ALA:HB3	2:60:B:PHE:HD1	10	1.48
(1,3544)	2:51:B:VAL:HG23	2:48:B:ARG:HB3	5	1.48
(1,2042)	2:5:B:LYS:HD3	2:44:B:PHE:HZ	9	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1614)	1:150:A:PRO:HB2	1:152:A:LEU:HD12	8	1.48
(1,1545)	1:136:A:LYS:HA	1:136:A:LYS:HE3	2	1.48
(1,1467)	1:145:A:THR:HG23	1:82:A:GLN:HE22	8	1.48
(1,705)	1:122:A:LYS:HE3	1:122:A:LYS:HB3	10	1.48
(1,185)	1:130:A:LEU:HD23	1:131:A:PHE:H	9	1.48
(1,185)	1:130:A:LEU:HD23	1:131:A:PHE:H	10	1.48
(1,56)	1:114:A:ILE:HD13	1:103:A:GLN:HE21	1	1.48
(1,3731)	2:12:C:ILE:HD13	2:13:C:VAL:HG12	8	1.47
(1,3672)	2:12:B:ILE:HG21	2:11:B:LEU:H	9	1.47
(1,3670)	2:3:B:ALA:HB2	2:60:C:PHE:HD1	10	1.47
(1,3553)	2:25:C:ILE:HD12	2:24:C:GLU:HB3	10	1.47
(1,2644)	2:20:B:VAL:HG13	2:33:B:LEU:HD21	3	1.47
(1,2628)	2:37:B:MET:HB3	2:17:B:SER:HB3	8	1.47
(1,2083)	2:25:C:ILE:HD12	2:19:C:ILE:HG23	8	1.47
(1,2063)	2:55:C:LEU:HD23	2:14:C:ASN:HB2	3	1.47
(1,2062)	2:55:B:LEU:HD22	2:14:B:ASN:HB2	9	1.47
(1,1758)	1:83:A:ALA:H	1:85:A:LYS:HG2	8	1.47
(1,1653)	1:126:A:LEU:HD11	1:126:A:LEU:HB3	4	1.47
(1,1653)	1:126:A:LEU:HD13	1:126:A:LEU:HB3	10	1.47
(1,1570)	1:139:A:PRO:HA	1:137:A:VAL:HG22	1	1.47
(1,804)	1:121:A:LEU:HD21	1:141:A:ASN:HD21	1	1.47
(1,52)	1:81:A:ILE:HD12	1:81:A:ILE:H	6	1.47
(1,47)	1:88:A:ILE:HD11	1:105:A:LEU:HA	10	1.47
(1,3970)	2:8:B:ILE:HD13	2:60:C:PHE:HE1	4	1.46
(1,3830)	2:40:B:ILE:HD11	2:13:B:VAL:HB	2	1.46
(1,3730)	2:12:B:ILE:HD13	2:13:B:VAL:HG13	10	1.46
(1,3718)	2:54:B:ILE:HG23	2:13:B:VAL:HG21	10	1.46
(1,3577)	2:33:C:LEU:HD22	2:19:C:ILE:HG21	9	1.46
(1,3553)	2:25:C:ILE:HD12	2:24:C:GLU:HB3	1	1.46
(1,2643)	2:25:C:ILE:HD11	2:20:C:VAL:HG13	3	1.46
(1,2158)	2:13:B:VAL:HG21	2:48:B:ARG:HD3	7	1.46
(1,1801)	1:82:A:GLN:HE22	1:81:A:ILE:HD12	5	1.46
(1,1653)	1:126:A:LEU:HD13	1:126:A:LEU:HB3	5	1.46
(1,1123)	1:87:A:SER:H	1:79:A:LYS:HD3	10	1.46
(1,4181)	1:120:A:LEU:HD12	2:31:B:ASP:H	6	1.45
(1,3928)	2:39:B:CYS:HB2	2:35:B:VAL:HB	6	1.45
(1,3874)	2:15:B:TYR:HA	2:12:C:ILE:HD12	8	1.45
(1,2645)	2:20:C:VAL:HG12	2:33:C:LEU:HD21	9	1.45
(1,2643)	2:25:C:ILE:HD11	2:20:C:VAL:HG11	2	1.45
(1,2639)	2:35:C:VAL:HG21	2:37:C:MET:HB3	1	1.45
(1,2544)	2:51:B:VAL:HG12	2:55:B:LEU:HG	1	1.45
(1,1653)	1:126:A:LEU:HD13	1:126:A:LEU:HB3	3	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,535)	1:150:A:PRO:HA	1:116:A:GLU:HG3	5	1.45
(1,56)	1:114:A:ILE:HD11	1:103:A:GLN:HE21	6	1.45
(1,3781)	2:13:C:VAL:HG23	2:16:C:PHE:HE2	8	1.44
(1,3573)	2:33:C:LEU:HD22	2:19:C:ILE:HB	7	1.44
(1,1670)	1:136:A:LYS:HA	1:136:A:LYS:HE3	5	1.44
(1,1570)	1:139:A:PRO:HA	1:137:A:VAL:HG22	7	1.44
(1,1449)	1:78:A:LEU:HD11	1:90:A:HIS:H	1	1.44
(1,4182)	1:120:A:LEU:HD23	2:38:B:ASP:H	4	1.43
(1,4181)	1:120:A:LEU:HD11	2:38:C:ASP:H	8	1.43
(1,3929)	2:39:C:CYS:HB3	2:35:B:VAL:HB	7	1.43
(1,3875)	2:15:C:TYR:HA	2:12:B:ILE:HD13	1	1.43
(1,3718)	2:54:B:ILE:HG23	2:13:B:VAL:HG21	1	1.43
(1,3620)	2:40:B:ILE:HA	2:36:C:ALA:HB2	3	1.43
(1,1653)	1:126:A:LEU:HD11	1:126:A:LEU:HB3	8	1.43
(1,1545)	1:136:A:LYS:HA	1:136:A:LYS:HE3	5	1.43
(1,632)	1:114:A:ILE:HB	1:106:A:ILE:HD13	1	1.43
(1,3934)	2:55:B:LEU:HD12	2:7:B:GLU:HG2	7	1.42
(1,3745)	2:40:C:ILE:HD11	2:36:C:ALA:HB1	4	1.42
(1,3673)	2:12:C:ILE:HG21	2:11:C:LEU:H	10	1.42
(1,3543)	2:51:C:VAL:HG23	2:13:C:VAL:HB	2	1.42
(1,2641)	2:33:C:LEU:HD13	2:20:C:VAL:HG13	1	1.42
(1,1653)	1:126:A:LEU:HD13	1:126:A:LEU:HB3	7	1.42
(1,1434)	1:83:A:ALA:HB1	1:84:A:PRO:HG2	2	1.42
(1,187)	1:120:A:LEU:HD21	1:119:A:LEU:H	10	1.42
(1,3672)	2:12:B:ILE:HG22	2:11:B:LEU:H	4	1.41
(1,2693)	2:50:C:ALA:HB2	2:47:C:GLU:HB2	4	1.41
(1,2615)	2:13:C:VAL:HG13	2:48:C:ARG:HG2	9	1.41
(1,2225)	2:7:C:GLU:HA	2:54:C:ILE:HG22	9	1.41
(1,1570)	1:139:A:PRO:HA	1:137:A:VAL:HG22	3	1.41
(1,474)	1:105:A:LEU:HA	1:108:A:GLU:HG3	6	1.41
(1,186)	1:120:A:LEU:HD21	1:120:A:LEU:H	9	1.41
(1,151)	1:135:A:LEU:HD12	1:135:A:LEU:H	7	1.41
(1,3740)	2:19:B:ILE:HD13	2:8:C:ILE:HG21	2	1.4
(1,3732)	2:12:B:ILE:HD13	2:40:B:ILE:HD12	10	1.4
(1,3730)	2:12:B:ILE:HD11	2:13:B:VAL:HG11	2	1.4
(1,3673)	2:12:C:ILE:HG22	2:11:C:LEU:H	5	1.4
(1,3577)	2:33:C:LEU:HD23	2:19:C:ILE:HG23	2	1.4
(1,3572)	2:33:B:LEU:HD22	2:19:B:ILE:HB	1	1.4
(1,3557)	2:25:C:ILE:HD12	2:5:B:LYS:HD2	2	1.4
(1,3554)	2:25:B:ILE:HD13	2:19:B:ILE:HB	3	1.4
(1,3183)	2:12:C:ILE:HD13	2:9:C:ALA:H	7	1.4
(1,2787)	2:20:C:VAL:HG11	2:34:C:ASN:HD22	7	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2158)	2:13:B:VAL:HG22	2:48:B:ARG:HD3	1	1.4
(1,2088)	2:8:B:ILE:HD12	2:19:C:ILE:HG12	2	1.4
(1,1434)	1:83:A:ALA:HB2	1:84:A:PRO:HG2	4	1.4
(1,1353)	1:121:A:LEU:HD13	1:141:A:ASN:HD21	6	1.4
(1,1353)	1:121:A:LEU:HD13	1:141:A:ASN:HD21	10	1.4
(1,834)	1:85:A:LYS:HE3	1:82:A:GLN:HA	8	1.4
(1,672)	1:121:A:LEU:HD23	1:144:A:ILE:HA	10	1.4
(1,460)	1:126:A:LEU:HD11	1:120:A:LEU:HA	2	1.4
(1,3929)	2:39:C:CYS:HB2	2:35:C:VAL:HB	4	1.39
(1,3874)	2:15:B:TYR:HA	2:12:C:ILE:HD13	7	1.39
(1,3741)	2:19:C:ILE:HD12	2:8:B:ILE:HG22	2	1.39
(1,3733)	2:12:C:ILE:HD13	2:40:C:ILE:HD12	7	1.39
(1,3731)	2:12:C:ILE:HD11	2:13:C:VAL:HG11	9	1.39
(1,3672)	2:12:B:ILE:HG22	2:11:B:LEU:H	7	1.39
(1,3670)	2:3:B:ALA:HB2	2:60:C:PHE:HD1	1	1.39
(1,3048)	2:50:B:ALA:H	2:13:B:VAL:HG12	9	1.39
(1,2698)	2:54:B:ILE:HG23	2:6:B:GLU:HG3	1	1.39
(1,2544)	2:51:B:VAL:HG13	2:55:B:LEU:HG	4	1.39
(1,2534)	2:36:B:ALA:HB2	2:40:C:ILE:HG13	7	1.39
(1,2490)	2:54:B:ILE:HG21	2:7:B:GLU:HG2	2	1.39
(1,2158)	2:13:B:VAL:HG22	2:48:B:ARG:HD3	9	1.39
(1,2083)	2:25:C:ILE:HD12	2:19:C:ILE:HG23	7	1.39
(1,2063)	2:55:C:LEU:HD23	2:14:C:ASN:HB2	7	1.39
(1,1651)	1:88:A:ILE:HG23	1:78:A:LEU:HB3	6	1.39
(1,700)	1:79:A:LYS:HE3	1:81:A:ILE:HA	3	1.39
(1,630)	1:78:A:LEU:HB2	1:146:A:VAL:HG23	8	1.39
(1,630)	1:78:A:LEU:HB2	1:146:A:VAL:HG22	10	1.39
(1,4182)	1:120:A:LEU:HD21	2:38:B:ASP:H	2	1.38
(1,4180)	1:147:A:MET:HE3	2:38:B:ASP:H	8	1.38
(1,3928)	2:39:B:CYS:HB3	2:35:C:VAL:HB	2	1.38
(1,3928)	2:39:B:CYS:HB2	2:35:B:VAL:HB	3	1.38
(1,3830)	2:40:B:ILE:HD11	2:13:B:VAL:HB	6	1.38
(1,3672)	2:12:B:ILE:HG23	2:11:B:LEU:H	5	1.38
(1,3672)	2:12:B:ILE:HG21	2:11:B:LEU:H	6	1.38
(1,3608)	2:38:B:ASP:HA	2:40:B:ILE:HD13	9	1.38
(1,3577)	2:33:C:LEU:HD23	2:19:C:ILE:HG23	8	1.38
(1,1651)	1:88:A:ILE:HG23	1:78:A:LEU:HB3	10	1.38
(1,1434)	1:83:A:ALA:HB2	1:84:A:PRO:HG2	9	1.38
(1,1123)	1:87:A:SER:H	1:79:A:LYS:HD3	9	1.38
(1,778)	1:128:A:ASP:HB2	1:99:A:LEU:HD23	6	1.38
(1,708)	1:122:A:LYS:HE3	1:121:A:LEU:HD11	5	1.38
(1,4015)	2:60:C:PHE:HD2	2:68:B:ILE:HD13	5	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3626)	2:41:B:SER:HB3	2:9:B:ALA:HB1	8	1.37
(1,3552)	2:25:B:ILE:HD13	2:24:B:GLU:HB3	1	1.37
(1,3049)	2:50:C:ALA:H	2:13:C:VAL:HG12	4	1.37
(1,2721)	2:54:C:ILE:HD13	2:6:C:GLU:HG3	2	1.37
(1,2546)	2:20:B:VAL:HG22	2:30:B:ALA:HB2	8	1.37
(1,2498)	2:25:B:ILE:HG23	2:20:B:VAL:HG12	1	1.37
(1,1653)	1:126:A:LEU:HD11	1:126:A:LEU:HB3	2	1.37
(1,1557)	1:81:A:ILE:HA	1:85:A:LYS:HD3	9	1.37
(1,1446)	1:97:A:THR:HG22	1:96:A:ASP:HB3	10	1.37
(1,183)	1:99:A:LEU:HD11	1:100:A:GLN:HE22	1	1.37
(1,118)	1:97:A:THR:HG23	1:97:A:THR:H	6	1.37
(1,3929)	2:39:C:CYS:HB2	2:35:C:VAL:HB	2	1.36
(1,3719)	2:54:C:ILE:HG23	2:13:C:VAL:HG22	5	1.36
(1,3542)	2:51:B:VAL:HG22	2:13:B:VAL:HB	3	1.36
(1,3325)	2:27:C:GLU:HG3	2:27:C:GLU:H	3	1.36
(1,2547)	2:20:C:VAL:HG21	2:30:C:ALA:HB2	1	1.36
(1,2545)	2:51:C:VAL:HG12	2:55:C:LEU:HG	1	1.36
(1,2299)	2:19:C:ILE:HA	2:22:C:LYS:HD3	9	1.36
(1,2088)	2:8:B:ILE:HD12	2:19:C:ILE:HG12	7	1.36
(1,2063)	2:55:C:LEU:HD21	2:14:C:ASN:HB2	1	1.36
(1,1803)	1:82:A:GLN:HE21	1:81:A:ILE:HG22	10	1.36
(1,1434)	1:83:A:ALA:HB3	1:82:A:GLN:HB2	10	1.36
(1,174)	1:132:A:LEU:HD21	1:92:A:PHE:HA	2	1.36
(1,25)	1:144:A:ILE:HD12	1:120:A:LEU:H	3	1.36
(1,4014)	2:60:B:PHE:HD2	2:68:C:ILE:HD11	1	1.35
(1,3731)	2:12:C:ILE:HD11	2:13:C:VAL:HG12	2	1.35
(1,3683)	2:12:C:ILE:HD13	2:16:B:PHE:HD1	6	1.35
(1,3555)	2:25:C:ILE:HD12	2:5:B:LYS:HB3	8	1.35
(1,2883)	2:13:C:VAL:HG11	2:41:C:SER:HB3	8	1.35
(1,834)	1:85:A:LYS:HE3	1:82:A:GLN:HA	5	1.35
(1,186)	1:120:A:LEU:HD22	1:120:A:LEU:H	5	1.35
(1,185)	1:130:A:LEU:HD23	1:131:A:PHE:H	4	1.35
(1,3928)	2:39:B:CYS:HB3	2:35:C:VAL:HB	8	1.34
(1,3875)	2:15:C:TYR:HA	2:12:B:ILE:HD12	5	1.34
(1,3626)	2:41:B:SER:HB3	2:9:B:ALA:HB3	10	1.34
(1,2883)	2:13:C:VAL:HG11	2:41:C:SER:HB3	2	1.34
(1,2720)	2:54:B:ILE:HD12	2:6:B:GLU:HG3	10	1.34
(1,2547)	2:20:C:VAL:HG22	2:30:C:ALA:HB3	6	1.34
(1,2083)	2:25:C:ILE:HD12	2:19:C:ILE:HG23	6	1.34
(1,1653)	1:126:A:LEU:HD13	1:126:A:LEU:HB3	1	1.34
(1,1653)	1:126:A:LEU:HD13	1:126:A:LEU:HB3	6	1.34
(1,1434)	1:83:A:ALA:HB2	1:84:A:PRO:HG2	7	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,898)	1:85:A:LYS:HB3	1:86:A:PHE:H	7	1.34
(1,150)	1:78:A:LEU:HD13	1:92:A:PHE:HZ	8	1.34
(1,118)	1:97:A:THR:HG23	1:97:A:THR:H	5	1.34
(1,4180)	1:147:A:MET:HE1	2:38:B:ASP:H	6	1.33
(1,4081)	2:13:C:VAL:H	2:41:C:SER:HA	4	1.33
(1,3313)	2:26:C:SER:H	2:44:B:PHE:HD1	9	1.33
(1,3221)	2:34:C:ASN:HA	2:17:C:SER:H	4	1.33
(1,2883)	2:13:C:VAL:HG11	2:41:C:SER:HB3	6	1.33
(1,2695)	2:54:C:ILE:HG23	2:46:C:PHE:HB2	10	1.33
(1,2545)	2:51:C:VAL:HG12	2:55:C:LEU:HG	10	1.33
(1,2426)	2:68:B:ILE:HD13	2:60:C:PHE:HD2	1	1.33
(1,2083)	2:25:C:ILE:HD12	2:19:C:ILE:HG22	10	1.33
(1,1295)	1:129:A:ASN:H	1:97:A:THR:HB	6	1.33
(1,778)	1:128:A:ASP:HB2	1:99:A:LEU:HD23	5	1.33
(1,728)	1:99:A:LEU:HG	1:103:A:GLN:HE22	5	1.33
(1,725)	1:148:A:ILE:HD12	1:80:A:LYS:HD3	9	1.33
(1,702)	1:122:A:LYS:HE3	1:122:A:LYS:H	4	1.33
(1,185)	1:130:A:LEU:HD22	1:131:A:PHE:H	1	1.33
(1,3684)	2:12:B:ILE:HD13	2:15:C:TYR:HD2	8	1.32
(1,3537)	2:55:C:LEU:HD21	2:55:C:LEU:H	9	1.32
(1,2645)	2:20:C:VAL:HG12	2:33:C:LEU:HD22	6	1.32
(1,1594)	1:142:A:SER:HB2	1:121:A:LEU:HD13	4	1.32
(1,1347)	1:141:A:ASN:HD22	1:121:A:LEU:HD12	9	1.32
(1,778)	1:128:A:ASP:HB2	1:99:A:LEU:HD23	1	1.32
(1,185)	1:130:A:LEU:HD23	1:131:A:PHE:H	5	1.32
(1,147)	1:132:A:LEU:HD23	1:98:A:ILE:H	5	1.32
(1,4187)	1:81:A:ILE:HG23	2:39:B:CYS:H	7	1.31
(1,3627)	2:41:C:SER:HB3	2:9:C:ALA:HB2	3	1.31
(1,3149)	2:5:C:LYS:HG3	2:6:C:GLU:H	10	1.31
(1,2644)	2:20:B:VAL:HG13	2:33:B:LEU:HD21	2	1.31
(1,2594)	2:57:B:LYS:HB3	2:68:C:ILE:HG13	2	1.31
(1,2182)	2:9:B:ALA:HA	2:40:B:ILE:HG23	4	1.31
(1,790)	1:126:A:LEU:HG	1:124:A:LYS:HE3	4	1.31
(1,778)	1:128:A:ASP:HB2	1:99:A:LEU:HD23	3	1.31
(1,709)	1:122:A:LYS:HE3	1:141:A:ASN:HA	9	1.31
(1,174)	1:132:A:LEU:HD22	1:92:A:PHE:HA	5	1.31
(1,54)	1:81:A:ILE:HD12	1:82:A:GLN:H	5	1.31
(1,25)	1:144:A:ILE:HD12	1:120:A:LEU:H	8	1.31
(1,3718)	2:54:B:ILE:HG23	2:13:B:VAL:HG21	5	1.3
(1,3443)	2:51:C:VAL:HA	2:54:C:ILE:H	9	1.3
(1,2645)	2:20:C:VAL:HG12	2:33:C:LEU:HD22	7	1.3
(1,2500)	2:25:B:ILE:HG23	2:20:B:VAL:HB	10	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2061)	2:55:C:LEU:HD22	2:14:C:ASN:H	4	1.3
(1,1434)	1:83:A:ALA:HB2	1:84:A:PRO:HG2	1	1.3
(1,1434)	1:83:A:ALA:HB2	1:84:A:PRO:HG2	6	1.3
(1,1423)	1:119:A:LEU:HD21	1:117:A:ILE:HB	7	1.3
(1,571)	1:93:A:SER:HB3	1:96:A:ASP:HB3	10	1.3
(1,151)	1:135:A:LEU:HD12	1:135:A:LEU:H	1	1.3
(1,26)	1:144:A:ILE:HD11	1:121:A:LEU:H	7	1.3
(1,4180)	1:147:A:MET:HE1	2:38:B:ASP:H	7	1.29
(1,3682)	2:12:B:ILE:HD12	2:16:C:PHE:HD1	5	1.29
(1,3626)	2:41:B:SER:HB3	2:9:B:ALA:HB1	2	1.29
(1,3313)	2:26:C:SER:H	2:44:B:PHE:HD1	10	1.29
(1,2642)	2:25:B:ILE:HD13	2:20:B:VAL:HG11	3	1.29
(1,2564)	2:33:B:LEU:HD12	2:19:B:ILE:HG22	6	1.29
(1,2500)	2:25:B:ILE:HG23	2:20:B:VAL:HB	9	1.29
(1,2192)	2:25:B:ILE:HD13	2:30:B:ALA:HA	8	1.29
(1,2115)	2:13:C:VAL:HG21	2:48:C:ARG:HG2	3	1.29
(1,898)	1:85:A:LYS:HB3	1:86:A:PHE:H	2	1.29
(1,778)	1:128:A:ASP:HB2	1:99:A:LEU:HD21	4	1.29
(1,735)	1:79:A:LYS:HD3	1:79:A:LYS:HA	3	1.29
(1,705)	1:122:A:LYS:HE3	1:122:A:LYS:HB3	3	1.29
(1,185)	1:130:A:LEU:HD23	1:131:A:PHE:H	7	1.29
(1,176)	1:132:A:LEU:HD22	1:96:A:ASP:HB2	6	1.29
(1,54)	1:81:A:ILE:HD12	1:82:A:GLN:H	9	1.29
(1,3741)	2:19:C:ILE:HD12	2:8:B:ILE:HG22	8	1.28
(1,3548)	2:55:B:LEU:HD11	2:12:B:ILE:HA	8	1.28
(1,3183)	2:12:C:ILE:HD13	2:9:C:ALA:H	6	1.28
(1,3183)	2:12:C:ILE:HD11	2:9:C:ALA:H	9	1.28
(1,2695)	2:54:C:ILE:HG21	2:46:C:PHE:HB2	7	1.28
(1,2062)	2:55:B:LEU:HD22	2:14:B:ASN:HB2	10	1.28
(1,2038)	2:5:B:LYS:HB3	2:44:B:PHE:HZ	4	1.28
(1,1808)	1:103:A:GLN:HE22	1:114:A:ILE:HG13	8	1.28
(1,778)	1:128:A:ASP:HB2	1:99:A:LEU:HD23	9	1.28
(1,571)	1:93:A:SER:HB3	1:96:A:ASP:HB3	1	1.28
(1,3875)	2:15:C:TYR:HA	2:12:B:ILE:HD12	10	1.27
(1,3795)	2:17:C:SER:HA	2:19:C:ILE:HG21	10	1.27
(1,3719)	2:54:C:ILE:HG21	2:13:C:VAL:HG23	2	1.27
(1,3572)	2:33:B:LEU:HD22	2:19:B:ILE:HB	9	1.27
(1,2640)	2:33:B:LEU:HD11	2:20:B:VAL:HG12	1	1.27
(1,2559)	2:55:C:LEU:HD23	2:13:C:VAL:HG21	9	1.27
(1,2061)	2:55:C:LEU:HD21	2:14:C:ASN:H	5	1.27
(1,1803)	1:82:A:GLN:HE21	1:81:A:ILE:HG22	3	1.27
(1,1801)	1:82:A:GLN:HE22	1:81:A:ILE:HG22	10	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1594)	1:142:A:SER:HB2	1:76:A:LEU:HD13	6	1.27
(1,1570)	1:139:A:PRO:HA	1:137:A:VAL:HG22	8	1.27
(1,1449)	1:78:A:LEU:HD11	1:90:A:HIS:H	6	1.27
(1,1328)	1:100:A:GLN:HE21	1:99:A:LEU:HD11	10	1.27
(1,736)	1:114:A:ILE:HG12	1:102:A:LYS:HB3	9	1.27
(1,720)	1:148:A:ILE:HD11	1:86:A:PHE:HZ	8	1.27
(1,704)	1:122:A:LYS:HE3	1:141:A:ASN:HD21	9	1.27
(1,185)	1:130:A:LEU:HD23	1:131:A:PHE:H	3	1.27
(1,118)	1:97:A:THR:HG22	1:97:A:THR:H	8	1.27
(1,4109)	2:21:C:GLU:H	2:22:C:LYS:HG3	7	1.26
(1,3627)	2:41:C:SER:HB3	2:9:C:ALA:HB2	6	1.26
(1,2954)	2:16:B:PHE:HZ	2:12:C:ILE:HD11	9	1.26
(1,2695)	2:54:C:ILE:HG21	2:46:C:PHE:HB2	8	1.26
(1,2491)	2:54:C:ILE:HG22	2:7:C:GLU:HG2	9	1.26
(1,2115)	2:13:C:VAL:HG21	2:48:C:ARG:HG2	10	1.26
(1,183)	1:99:A:LEU:HD11	1:100:A:GLN:HE22	4	1.26
(1,174)	1:132:A:LEU:HD22	1:92:A:PHE:HA	8	1.26
(1,48)	1:88:A:ILE:HD12	1:90:A:HIS:HE1	6	1.26
(1,4180)	1:147:A:MET:HE3	2:38:B:ASP:H	4	1.25
(1,4175)	1:125:A:VAL:HB	2:39:C:CYS:HG	9	1.25
(1,3555)	2:25:C:ILE:HD12	2:19:C:ILE:HB	2	1.25
(1,3477)	2:55:C:LEU:HD21	2:14:C:ASN:HD21	4	1.25
(1,3183)	2:12:C:ILE:HD13	2:9:C:ALA:H	8	1.25
(1,2882)	2:13:B:VAL:HG13	2:41:B:SER:HB3	8	1.25
(1,2882)	2:13:B:VAL:HG12	2:41:B:SER:HB3	9	1.25
(1,2114)	2:13:B:VAL:HG22	2:48:B:ARG:HG2	5	1.25
(1,1295)	1:129:A:ASN:H	1:97:A:THR:HB	8	1.25
(1,898)	1:85:A:LYS:HB3	1:86:A:PHE:H	1	1.25
(1,786)	1:126:A:LEU:HD11	1:124:A:LYS:HD3	4	1.25
(1,85)	1:73:A:MET:HE1	1:73:A:MET:HA	5	1.25
(1,4187)	1:81:A:ILE:HG23	2:36:C:ALA:H	6	1.24
(1,3934)	2:55:B:LEU:HD12	2:7:B:GLU:HG2	9	1.24
(1,3794)	2:18:B:SER:HB3	2:19:B:ILE:HG22	5	1.24
(1,3627)	2:41:C:SER:HB3	2:9:C:ALA:HB2	8	1.24
(1,3555)	2:25:C:ILE:HD12	2:5:B:LYS:HB3	10	1.24
(1,3548)	2:55:B:LEU:HD11	2:12:B:ILE:HA	7	1.24
(1,3101)	2:23:C:LYS:HG3	2:23:C:LYS:H	7	1.24
(1,2644)	2:20:B:VAL:HG11	2:33:B:LEU:HD22	5	1.24
(1,2500)	2:25:B:ILE:HG23	2:20:B:VAL:HB	1	1.24
(1,2246)	2:11:B:LEU:HA	2:12:B:ILE:HD12	3	1.24
(1,1423)	1:119:A:LEU:HD21	1:126:A:LEU:HB3	10	1.24
(1,1356)	1:151:A:ASN:HA	1:151:A:ASN:HD22	1	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,174)	1:132:A:LEU:HD22	1:92:A:PHE:HA	4	1.24
(1,3732)	2:12:B:ILE:HD11	2:40:B:ILE:HG21	1	1.23
(1,3627)	2:41:C:SER:HB3	2:9:C:ALA:HB2	2	1.23
(1,3626)	2:41:B:SER:HB3	2:9:B:ALA:HB1	6	1.23
(1,3325)	2:27:C:GLU:HG3	2:27:C:GLU:H	10	1.23
(1,2211)	2:22:C:LYS:HA	2:24:C:GLU:HB2	1	1.23
(1,2089)	2:8:C:ILE:HD13	2:19:B:ILE:HG12	7	1.23
(1,2082)	2:25:B:ILE:HD11	2:19:B:ILE:HG23	7	1.23
(1,2062)	2:55:B:LEU:HD22	2:14:B:ASN:HB2	4	1.23
(1,1594)	1:142:A:SER:HB2	1:121:A:LEU:HD12	9	1.23
(1,1449)	1:78:A:LEU:HD11	1:90:A:HIS:H	3	1.23
(1,1021)	1:103:A:GLN:HG3	1:103:A:GLN:H	3	1.23
(1,735)	1:79:A:LYS:HD3	1:79:A:LYS:HA	9	1.23
(1,4086)	2:15:B:TYR:H	2:12:C:ILE:HD13	9	1.22
(1,3934)	2:55:B:LEU:HD12	2:7:B:GLU:HG2	10	1.22
(1,3928)	2:39:B:CYS:HB3	2:35:C:VAL:HB	4	1.22
(1,3731)	2:12:C:ILE:HD13	2:13:C:VAL:HG12	3	1.22
(1,3608)	2:38:B:ASP:HA	2:40:B:ILE:HD11	4	1.22
(1,3151)	2:5:C:LYS:HG2	2:6:C:GLU:H	10	1.22
(1,3101)	2:23:C:LYS:HG3	2:23:C:LYS:H	2	1.22
(1,3100)	2:23:B:LYS:HG3	2:23:B:LYS:H	7	1.22
(1,3048)	2:50:B:ALA:H	2:13:B:VAL:HG12	10	1.22
(1,2629)	2:37:C:MET:HB3	2:17:C:SER:HB3	7	1.22
(1,1799)	1:142:A:SER:H	1:121:A:LEU:HD13	2	1.22
(1,1648)	1:135:A:LEU:HA	1:135:A:LEU:HD12	9	1.22
(1,1123)	1:87:A:SER:H	1:79:A:LYS:HD3	4	1.22
(1,782)	1:98:A:ILE:HG21	1:98:A:ILE:HG12	7	1.22
(1,736)	1:114:A:ILE:HG12	1:102:A:LYS:HB3	5	1.22
(1,702)	1:122:A:LYS:HE3	1:122:A:LYS:H	1	1.22
(1,630)	1:78:A:LEU:HB2	1:146:A:VAL:HG22	9	1.22
(1,571)	1:93:A:SER:HB3	1:96:A:ASP:HB3	2	1.22
(1,571)	1:93:A:SER:HB3	1:96:A:ASP:HB3	6	1.22
(1,185)	1:130:A:LEU:HD23	1:131:A:PHE:H	6	1.22
(1,151)	1:135:A:LEU:HD12	1:135:A:LEU:H	10	1.22
(1,3934)	2:55:B:LEU:HD11	2:7:B:GLU:HG2	3	1.21
(1,3671)	2:3:C:ALA:HB3	2:60:B:PHE:HD1	5	1.21
(1,3608)	2:38:B:ASP:HA	2:13:B:VAL:HG22	10	1.21
(1,3554)	2:25:B:ILE:HD13	2:5:C:LYS:HB3	1	1.21
(1,3554)	2:25:B:ILE:HD13	2:5:C:LYS:HB3	2	1.21
(1,3552)	2:25:B:ILE:HD12	2:24:B:GLU:HB3	10	1.21
(1,2713)	2:54:C:ILE:HD11	2:51:C:VAL:H	9	1.21
(1,2645)	2:20:C:VAL:HG12	2:33:C:LEU:HD22	8	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2553)	2:35:C:VAL:HG13	2:37:C:MET:HB3	7	1.21
(1,1021)	1:103:A:GLN:HG3	1:103:A:GLN:H	8	1.21
(1,795)	1:80:A:LYS:HE3	1:86:A:PHE:HZ	10	1.21
(1,4015)	2:60:C:PHE:HD1	2:68:B:ILE:HD12	9	1.2
(1,3830)	2:40:B:ILE:HD11	2:13:B:VAL:HB	3	1.2
(1,3719)	2:54:C:ILE:HG22	2:13:C:VAL:HG23	4	1.2
(1,3719)	2:54:C:ILE:HG21	2:13:C:VAL:HG23	8	1.2
(1,3620)	2:40:B:ILE:HA	2:36:C:ALA:HB2	10	1.2
(1,3608)	2:38:B:ASP:HA	2:40:B:ILE:HD13	1	1.2
(1,3556)	2:25:B:ILE:HD13	2:5:C:LYS:HD2	9	1.2
(1,3554)	2:25:B:ILE:HD13	2:5:C:LYS:HB3	9	1.2
(1,3548)	2:55:B:LEU:HD11	2:12:B:ILE:HA	6	1.2
(1,3544)	2:51:B:VAL:HG21	2:48:B:ARG:HB3	2	1.2
(1,2941)	2:44:C:PHE:HZ	2:33:B:LEU:HD22	7	1.2
(1,2883)	2:13:C:VAL:HG13	2:41:C:SER:HB3	1	1.2
(1,1399)	1:80:A:LYS:HE3	1:148:A:ILE:H	9	1.2
(1,778)	1:128:A:ASP:HB2	1:99:A:LEU:HD23	8	1.2
(1,8)	1:120:A:LEU:HD12	1:147:A:MET:HG3	5	1.2
(1,4187)	1:81:A:ILE:HG23	2:36:C:ALA:H	10	1.19
(1,4182)	1:120:A:LEU:HD22	2:38:B:ASP:H	7	1.19
(1,4052)	2:55:B:LEU:HD22	2:8:B:ILE:H	5	1.19
(1,3874)	2:15:B:TYR:HA	2:12:C:ILE:HD12	3	1.19
(1,3794)	2:17:B:SER:HA	2:19:B:ILE:HG23	9	1.19
(1,3780)	2:13:B:VAL:HG21	2:16:B:PHE:HE2	5	1.19
(1,3770)	2:20:B:VAL:HG23	2:19:B:ILE:HA	1	1.19
(1,3555)	2:25:C:ILE:HD11	2:19:C:ILE:HB	3	1.19
(1,3553)	2:25:C:ILE:HD12	2:24:C:GLU:HB3	4	1.19
(1,3259)	2:22:C:LYS:HG3	2:22:C:LYS:H	7	1.19
(1,3101)	2:23:C:LYS:HG3	2:23:C:LYS:H	6	1.19
(1,2564)	2:33:B:LEU:HD11	2:19:B:ILE:HG23	3	1.19
(1,2547)	2:20:C:VAL:HG22	2:30:C:ALA:HB3	3	1.19
(1,2158)	2:13:B:VAL:HG23	2:48:B:ARG:HD3	3	1.19
(1,1068)	1:119:A:LEU:HD23	1:119:A:LEU:H	5	1.19
(1,782)	1:98:A:ILE:HG23	1:98:A:ILE:HG12	2	1.19
(1,501)	1:81:A:ILE:HA	1:85:A:LYS:HE3	2	1.19
(1,201)	1:144:A:ILE:HG22	1:120:A:LEU:H	2	1.19
(1,185)	1:130:A:LEU:HD22	1:131:A:PHE:H	8	1.19
(1,174)	1:132:A:LEU:HD22	1:92:A:PHE:HA	7	1.19
(1,13)	1:119:A:LEU:HD21	1:98:A:ILE:HA	7	1.19
(1,4175)	1:125:A:VAL:HG21	2:31:B:ASP:HB3	7	1.18
(1,4085)	2:14:C:ASN:H	2:12:C:ILE:HG22	10	1.18
(1,3718)	2:54:B:ILE:HG22	2:13:B:VAL:HG23	8	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3627)	2:41:C:SER:HB3	2:9:C:ALA:HB2	10	1.18
(1,3626)	2:41:B:SER:HB3	2:9:B:ALA:HB3	1	1.18
(1,3555)	2:25:C:ILE:HD12	2:19:C:ILE:HB	9	1.18
(1,3554)	2:25:B:ILE:HD13	2:19:B:ILE:HB	7	1.18
(1,3312)	2:26:B:SER:H	2:44:C:PHE:HD1	4	1.18
(1,3100)	2:23:B:LYS:HG3	2:23:B:LYS:H	8	1.18
(1,2950)	2:60:B:PHE:HD2	2:54:B:ILE:HB	6	1.18
(1,2553)	2:35:C:VAL:HG12	2:37:C:MET:HB3	10	1.18
(1,2062)	2:55:B:LEU:HD21	2:14:B:ASN:HB2	3	1.18
(1,1457)	1:120:A:LEU:HD23	1:118:A:LYS:HE3	4	1.18
(1,1446)	1:97:A:THR:HG22	1:96:A:ASP:HB3	4	1.18
(1,782)	1:98:A:ILE:HG23	1:98:A:ILE:HG12	4	1.18
(1,782)	1:98:A:ILE:HG23	1:98:A:ILE:HG12	6	1.18
(1,655)	1:81:A:ILE:HG12	1:145:A:THR:HA	2	1.18
(1,630)	1:78:A:LEU:HB2	1:146:A:VAL:HG22	1	1.18
(1,571)	1:93:A:SER:HB3	1:96:A:ASP:HB3	8	1.18
(1,85)	1:73:A:MET:HE1	1:73:A:MET:HA	6	1.18
(1,55)	1:114:A:ILE:HD11	1:103:A:GLN:HE22	3	1.18
(1,35)	1:106:A:ILE:HD12	1:113:A:HIS:HA	9	1.18
(1,4084)	2:55:B:LEU:HD21	2:14:B:ASN:H	7	1.17
(1,4052)	2:55:B:LEU:HD22	2:8:B:ILE:H	4	1.17
(1,4015)	2:60:C:PHE:HD1	2:8:C:ILE:HD11	2	1.17
(1,3932)	2:18:B:SER:HB3	2:15:B:TYR:HB3	4	1.17
(1,3745)	2:40:C:ILE:HD12	2:36:C:ALA:HB3	6	1.17
(1,3740)	2:19:B:ILE:HD11	2:8:C:ILE:HG21	4	1.17
(1,3548)	2:55:B:LEU:HD11	2:12:B:ILE:HA	2	1.17
(1,2498)	2:25:B:ILE:HG21	2:20:B:VAL:HG12	5	1.17
(1,2159)	2:13:C:VAL:HG21	2:48:C:ARG:HD3	7	1.17
(1,2115)	2:13:C:VAL:HG21	2:48:C:ARG:HG2	8	1.17
(1,2089)	2:8:C:ILE:HD12	2:19:B:ILE:HG12	3	1.17
(1,2082)	2:25:B:ILE:HD13	2:19:B:ILE:HG22	4	1.17
(1,782)	1:98:A:ILE:HG23	1:98:A:ILE:HG12	8	1.17
(1,735)	1:79:A:LYS:HD3	1:79:A:LYS:HA	2	1.17
(1,735)	1:79:A:LYS:HD3	1:79:A:LYS:HA	8	1.17
(1,55)	1:114:A:ILE:HD11	1:103:A:GLN:HE22	8	1.17
(1,47)	1:88:A:ILE:HD13	1:105:A:LEU:HA	2	1.17
(1,3850)	2:40:B:ILE:HG21	2:13:B:VAL:HB	2	1.16
(1,3795)	2:17:C:SER:HA	2:19:C:ILE:HG23	5	1.16
(1,3627)	2:41:C:SER:HB3	2:9:C:ALA:HB2	9	1.16
(1,3621)	2:40:C:ILE:HA	2:36:B:ALA:HB1	3	1.16
(1,3620)	2:40:B:ILE:HA	2:36:C:ALA:HB2	8	1.16
(1,2695)	2:54:C:ILE:HG23	2:46:C:PHE:HB2	1	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2630)	2:51:B:VAL:HB	2:55:B:LEU:HG	1	1.16
(1,2082)	2:25:B:ILE:HD13	2:19:B:ILE:HG21	1	1.16
(1,1651)	1:88:A:ILE:HG21	1:89:A:GLU:HG3	7	1.16
(1,1041)	1:108:A:GLU:HG3	1:108:A:GLU:H	6	1.16
(1,804)	1:121:A:LEU:HD21	1:141:A:ASN:HD21	7	1.16
(1,735)	1:79:A:LYS:HD3	1:79:A:LYS:HA	10	1.16
(1,150)	1:78:A:LEU:HD13	1:92:A:PHE:HZ	9	1.16
(1,4085)	2:14:C:ASN:H	2:12:C:ILE:HG23	5	1.15
(1,4084)	2:14:B:ASN:H	2:12:B:ILE:HG22	9	1.15
(1,3658)	2:51:B:VAL:HG21	2:46:B:PHE:HE2	2	1.15
(1,3555)	2:25:C:ILE:HD12	2:5:B:LYS:HB3	1	1.15
(1,3547)	2:51:C:VAL:HG23	2:50:C:ALA:HB3	1	1.15
(1,3100)	2:23:B:LYS:HG3	2:23:B:LYS:H	2	1.15
(1,2891)	2:21:C:GLU:HA	2:23:C:LYS:HE3	5	1.15
(1,2883)	2:13:C:VAL:HG13	2:41:C:SER:HB3	9	1.15
(1,2640)	2:33:B:LEU:HD12	2:20:B:VAL:HG11	6	1.15
(1,2547)	2:20:C:VAL:HG21	2:30:C:ALA:HB3	9	1.15
(1,2063)	2:55:C:LEU:HD23	2:14:C:ASN:HB2	2	1.15
(1,1829)	1:147:A:MET:H	1:146:A:VAL:HG21	5	1.15
(1,1809)	1:103:A:GLN:HE22	1:99:A:LEU:HD11	3	1.15
(1,1651)	1:88:A:ILE:HG21	1:89:A:GLU:HG3	1	1.15
(1,1614)	1:150:A:PRO:HB2	1:152:A:LEU:HD12	9	1.15
(1,1123)	1:87:A:SER:H	1:79:A:LYS:HD3	2	1.15
(1,782)	1:98:A:ILE:HG22	1:98:A:ILE:HG12	5	1.15
(1,118)	1:97:A:THR:HG22	1:97:A:THR:H	9	1.15
(1,56)	1:114:A:ILE:HD12	1:103:A:GLN:HE21	4	1.15
(1,35)	1:106:A:ILE:HD13	1:113:A:HIS:HA	8	1.15
(1,4179)	1:147:A:MET:HE3	2:35:B:VAL:H	10	1.14
(1,4015)	2:60:C:PHE:HD2	2:68:B:ILE:HD13	10	1.14
(1,3552)	2:25:B:ILE:HD13	2:24:B:GLU:HB3	5	1.14
(1,3547)	2:51:C:VAL:HG22	2:50:C:ALA:HB3	9	1.14
(1,3313)	2:26:C:SER:H	2:44:B:PHE:HD1	1	1.14
(1,3101)	2:23:C:LYS:HG3	2:23:C:LYS:H	8	1.14
(1,3100)	2:23:B:LYS:HG3	2:23:B:LYS:H	3	1.14
(1,2645)	2:20:C:VAL:HG12	2:33:C:LEU:HD22	3	1.14
(1,2638)	2:35:B:VAL:HG22	2:37:B:MET:HB3	1	1.14
(1,2564)	2:33:B:LEU:HD12	2:19:B:ILE:HG22	2	1.14
(1,2564)	2:33:B:LEU:HD13	2:19:B:ILE:HG23	8	1.14
(1,2546)	2:20:B:VAL:HG22	2:30:B:ALA:HB2	6	1.14
(1,2250)	2:11:B:LEU:HA	2:55:B:LEU:HB3	6	1.14
(1,2062)	2:55:B:LEU:HD22	2:14:B:ASN:HB2	5	1.14
(1,2055)	2:55:C:LEU:HG	2:55:C:LEU:H	9	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1820)	1:129:A:ASN:HD21	1:99:A:LEU:HD12	7	1.14
(1,1557)	1:81:A:ILE:HA	1:85:A:LYS:HD3	1	1.14
(1,1461)	1:120:A:LEU:HD22	1:145:A:THR:H	1	1.14
(1,1423)	1:119:A:LEU:HD22	1:117:A:ILE:HB	6	1.14
(1,1021)	1:103:A:GLN:HG3	1:103:A:GLN:H	10	1.14
(1,803)	1:99:A:LEU:HG	1:103:A:GLN:HE21	8	1.14
(1,151)	1:135:A:LEU:HD12	1:135:A:LEU:H	8	1.14
(1,3718)	2:54:B:ILE:HG22	2:13:B:VAL:HG22	3	1.13
(1,3627)	2:41:C:SER:HB3	2:9:C:ALA:HB2	1	1.13
(1,3573)	2:33:C:LEU:HD22	2:19:C:ILE:HB	3	1.13
(1,3542)	2:51:B:VAL:HG23	2:49:B:GLU:HG3	5	1.13
(1,2533)	2:36:C:ALA:HB2	2:35:C:VAL:HB	8	1.13
(1,1455)	1:132:A:LEU:HD21	1:94:A:PRO:HA	10	1.13
(1,1356)	1:151:A:ASN:HA	1:151:A:ASN:HD22	5	1.13
(1,1021)	1:103:A:GLN:HG3	1:103:A:GLN:H	4	1.13
(1,702)	1:122:A:LYS:HE3	1:122:A:LYS:H	6	1.13
(1,174)	1:132:A:LEU:HD22	1:92:A:PHE:HA	3	1.13
(1,3935)	2:55:C:LEU:HD12	2:7:C:GLU:HG2	1	1.12
(1,3935)	2:55:C:LEU:HD12	2:7:C:GLU:HG2	5	1.12
(1,3875)	2:15:C:TYR:HA	2:12:C:ILE:HD11	3	1.12
(1,3719)	2:54:C:ILE:HG21	2:13:C:VAL:HG23	6	1.12
(1,3100)	2:23:B:LYS:HG3	2:23:B:LYS:H	6	1.12
(1,3048)	2:50:B:ALA:H	2:13:B:VAL:HG12	4	1.12
(1,2641)	2:33:C:LEU:HD13	2:20:C:VAL:HG12	10	1.12
(1,2638)	2:35:B:VAL:HG21	2:37:B:MET:HB3	10	1.12
(1,2532)	2:36:B:ALA:HB3	2:35:B:VAL:HB	4	1.12
(1,2498)	2:25:B:ILE:HG23	2:20:B:VAL:HG12	10	1.12
(1,1557)	1:81:A:ILE:HA	1:85:A:LYS:HD3	6	1.12
(1,782)	1:98:A:ILE:HG23	1:98:A:ILE:HG12	1	1.12
(1,698)	1:79:A:LYS:HE3	1:81:A:ILE:HG21	5	1.12
(1,571)	1:93:A:SER:HB3	1:96:A:ASP:HB3	5	1.12
(1,461)	1:96:A:ASP:HA	1:97:A:THR:HG22	5	1.12
(1,139)	1:125:A:VAL:HG23	1:125:A:VAL:HA	1	1.12
(1,4090)	2:16:B:PHE:H	2:12:C:ILE:HD12	6	1.11
(1,3970)	2:8:B:ILE:HD13	2:60:C:PHE:HE1	5	1.11
(1,3740)	2:19:B:ILE:HD13	2:8:C:ILE:HG21	6	1.11
(1,3733)	2:12:C:ILE:HD13	2:40:C:ILE:HG22	3	1.11
(1,3549)	2:55:C:LEU:HD12	2:12:C:ILE:HA	2	1.11
(1,3101)	2:23:C:LYS:HG3	2:23:C:LYS:H	3	1.11
(1,2546)	2:20:B:VAL:HG22	2:30:B:ALA:HB2	3	1.11
(1,2501)	2:25:C:ILE:HG22	2:20:C:VAL:HB	10	1.11
(1,2388)	2:20:B:VAL:HG21	2:34:B:ASN:HD22	1	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2083)	2:25:C:ILE:HD12	2:19:C:ILE:HG21	5	1.11
(1,2062)	2:55:B:LEU:HD21	2:14:B:ASN:HB2	6	1.11
(1,1593)	1:142:A:SER:HB2	1:137:A:VAL:HB	5	1.11
(1,1446)	1:97:A:THR:HG22	1:96:A:ASP:HB3	3	1.11
(1,1172)	1:85:A:LYS:HE3	1:83:A:ALA:H	5	1.11
(1,1158)	1:150:A:PRO:HB3	1:152:A:LEU:H	2	1.11
(1,1021)	1:103:A:GLN:HG3	1:103:A:GLN:H	6	1.11
(1,898)	1:85:A:LYS:HB3	1:86:A:PHE:H	6	1.11
(1,782)	1:98:A:ILE:HG23	1:98:A:ILE:HG12	10	1.11
(1,778)	1:128:A:ASP:HB2	1:99:A:LEU:HD23	7	1.11
(1,736)	1:114:A:ILE:HG12	1:102:A:LYS:HB3	6	1.11
(1,698)	1:79:A:LYS:HE3	1:81:A:ILE:HG21	6	1.11
(1,697)	1:79:A:LYS:HE3	1:79:A:LYS:HG3	6	1.11
(1,174)	1:132:A:LEU:HD22	1:92:A:PHE:HA	6	1.11
(1,4109)	2:21:C:GLU:H	2:22:C:LYS:HG3	5	1.1
(1,3794)	2:17:B:SER:HA	2:19:B:ILE:HG23	10	1.1
(1,3718)	2:54:B:ILE:HG23	2:13:B:VAL:HG21	9	1.1
(1,3629)	2:17:C:SER:HA	2:19:C:ILE:HG23	4	1.1
(1,3608)	2:38:B:ASP:HA	2:40:B:ILE:HD13	5	1.1
(1,3221)	2:34:C:ASN:HA	2:17:C:SER:H	1	1.1
(1,2882)	2:13:B:VAL:HG13	2:41:B:SER:HB3	2	1.1
(1,2638)	2:35:B:VAL:HG22	2:37:B:MET:HB3	9	1.1
(1,2546)	2:20:B:VAL:HG22	2:30:B:ALA:HB2	2	1.1
(1,2532)	2:36:B:ALA:HB1	2:35:B:VAL:HB	9	1.1
(1,2498)	2:25:B:ILE:HG23	2:20:B:VAL:HG13	4	1.1
(1,2211)	2:22:C:LYS:HA	2:24:C:GLU:HB2	10	1.1
(1,2042)	2:5:B:LYS:HD3	2:44:B:PHE:HZ	8	1.1
(1,1809)	1:103:A:GLN:HE22	1:114:A:ILE:HG23	5	1.1
(1,1353)	1:121:A:LEU:HD13	1:141:A:ASN:HD21	8	1.1
(1,1198)	1:113:A:HIS:H	1:116:A:GLU:HB3	6	1.1
(1,782)	1:98:A:ILE:HG23	1:98:A:ILE:HG12	3	1.1
(1,778)	1:128:A:ASP:HB2	1:99:A:LEU:HD23	10	1.1
(1,732)	1:81:A:ILE:HA	1:79:A:LYS:HD3	5	1.1
(1,630)	1:78:A:LEU:HB2	1:146:A:VAL:HG22	7	1.1
(1,229)	1:118:A:LYS:HB2	1:118:A:LYS:HE3	1	1.1
(1,157)	1:99:A:LEU:HD23	1:103:A:GLN:HE22	2	1.1
(1,4187)	1:81:A:ILE:HG23	2:39:B:CYS:H	1	1.09
(1,4183)	1:120:A:LEU:HD11	2:35:C:VAL:H	9	1.09
(1,4081)	2:13:C:VAL:H	2:41:C:SER:HA	6	1.09
(1,3817)	2:6:C:GLU:HB2	2:46:C:PHE:HD2	2	1.09
(1,3718)	2:54:B:ILE:HG22	2:13:B:VAL:HG23	6	1.09
(1,3672)	2:12:B:ILE:HG21	2:11:B:LEU:H	8	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3573)	2:33:C:LEU:HD21	2:19:C:ILE:HB	9	1.09
(1,3544)	2:51:B:VAL:HG23	2:48:B:ARG:HB3	1	1.09
(1,2941)	2:44:C:PHE:HZ	2:33:B:LEU:HD21	4	1.09
(1,2882)	2:13:B:VAL:HG12	2:41:B:SER:HB3	5	1.09
(1,2595)	2:57:C:LYS:HB3	2:68:B:ILE:HG13	1	1.09
(1,2553)	2:35:C:VAL:HG12	2:37:C:MET:HB3	8	1.09
(1,2533)	2:36:C:ALA:HB2	2:35:C:VAL:HB	6	1.09
(1,2500)	2:25:B:ILE:HG23	2:20:B:VAL:HB	5	1.09
(1,2179)	2:9:C:ALA:HA	2:12:C:ILE:HD13	7	1.09
(1,1594)	1:142:A:SER:HB2	1:121:A:LEU:HD13	8	1.09
(1,1457)	1:120:A:LEU:HD21	1:118:A:LYS:HE3	7	1.09
(1,735)	1:79:A:LYS:HD3	1:79:A:LYS:HA	5	1.09
(1,118)	1:97:A:THR:HG22	1:97:A:THR:H	1	1.09
(1,3)	1:120:A:LEU:HD11	1:119:A:LEU:H	5	1.09
(1,4180)	1:147:A:MET:HE3	2:38:B:ASP:H	10	1.08
(1,3732)	2:12:B:ILE:HD11	2:40:B:ILE:HD12	5	1.08
(1,3573)	2:33:C:LEU:HD22	2:19:C:ILE:HB	2	1.08
(1,3554)	2:25:B:ILE:HD11	2:19:B:ILE:HB	6	1.08
(1,3546)	2:51:B:VAL:HG23	2:50:B:ALA:HB3	4	1.08
(1,3312)	2:26:B:SER:H	2:44:C:PHE:HD1	10	1.08
(1,2594)	2:57:B:LYS:HB3	2:68:C:ILE:HG13	3	1.08
(1,2250)	2:11:B:LEU:HA	2:55:B:LEU:HB3	2	1.08
(1,2250)	2:11:B:LEU:HA	2:55:B:LEU:HB3	7	1.08
(1,2083)	2:25:C:ILE:HD12	2:19:C:ILE:HG23	3	1.08
(1,1623)	1:126:A:LEU:HG	1:127:A:HIS:HB2	5	1.08
(1,1593)	1:142:A:SER:HB2	1:137:A:VAL:HB	6	1.08
(1,1435)	1:98:A:ILE:HG23	1:128:A:ASP:H	10	1.08
(1,1021)	1:103:A:GLN:HG3	1:103:A:GLN:H	2	1.08
(1,1021)	1:103:A:GLN:HG3	1:103:A:GLN:H	7	1.08
(1,151)	1:135:A:LEU:HD12	1:135:A:LEU:H	9	1.08
(1,73)	1:88:A:ILE:HG22	1:90:A:HIS:HE1	6	1.08
(1,57)	1:81:A:ILE:HD13	1:145:A:THR:HB	10	1.08
(1,3933)	2:18:C:SER:HB3	2:15:C:TYR:HB3	6	1.07
(1,3889)	2:18:C:SER:HB3	2:22:C:LYS:HG2	3	1.07
(1,3745)	2:40:C:ILE:HD13	2:36:B:ALA:HB2	10	1.07
(1,3719)	2:54:C:ILE:HG21	2:13:C:VAL:HG23	3	1.07
(1,3684)	2:12:B:ILE:HD11	2:15:C:TYR:HD2	4	1.07
(1,3608)	2:38:B:ASP:HA	2:40:B:ILE:HD11	6	1.07
(1,2882)	2:13:B:VAL:HG12	2:41:B:SER:HB3	6	1.07
(1,2552)	2:35:B:VAL:HG12	2:37:B:MET:HB3	3	1.07
(1,2547)	2:20:C:VAL:HG22	2:30:C:ALA:HB3	2	1.07
(1,2242)	2:11:B:LEU:HA	2:54:B:ILE:HB	4	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1346)	1:141:A:ASN:HD22	1:138:A:THR:HG23	5	1.07
(1,735)	1:79:A:LYS:HD3	1:79:A:LYS:HA	1	1.07
(1,717)	1:120:A:LEU:HG	1:125:A:VAL:HA	9	1.07
(1,702)	1:122:A:LYS:HE3	1:122:A:LYS:H	2	1.07
(1,80)	1:148:A:ILE:HG21	1:112:A:SER:HA	4	1.07
(1,4084)	2:14:B:ASN:H	2:12:B:ILE:HG21	5	1.06
(1,3719)	2:54:C:ILE:HG21	2:13:C:VAL:HG23	7	1.06
(1,3621)	2:40:C:ILE:HA	2:36:B:ALA:HB1	5	1.06
(1,3621)	2:40:C:ILE:HA	2:36:B:ALA:HB1	8	1.06
(1,3609)	2:38:C:ASP:HA	2:40:C:ILE:HD12	5	1.06
(1,2882)	2:13:B:VAL:HG13	2:41:B:SER:HB3	3	1.06
(1,2694)	2:54:B:ILE:HG22	2:46:B:PHE:HB2	6	1.06
(1,2533)	2:36:C:ALA:HB2	2:35:C:VAL:HB	9	1.06
(1,2532)	2:36:B:ALA:HB1	2:35:B:VAL:HB	10	1.06
(1,2299)	2:19:C:ILE:HA	2:22:C:LYS:HD3	8	1.06
(1,2083)	2:25:C:ILE:HD12	2:19:C:ILE:HG23	2	1.06
(1,1593)	1:142:A:SER:HB2	1:137:A:VAL:HB	4	1.06
(1,786)	1:126:A:LEU:HD12	1:124:A:LYS:HD3	10	1.06
(1,732)	1:81:A:ILE:HA	1:79:A:LYS:HD3	10	1.06
(1,703)	1:122:A:LYS:HE3	1:141:A:ASN:HD22	10	1.06
(1,630)	1:78:A:LEU:HB2	1:146:A:VAL:HG22	3	1.06
(1,176)	1:132:A:LEU:HD22	1:96:A:ASP:HB2	4	1.06
(1,80)	1:148:A:ILE:HG22	1:112:A:SER:HA	7	1.06
(1,3628)	2:18:B:SER:HB3	2:19:B:ILE:HD12	4	1.05
(1,3621)	2:40:C:ILE:HA	2:36:B:ALA:HB1	1	1.05
(1,2693)	2:50:C:ALA:HB3	2:47:C:GLU:HB2	3	1.05
(1,2645)	2:20:C:VAL:HG12	2:33:C:LEU:HD21	5	1.05
(1,2638)	2:35:B:VAL:HG21	2:37:B:MET:HB3	6	1.05
(1,2532)	2:36:B:ALA:HB1	2:35:B:VAL:HB	2	1.05
(1,2298)	2:19:B:ILE:HA	2:22:B:LYS:HD3	3	1.05
(1,2127)	2:54:C:ILE:HB	2:13:C:VAL:HG21	5	1.05
(1,2083)	2:25:C:ILE:HD12	2:19:C:ILE:HG21	1	1.05
(1,1653)	1:126:A:LEU:HD12	1:124:A:LYS:HD3	9	1.05
(1,672)	1:121:A:LEU:HD21	1:144:A:ILE:HA	2	1.05
(1,179)	1:120:A:LEU:HD21	1:147:A:MET:HG3	1	1.05
(1,174)	1:132:A:LEU:HD22	1:92:A:PHE:HA	9	1.05
(1,174)	1:132:A:LEU:HD22	1:92:A:PHE:HA	10	1.05
(1,162)	1:78:A:LEU:HD23	1:92:A:PHE:HZ	8	1.05
(1,4183)	1:120:A:LEU:HD11	2:35:C:VAL:H	1	1.04
(1,3928)	2:39:B:CYS:HB3	2:35:C:VAL:HB	7	1.04
(1,3851)	2:40:C:ILE:HG22	2:13:C:VAL:HB	7	1.04
(1,3771)	2:30:C:ALA:HA	2:20:C:VAL:HG23	4	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3770)	2:30:B:ALA:HA	2:20:B:VAL:HG22	8	1.04
(1,3621)	2:40:C:ILE:HA	2:36:B:ALA:HB1	6	1.04
(1,3572)	2:33:B:LEU:HD22	2:19:B:ILE:HB	5	1.04
(1,3547)	2:51:C:VAL:HG22	2:50:C:ALA:HB1	4	1.04
(1,3547)	2:51:C:VAL:HG23	2:50:C:ALA:HB3	5	1.04
(1,3547)	2:51:C:VAL:HG22	2:55:C:LEU:HG	10	1.04
(1,3546)	2:51:B:VAL:HG23	2:50:B:ALA:HB3	10	1.04
(1,2883)	2:13:C:VAL:HG13	2:41:C:SER:HB3	10	1.04
(1,2533)	2:36:C:ALA:HB3	2:35:C:VAL:HB	4	1.04
(1,2499)	2:25:C:ILE:HG21	2:20:C:VAL:HG13	8	1.04
(1,2409)	2:19:C:ILE:HG21	2:44:B:PHE:HZ	9	1.04
(1,2083)	2:25:C:ILE:HD12	2:19:C:ILE:HG21	9	1.04
(1,2063)	2:55:C:LEU:HD23	2:14:C:ASN:HB2	8	1.04
(1,47)	1:88:A:ILE:HD13	1:105:A:LEU:HA	9	1.04
(1,3971)	2:8:C:ILE:HD11	2:60:B:PHE:HE1	4	1.03
(1,3795)	2:17:C:SER:HA	2:19:C:ILE:HG22	8	1.03
(1,3555)	2:25:C:ILE:HD12	2:19:C:ILE:HB	4	1.03
(1,3553)	2:25:C:ILE:HD12	2:24:C:GLU:HB3	9	1.03
(1,3045)	2:47:C:GLU:HB2	2:50:C:ALA:H	4	1.03
(1,2534)	2:36:B:ALA:HB3	2:40:C:ILE:HG13	8	1.03
(1,2533)	2:36:C:ALA:HB2	2:35:C:VAL:HB	5	1.03
(1,2490)	2:54:B:ILE:HG21	2:7:B:GLU:HG2	8	1.03
(1,2389)	2:20:C:VAL:HG21	2:34:C:ASN:HD22	10	1.03
(1,2381)	2:55:C:LEU:HD12	2:60:C:PHE:HD1	9	1.03
(1,2158)	2:13:B:VAL:HG21	2:48:B:ARG:HD3	8	1.03
(1,2127)	2:54:C:ILE:HB	2:13:C:VAL:HG22	4	1.03
(1,2082)	2:25:B:ILE:HD11	2:19:B:ILE:HG23	6	1.03
(1,2061)	2:55:C:LEU:HD23	2:14:C:ASN:H	9	1.03
(1,2042)	2:5:B:LYS:HD3	2:44:B:PHE:HZ	1	1.03
(1,1661)	1:149:A:LYS:HE3	1:149:A:LYS:HD3	5	1.03
(1,1593)	1:142:A:SER:HB2	1:137:A:VAL:HB	1	1.03
(1,1434)	1:83:A:ALA:HB3	1:82:A:GLN:HB2	8	1.03
(1,1060)	1:116:A:GLU:HG2	1:116:A:GLU:H	2	1.03
(1,782)	1:98:A:ILE:HG23	1:98:A:ILE:HG12	9	1.03
(1,229)	1:118:A:LYS:HB2	1:118:A:LYS:HE3	3	1.03
(1,174)	1:132:A:LEU:HD22	1:92:A:PHE:HA	1	1.03
(1,118)	1:97:A:THR:HG22	1:97:A:THR:H	2	1.03
(1,80)	1:148:A:ILE:HG22	1:112:A:SER:HA	3	1.03
(1,13)	1:119:A:LEU:HD21	1:98:A:ILE:HA	8	1.03
(1,4052)	2:55:B:LEU:HD22	2:8:B:ILE:H	10	1.02
(1,3874)	2:15:B:TYR:HA	2:12:B:ILE:HD11	10	1.02
(1,3718)	2:54:B:ILE:HG22	2:13:B:VAL:HG23	7	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3544)	2:51:B:VAL:HG23	2:48:B:ARG:HB3	10	1.02
(1,3313)	2:26:C:SER:H	2:44:B:PHE:HD1	4	1.02
(1,3313)	2:26:C:SER:H	2:44:B:PHE:HD1	5	1.02
(1,3183)	2:12:C:ILE:HD13	2:9:C:ALA:H	3	1.02
(1,3119)	2:48:C:ARG:HB3	2:49:C:GLU:H	8	1.02
(1,3049)	2:50:C:ALA:H	2:13:C:VAL:HG11	6	1.02
(1,2950)	2:60:B:PHE:HD1	2:54:B:ILE:HB	2	1.02
(1,2948)	2:60:B:PHE:HD1	2:7:B:GLU:HB3	4	1.02
(1,2501)	2:25:C:ILE:HG22	2:20:C:VAL:HB	1	1.02
(1,2251)	2:11:C:LEU:HA	2:55:C:LEU:HB3	9	1.02
(1,2042)	2:5:B:LYS:HD3	2:44:B:PHE:HZ	4	1.02
(1,2013)	2:47:C:GLU:HG3	2:47:C:GLU:H	4	1.02
(1,1648)	1:135:A:LEU:HA	1:135:A:LEU:HD12	1	1.02
(1,1648)	1:135:A:LEU:HA	1:135:A:LEU:HD12	7	1.02
(1,1648)	1:135:A:LEU:HA	1:135:A:LEU:HD12	10	1.02
(1,1021)	1:103:A:GLN:HG3	1:103:A:GLN:H	1	1.02
(1,1021)	1:103:A:GLN:HG3	1:103:A:GLN:H	9	1.02
(1,262)	1:80:A:LYS:HD3	1:86:A:PHE:HZ	10	1.02
(1,151)	1:135:A:LEU:HD12	1:135:A:LEU:H	3	1.02
(1,150)	1:78:A:LEU:HD13	1:92:A:PHE:HZ	4	1.02
(1,8)	1:120:A:LEU:HD13	1:147:A:MET:HG3	3	1.02
(1,4175)	1:125:A:VAL:HG21	2:31:B:ASP:HB3	3	1.01
(1,4081)	2:13:C:VAL:H	2:41:C:SER:HA	3	1.01
(1,3875)	2:15:C:TYR:HA	2:12:C:ILE:HD11	7	1.01
(1,3794)	2:17:B:SER:HA	2:19:B:ILE:HG23	1	1.01
(1,3732)	2:12:B:ILE:HD11	2:40:B:ILE:HG22	2	1.01
(1,3719)	2:54:C:ILE:HG23	2:13:C:VAL:HG22	1	1.01
(1,3672)	2:12:B:ILE:HG22	2:11:B:LEU:H	3	1.01
(1,3609)	2:38:C:ASP:HA	2:40:C:ILE:HD11	6	1.01
(1,3573)	2:33:C:LEU:HD22	2:19:C:ILE:HB	8	1.01
(1,3552)	2:25:B:ILE:HD13	2:24:B:GLU:HB3	4	1.01
(1,3547)	2:51:C:VAL:HG23	2:50:C:ALA:HB2	3	1.01
(1,3546)	2:51:B:VAL:HG23	2:50:B:ALA:HB2	1	1.01
(1,3324)	2:27:B:GLU:HG3	2:27:B:GLU:H	9	1.01
(1,3220)	2:34:B:ASN:HA	2:17:B:SER:H	9	1.01
(1,3151)	2:5:C:LYS:HG2	2:6:C:GLU:H	9	1.01
(1,3129)	2:55:C:LEU:HD21	2:55:C:LEU:H	9	1.01
(1,2882)	2:13:B:VAL:HG12	2:41:B:SER:HB3	4	1.01
(1,2645)	2:20:C:VAL:HG13	2:33:C:LEU:HD22	2	1.01
(1,2642)	2:25:B:ILE:HD13	2:20:B:VAL:HG11	6	1.01
(1,2247)	2:11:C:LEU:HA	2:12:C:ILE:HD11	3	1.01
(1,2064)	2:55:B:LEU:HD22	2:51:B:VAL:HB	4	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1449)	1:78:A:LEU:HD11	1:90:A:HIS:H	8	1.01
(1,1441)	1:77:A:THR:HG22	1:143:A:THR:HA	2	1.01
(1,1435)	1:98:A:ILE:HG23	1:128:A:ASP:H	3	1.01
(1,704)	1:122:A:LYS:HE3	1:141:A:ASN:HD21	1	1.01
(1,695)	1:79:A:LYS:HE3	1:81:A:ILE:HB	10	1.01
(1,672)	1:121:A:LEU:HD23	1:144:A:ILE:HA	8	1.01
(1,610)	1:108:A:GLU:HG3	1:107:A:SER:HB3	6	1.01
(1,4081)	2:13:C:VAL:H	2:41:C:SER:HA	2	1.0
(1,3962)	2:36:B:ALA:HB3	2:40:C:ILE:HA	2	1.0
(1,3819)	2:6:C:GLU:HB3	2:46:C:PHE:HD2	10	1.0
(1,3818)	2:6:B:GLU:HB3	2:46:B:PHE:HD1	2	1.0
(1,3119)	2:48:C:ARG:HB3	2:49:C:GLU:H	3	1.0
(1,2829)	2:6:C:GLU:HG2	2:9:C:ALA:HB3	6	1.0
(1,2640)	2:33:B:LEU:HD11	2:20:B:VAL:HG11	9	1.0
(1,2127)	2:54:C:ILE:HB	2:13:C:VAL:HG22	1	1.0
(1,2089)	2:8:C:ILE:HD13	2:19:B:ILE:HG12	2	1.0
(1,2082)	2:25:B:ILE:HD11	2:19:B:ILE:HG21	10	1.0
(1,1593)	1:142:A:SER:HB2	1:137:A:VAL:HB	3	1.0
(1,720)	1:148:A:ILE:HD11	1:86:A:PHE:HZ	3	1.0
(1,672)	1:121:A:LEU:HD23	1:144:A:ILE:HA	7	1.0
(1,4181)	1:120:A:LEU:HD12	2:38:C:ASP:H	10	0.99
(1,4052)	2:55:B:LEU:HD22	2:8:B:ILE:H	9	0.99
(1,4050)	2:54:B:ILE:HB	2:50:B:ALA:H	10	0.99
(1,3850)	2:40:B:ILE:HG21	2:13:B:VAL:HB	8	0.99
(1,3672)	2:12:B:ILE:HG23	2:11:B:LEU:H	1	0.99
(1,3556)	2:25:B:ILE:HD13	2:5:C:LYS:HD2	4	0.99
(1,2883)	2:13:C:VAL:HG13	2:41:C:SER:HB3	5	0.99
(1,2882)	2:13:B:VAL:HG12	2:41:B:SER:HB3	1	0.99
(1,2090)	2:8:B:ILE:HD11	2:3:B:ALA:HB3	5	0.99
(1,2088)	2:8:B:ILE:HD11	2:19:C:ILE:HG12	6	0.99
(1,2062)	2:55:B:LEU:HD21	2:14:B:ASN:HB2	7	0.99
(1,2042)	2:5:B:LYS:HD3	2:44:B:PHE:HZ	6	0.99
(1,1820)	1:129:A:ASN:HD21	1:99:A:LEU:HD12	8	0.99
(1,725)	1:148:A:ILE:HD13	1:80:A:LYS:HD3	5	0.99
(1,531)	1:137:A:VAL:HA	1:138:A:THR:HG21	5	0.99
(1,151)	1:135:A:LEU:HD12	1:135:A:LEU:H	6	0.99
(1,135)	1:125:A:VAL:HG23	1:118:A:LYS:HE3	2	0.99
(1,56)	1:114:A:ILE:HD11	1:103:A:GLN:HE21	10	0.99
(1,3935)	2:55:C:LEU:HD12	2:7:C:GLU:HG2	10	0.98
(1,3745)	2:40:C:ILE:HD13	2:36:C:ALA:HB3	2	0.98
(1,3620)	2:40:B:ILE:HA	2:36:C:ALA:HB2	1	0.98
(1,3546)	2:51:B:VAL:HG22	2:55:B:LEU:HG	5	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3322)	2:25:B:ILE:HG12	2:26:B:SER:H	2	0.98
(1,3221)	2:34:C:ASN:HA	2:17:C:SER:H	5	0.98
(1,2950)	2:60:B:PHE:HD2	2:54:B:ILE:HB	3	0.98
(1,2720)	2:54:B:ILE:HD12	2:6:B:GLU:HG3	6	0.98
(1,2628)	2:37:B:MET:HB3	2:17:B:SER:HB3	6	0.98
(1,2558)	2:55:B:LEU:HD22	2:13:B:VAL:HG21	1	0.98
(1,2544)	2:51:B:VAL:HG12	2:55:B:LEU:HG	10	0.98
(1,2532)	2:36:B:ALA:HB1	2:35:B:VAL:HB	8	0.98
(1,2250)	2:11:B:LEU:HA	2:55:B:LEU:HB3	1	0.98
(1,2250)	2:11:B:LEU:HA	2:55:B:LEU:HB3	3	0.98
(1,2250)	2:11:B:LEU:HA	2:55:B:LEU:HB3	8	0.98
(1,2147)	2:23:C:LYS:HE3	2:23:C:LYS:HG3	7	0.98
(1,2126)	2:54:B:ILE:HB	2:13:B:VAL:HG22	4	0.98
(1,2039)	2:5:C:LYS:HB3	2:44:C:PHE:HZ	8	0.98
(1,1614)	1:90:A:HIS:HB2	1:76:A:LEU:HD13	2	0.98
(1,1441)	1:77:A:THR:HG23	1:143:A:THR:HA	7	0.98
(1,1423)	1:119:A:LEU:HD22	1:117:A:ILE:HB	1	0.98
(1,1353)	1:121:A:LEU:HD13	1:141:A:ASN:HD21	3	0.98
(1,1295)	1:129:A:ASN:H	1:97:A:THR:HB	1	0.98
(1,786)	1:126:A:LEU:HD13	1:124:A:LYS:HD3	5	0.98
(1,672)	1:121:A:LEU:HD23	1:144:A:ILE:HA	4	0.98
(1,176)	1:132:A:LEU:HD22	1:96:A:ASP:HB2	1	0.98
(1,151)	1:135:A:LEU:HD12	1:135:A:LEU:H	4	0.98
(1,151)	1:135:A:LEU:HD11	1:135:A:LEU:H	5	0.98
(1,85)	1:73:A:MET:HE1	1:73:A:MET:HA	3	0.98
(1,53)	1:114:A:ILE:HD11	1:103:A:GLN:H	9	0.98
(1,35)	1:106:A:ILE:HD11	1:113:A:HIS:HA	7	0.98
(1,4187)	1:81:A:ILE:HG23	2:39:B:CYS:H	5	0.97
(1,4081)	2:13:C:VAL:H	2:41:C:SER:HA	8	0.97
(1,4050)	2:54:B:ILE:HB	2:50:B:ALA:H	3	0.97
(1,3875)	2:15:C:TYR:HA	2:12:B:ILE:HD13	2	0.97
(1,3718)	2:54:B:ILE:HG22	2:13:B:VAL:HG23	2	0.97
(1,3609)	2:38:C:ASP:HA	2:40:C:ILE:HD11	3	0.97
(1,3609)	2:38:C:ASP:HA	2:13:C:VAL:HG21	10	0.97
(1,3546)	2:51:B:VAL:HG23	2:50:B:ALA:HB2	9	0.97
(1,2882)	2:13:B:VAL:HG12	2:41:B:SER:HB3	10	0.97
(1,2639)	2:35:C:VAL:HG23	2:37:C:MET:HB3	9	0.97
(1,2628)	2:37:B:MET:HB3	2:17:B:SER:HB3	2	0.97
(1,2562)	2:11:B:LEU:HD23	2:55:B:LEU:HD21	5	0.97
(1,2540)	2:36:B:ALA:HB3	2:33:B:LEU:HD13	1	0.97
(1,2499)	2:25:C:ILE:HG22	2:20:C:VAL:HG13	10	0.97
(1,2498)	2:25:B:ILE:HG23	2:20:B:VAL:HG12	9	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2147)	2:23:C:LYS:HE3	2:23:C:LYS:HG3	3	0.97
(1,1467)	1:145:A:THR:HG23	1:82:A:GLN:HE22	9	0.97
(1,1123)	1:87:A:SER:H	1:79:A:LYS:HD3	7	0.97
(1,672)	1:121:A:LEU:HD23	1:144:A:ILE:HA	9	0.97
(1,4086)	2:15:B:TYR:H	2:12:C:ILE:HD12	6	0.96
(1,3929)	2:39:C:CYS:HB3	2:35:B:VAL:HB	8	0.96
(1,3874)	2:15:B:TYR:HA	2:12:C:ILE:HD12	5	0.96
(1,3738)	2:68:B:ILE:HD13	2:11:C:LEU:HD22	10	0.96
(1,3684)	2:12:B:ILE:HD11	2:15:B:TYR:HD2	5	0.96
(1,3608)	2:38:B:ASP:HA	2:40:B:ILE:HD11	7	0.96
(1,2695)	2:54:C:ILE:HG21	2:46:C:PHE:HB2	6	0.96
(1,2638)	2:35:B:VAL:HG21	2:37:B:MET:HB3	2	0.96
(1,2629)	2:37:C:MET:HB3	2:17:C:SER:HB3	8	0.96
(1,2552)	2:35:B:VAL:HG11	2:37:B:MET:HB3	2	0.96
(1,2535)	2:36:C:ALA:HB2	2:40:B:ILE:HG13	3	0.96
(1,2533)	2:36:C:ALA:HB2	2:35:C:VAL:HB	2	0.96
(1,2532)	2:36:B:ALA:HB1	2:35:B:VAL:HB	7	0.96
(1,2309)	2:52:C:SER:HA	2:55:C:LEU:HD11	10	0.96
(1,2147)	2:23:C:LYS:HE3	2:23:C:LYS:HG3	6	0.96
(1,2147)	2:23:C:LYS:HE3	2:23:C:LYS:HG3	10	0.96
(1,2061)	2:55:C:LEU:HD21	2:14:C:ASN:H	1	0.96
(1,1670)	1:136:A:LYS:HA	1:136:A:LYS:HE3	6	0.96
(1,1295)	1:129:A:ASN:H	1:97:A:THR:HB	9	0.96
(1,807)	1:143:A:THR:HA	1:76:A:LEU:HG	2	0.96
(1,736)	1:114:A:ILE:HG12	1:102:A:LYS:HB3	10	0.96
(1,264)	1:81:A:ILE:HG13	1:81:A:ILE:H	2	0.96
(1,151)	1:135:A:LEU:HD12	1:135:A:LEU:H	2	0.96
(1,56)	1:114:A:ILE:HD11	1:103:A:GLN:HE21	7	0.96
(1,4175)	1:125:A:VAL:HG21	2:31:B:ASP:OD2	6	0.95
(1,3983)	2:15:C:TYR:HD2	2:12:B:ILE:HD12	5	0.95
(1,3549)	2:55:C:LEU:HD11	2:12:C:ILE:HA	7	0.95
(1,3546)	2:51:B:VAL:HG22	2:50:B:ALA:HB2	3	0.95
(1,3313)	2:26:C:SER:H	2:44:B:PHE:HD1	7	0.95
(1,3313)	2:26:C:SER:H	2:44:B:PHE:HD1	8	0.95
(1,3221)	2:34:C:ASN:HA	2:17:C:SER:H	7	0.95
(1,2951)	2:60:C:PHE:HD2	2:54:C:ILE:HB	3	0.95
(1,2615)	2:13:C:VAL:HG12	2:48:C:ARG:HG2	5	0.95
(1,2614)	2:13:B:VAL:HG12	2:48:B:ARG:HG2	1	0.95
(1,2533)	2:36:C:ALA:HB2	2:35:C:VAL:HB	7	0.95
(1,2243)	2:11:C:LEU:HA	2:54:C:ILE:HB	4	0.95
(1,2179)	2:9:C:ALA:HA	2:12:C:ILE:HD13	8	0.95
(1,2159)	2:13:C:VAL:HG21	2:48:C:ARG:HD3	6	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2147)	2:23:C:LYS:HE3	2:23:C:LYS:HG3	5	0.95
(1,2126)	2:54:B:ILE:HB	2:13:B:VAL:HG21	10	0.95
(1,2060)	2:55:B:LEU:HD22	2:14:B:ASN:H	10	0.95
(1,1820)	1:129:A:ASN:HD21	1:99:A:LEU:HD12	9	0.95
(1,1656)	1:124:A:LYS:HD3	1:121:A:LEU:HD22	8	0.95
(1,698)	1:79:A:LYS:HE3	1:81:A:ILE:HG21	9	0.95
(1,461)	1:96:A:ASP:HA	1:97:A:THR:HG22	6	0.95
(1,150)	1:78:A:LEU:HD13	1:92:A:PHE:HZ	10	0.95
(1,119)	1:97:A:THR:HG22	1:131:A:PHE:HD2	5	0.95
(1,85)	1:73:A:MET:HE2	1:73:A:MET:HA	1	0.95
(1,3982)	2:15:B:TYR:HD2	2:12:C:ILE:HD11	9	0.94
(1,3851)	2:40:C:ILE:HG21	2:13:C:VAL:HB	3	0.94
(1,3795)	2:17:C:SER:HA	2:19:C:ILE:HG23	9	0.94
(1,3794)	2:17:B:SER:HA	2:19:B:ILE:HG22	6	0.94
(1,3719)	2:54:C:ILE:HG23	2:13:C:VAL:HG23	10	0.94
(1,3220)	2:34:B:ASN:HA	2:17:B:SER:H	8	0.94
(1,2694)	2:54:B:ILE:HG22	2:46:B:PHE:HB2	7	0.94
(1,2639)	2:35:C:VAL:HG22	2:37:C:MET:HB3	7	0.94
(1,2638)	2:35:B:VAL:HG21	2:37:B:MET:HB3	7	0.94
(1,2146)	2:23:B:LYS:HE3	2:23:B:LYS:HG3	1	0.94
(1,2082)	2:25:B:ILE:HD13	2:19:B:ILE:HG23	8	0.94
(1,2082)	2:25:B:ILE:HD13	2:19:B:ILE:HG21	9	0.94
(1,1809)	1:103:A:GLN:HE22	1:99:A:LEU:HD12	9	0.94
(1,1593)	1:142:A:SER:HB2	1:137:A:VAL:HB	7	0.94
(1,1545)	1:136:A:LYS:HA	1:136:A:LYS:HE3	6	0.94
(1,1265)	1:107:A:SER:H	1:108:A:GLU:HG3	6	0.94
(1,785)	1:122:A:LYS:HD3	1:121:A:LEU:HD12	3	0.94
(1,720)	1:148:A:ILE:HD11	1:86:A:PHE:HZ	7	0.94
(1,630)	1:78:A:LEU:HB2	1:146:A:VAL:HG22	5	0.94
(1,511)	1:139:A:PRO:HD2	1:138:A:THR:HB	7	0.94
(1,110)	1:126:A:LEU:HD11	1:125:A:VAL:HA	2	0.94
(1,85)	1:73:A:MET:HE2	1:73:A:MET:HA	7	0.94
(1,4180)	1:147:A:MET:HE1	2:38:B:ASP:H	1	0.93
(1,3819)	2:6:C:GLU:HB3	2:46:C:PHE:HD2	8	0.93
(1,3673)	2:12:C:ILE:HG22	2:11:C:LEU:H	9	0.93
(1,3620)	2:40:B:ILE:HA	2:36:C:ALA:HB2	7	0.93
(1,3554)	2:25:B:ILE:HD13	2:19:B:ILE:HB	8	0.93
(1,3542)	2:51:B:VAL:HG23	2:49:B:GLU:HG3	9	0.93
(1,2695)	2:54:C:ILE:HG21	2:46:C:PHE:HB2	3	0.93
(1,2532)	2:36:B:ALA:HB1	2:35:B:VAL:HB	5	0.93
(1,2250)	2:11:B:LEU:HA	2:55:B:LEU:HB3	4	0.93
(1,2147)	2:23:C:LYS:HE3	2:23:C:LYS:HG3	9	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2146)	2:23:B:LYS:HE3	2:23:B:LYS:HG3	5	0.93
(1,2146)	2:23:B:LYS:HE3	2:23:B:LYS:HG3	7	0.93
(1,1660)	1:125:A:VAL:HG23	1:118:A:LYS:HE3	2	0.93
(1,1441)	1:77:A:THR:HG23	1:143:A:THR:HA	3	0.93
(1,898)	1:85:A:LYS:HB3	1:86:A:PHE:H	10	0.93
(1,229)	1:118:A:LYS:HB2	1:118:A:LYS:HE3	6	0.93
(1,4085)	2:14:C:ASN:H	2:12:C:ILE:HG23	1	0.92
(1,4084)	2:14:B:ASN:H	2:12:B:ILE:HG22	4	0.92
(1,3971)	2:8:C:ILE:HD12	2:60:B:PHE:HE1	10	0.92
(1,3730)	2:12:B:ILE:HD11	2:13:B:VAL:HG13	1	0.92
(1,3673)	2:12:C:ILE:HG23	2:11:C:LEU:H	6	0.92
(1,3608)	2:38:B:ASP:HA	2:40:B:ILE:HD11	3	0.92
(1,3553)	2:25:C:ILE:HD12	2:24:C:GLU:HB3	8	0.92
(1,3546)	2:51:B:VAL:HG23	2:55:B:LEU:HG	2	0.92
(1,3149)	2:5:C:LYS:HG3	2:6:C:GLU:H	9	0.92
(1,2640)	2:33:B:LEU:HD12	2:20:B:VAL:HG12	4	0.92
(1,2605)	2:14:C:ASN:HB2	2:51:C:VAL:HG12	9	0.92
(1,2559)	2:55:C:LEU:HD21	2:13:C:VAL:HG23	10	0.92
(1,2532)	2:36:B:ALA:HB1	2:35:B:VAL:HB	6	0.92
(1,2500)	2:25:B:ILE:HG23	2:20:B:VAL:HB	4	0.92
(1,2499)	2:25:C:ILE:HG22	2:20:C:VAL:HG13	1	0.92
(1,2483)	2:25:C:ILE:HB	2:19:C:ILE:HG21	10	0.92
(1,2244)	2:55:B:LEU:HD22	2:11:B:LEU:HA	1	0.92
(1,2147)	2:23:C:LYS:HE3	2:23:C:LYS:HG3	2	0.92
(1,2146)	2:23:B:LYS:HE3	2:23:B:LYS:HG3	10	0.92
(1,2060)	2:55:B:LEU:HD22	2:14:B:ASN:H	4	0.92
(1,2060)	2:55:B:LEU:HD22	2:14:B:ASN:H	9	0.92
(1,1801)	1:82:A:GLN:HE22	1:81:A:ILE:HG22	6	0.92
(1,749)	1:124:A:LYS:HG2	1:125:A:VAL:HA	1	0.92
(1,51)	1:88:A:ILE:HD13	1:92:A:PHE:HZ	5	0.92
(1,4053)	2:55:C:LEU:HD21	2:8:C:ILE:H	1	0.91
(1,4050)	2:54:B:ILE:HB	2:50:B:ALA:H	9	0.91
(1,3830)	2:40:B:ILE:HD13	2:13:B:VAL:HB	1	0.91
(1,3733)	2:12:C:ILE:HD13	2:40:C:ILE:HG22	2	0.91
(1,3723)	2:25:C:ILE:HG22	2:5:B:LYS:HE3	1	0.91
(1,3673)	2:12:C:ILE:HG23	2:11:C:LEU:H	2	0.91
(1,3555)	2:25:C:ILE:HD12	2:5:B:LYS:HB3	6	0.91
(1,3049)	2:50:C:ALA:H	2:13:C:VAL:HG13	5	0.91
(1,2639)	2:35:C:VAL:HG23	2:37:C:MET:HB3	10	0.91
(1,2628)	2:37:B:MET:HB3	2:17:B:SER:HB3	3	0.91
(1,2595)	2:57:C:LYS:HB3	2:68:B:ILE:HG13	7	0.91
(1,2565)	2:33:C:LEU:HD11	2:19:C:ILE:HG22	10	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2242)	2:11:B:LEU:HA	2:54:B:ILE:HB	6	0.91
(1,2179)	2:9:C:ALA:HA	2:12:C:ILE:HD13	6	0.91
(1,1683)	1:77:A:THR:H	1:76:A:LEU:HD12	8	0.91
(1,1632)	1:147:A:MET:HG3	1:120:A:LEU:HB2	4	0.91
(1,1455)	1:132:A:LEU:HD21	1:94:A:PRO:HA	8	0.91
(1,1423)	1:119:A:LEU:HD22	1:117:A:ILE:HB	4	0.91
(1,1408)	1:148:A:ILE:HG22	1:149:A:LYS:H	2	0.91
(1,803)	1:99:A:LEU:HG	1:103:A:GLN:HE21	5	0.91
(1,58)	1:114:A:ILE:HD12	1:99:A:LEU:HA	9	0.91
(1,13)	1:119:A:LEU:HD21	1:98:A:ILE:HA	4	0.91
(1,3)	1:120:A:LEU:HD12	1:119:A:LEU:H	9	0.91
(3,33)	1:149:A:LYS:H	1:116:A:GLU:O	10	0.9
(1,4080)	2:13:B:VAL:H	2:41:B:SER:HA	8	0.9
(1,3874)	2:15:B:TYR:HA	2:12:C:ILE:HD12	1	0.9
(1,3850)	2:40:B:ILE:HG22	2:13:B:VAL:HB	3	0.9
(1,3830)	2:40:B:ILE:HD11	2:13:B:VAL:HB	8	0.9
(1,3795)	2:17:C:SER:HA	2:19:C:ILE:HG23	1	0.9
(1,3544)	2:51:B:VAL:HG23	2:48:B:ARG:HB3	9	0.9
(1,3183)	2:12:C:ILE:HD13	2:9:C:ALA:H	2	0.9
(1,2937)	2:6:C:GLU:HG2	2:44:C:PHE:HD1	10	0.9
(1,2693)	2:50:C:ALA:HB1	2:47:C:GLU:HB2	1	0.9
(1,2638)	2:35:B:VAL:HG21	2:37:B:MET:HB3	5	0.9
(1,2565)	2:33:C:LEU:HD11	2:19:C:ILE:HG23	7	0.9
(1,2532)	2:36:B:ALA:HB1	2:35:B:VAL:HB	3	0.9
(1,2242)	2:11:B:LEU:HA	2:54:B:ILE:HB	1	0.9
(1,2147)	2:23:C:LYS:HE3	2:23:C:LYS:HG3	1	0.9
(1,1656)	1:124:A:LYS:HD3	1:121:A:LEU:HD22	1	0.9
(1,1651)	1:88:A:ILE:HG21	1:89:A:GLU:HG3	3	0.9
(1,698)	1:79:A:LYS:HE3	1:81:A:ILE:HG21	1	0.9
(1,176)	1:132:A:LEU:HD22	1:96:A:ASP:HB2	8	0.9
(1,4188)	1:79:A:LYS:HE2	2:35:C:VAL:H	8	0.89
(1,3875)	2:15:C:TYR:HA	2:12:B:ILE:HD11	4	0.89
(1,3875)	2:15:C:TYR:HA	2:12:C:ILE:HD11	8	0.89
(1,3850)	2:40:B:ILE:HG21	2:13:B:VAL:HB	7	0.89
(1,3819)	2:6:C:GLU:HB3	2:46:C:PHE:HD2	1	0.89
(1,3795)	2:17:C:SER:HA	2:19:C:ILE:HG22	6	0.89
(1,3794)	2:17:B:SER:HA	2:19:B:ILE:HG22	2	0.89
(1,3794)	2:17:B:SER:HA	2:19:B:ILE:HG22	8	0.89
(1,3771)	2:30:C:ALA:HA	2:20:C:VAL:HG21	9	0.89
(1,3770)	2:20:B:VAL:HG21	2:19:B:ILE:HA	4	0.89
(1,3325)	2:27:C:GLU:HG3	2:27:C:GLU:H	1	0.89
(1,3221)	2:34:C:ASN:HA	2:17:C:SER:H	6	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2638)	2:35:B:VAL:HG21	2:37:B:MET:HB3	8	0.89
(1,2546)	2:20:B:VAL:HG22	2:30:B:ALA:HB2	7	0.89
(1,2533)	2:36:C:ALA:HB2	2:35:C:VAL:HB	3	0.89
(1,2182)	2:9:B:ALA:HA	2:40:B:ILE:HG22	2	0.89
(1,2064)	2:55:B:LEU:HD21	2:51:B:VAL:HB	3	0.89
(1,1818)	1:99:A:LEU:HD23	1:129:A:ASN:HD22	10	0.89
(1,1632)	1:147:A:MET:HG3	1:120:A:LEU:HB2	6	0.89
(1,1557)	1:81:A:ILE:HA	1:85:A:LYS:HD3	7	0.89
(1,1140)	1:82:A:GLN:HG2	1:82:A:GLN:H	3	0.89
(1,1041)	1:108:A:GLU:HG3	1:108:A:GLU:H	7	0.89
(1,867)	1:145:A:THR:HG22	1:145:A:THR:H	1	0.89
(1,736)	1:114:A:ILE:HG12	1:102:A:LYS:HB3	8	0.89
(1,642)	1:97:A:THR:HG23	1:100:A:GLN:HG3	6	0.89
(1,620)	1:73:A:MET:HB3	1:92:A:PHE:HA	2	0.89
(1,54)	1:81:A:ILE:HD12	1:82:A:GLN:H	7	0.89
(1,4179)	1:147:A:MET:HE3	2:35:C:VAL:H	2	0.88
(1,4175)	1:125:A:VAL:HG21	2:31:B:ASP:HB3	4	0.88
(1,3983)	2:15:C:TYR:HD2	2:12:B:ILE:HD11	4	0.88
(1,3929)	2:39:C:CYS:HB3	2:35:B:VAL:HB	3	0.88
(1,3684)	2:12:B:ILE:HD12	2:15:B:TYR:HD2	3	0.88
(1,3575)	2:33:C:LEU:HB2	2:33:C:LEU:HD21	3	0.88
(1,3553)	2:25:C:ILE:HD12	2:24:C:GLU:HB3	2	0.88
(1,2775)	2:71:C:SER:HB3	2:68:C:ILE:H	5	0.88
(1,2638)	2:35:B:VAL:HG23	2:37:B:MET:HB3	3	0.88
(1,2564)	2:33:B:LEU:HD13	2:19:B:ILE:HG23	7	0.88
(1,2501)	2:25:C:ILE:HG21	2:20:C:VAL:HB	8	0.88
(1,2473)	2:12:C:ILE:HG22	2:13:C:VAL:HG12	10	0.88
(1,2193)	2:25:C:ILE:HD11	2:30:C:ALA:HA	1	0.88
(1,1428)	1:106:A:ILE:HD12	1:102:A:LYS:HB3	4	0.88
(1,736)	1:114:A:ILE:HG12	1:102:A:LYS:HB3	4	0.88
(1,700)	1:79:A:LYS:HE3	1:81:A:ILE:HA	5	0.88
(1,54)	1:81:A:ILE:HD11	1:82:A:GLN:H	8	0.88
(1,4188)	1:79:A:LYS:HE2	2:35:C:VAL:H	6	0.87
(1,4180)	1:147:A:MET:HE2	2:38:B:ASP:H	9	0.87
(1,4050)	2:54:B:ILE:HB	2:50:B:ALA:H	1	0.87
(1,3771)	2:20:C:VAL:HG23	2:19:C:ILE:HA	1	0.87
(1,3575)	2:33:C:LEU:HB2	2:33:C:LEU:HD22	2	0.87
(1,3557)	2:25:C:ILE:HD12	2:5:B:LYS:HD2	9	0.87
(1,3546)	2:51:B:VAL:HG23	2:55:B:LEU:HG	8	0.87
(1,3543)	2:51:C:VAL:HG22	2:49:C:GLU:HG3	9	0.87
(1,3119)	2:48:C:ARG:HB3	2:49:C:GLU:H	1	0.87
(1,2642)	2:25:B:ILE:HD13	2:20:B:VAL:HG11	7	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2243)	2:11:C:LEU:HA	2:54:C:ILE:HB	5	0.87
(1,2127)	2:54:C:ILE:HB	2:13:C:VAL:HG23	6	0.87
(1,2038)	2:5:B:LYS:HB3	2:44:B:PHE:HZ	9	0.87
(1,1449)	1:78:A:LEU:HD11	1:90:A:HIS:H	9	0.87
(1,1449)	1:78:A:LEU:HD11	1:90:A:HIS:H	10	0.87
(1,702)	1:122:A:LYS:HE3	1:122:A:LYS:H	8	0.87
(1,531)	1:137:A:VAL:HA	1:138:A:THR:HG23	7	0.87
(1,101)	1:77:A:THR:HG23	1:87:A:SER:HB3	6	0.87
(1,3)	1:120:A:LEU:HD13	1:119:A:LEU:H	1	0.87
(1,4188)	1:79:A:LYS:HE2	2:35:C:VAL:H	5	0.86
(1,4188)	1:79:A:LYS:HE2	2:35:C:VAL:H	7	0.86
(1,4169)	1:81:A:ILE:HD11	2:31:C:ASP:OD2	4	0.86
(1,4091)	2:16:C:PHE:H	2:12:B:ILE:HD12	10	0.86
(1,4050)	2:54:B:ILE:HB	2:50:B:ALA:H	5	0.86
(1,3818)	2:6:B:GLU:HB3	2:46:B:PHE:HD2	9	0.86
(1,3722)	2:25:B:ILE:HG23	2:5:C:LYS:HE3	1	0.86
(1,3620)	2:40:B:ILE:HA	2:36:C:ALA:HB2	2	0.86
(1,3620)	2:40:B:ILE:HA	2:36:C:ALA:HB2	6	0.86
(1,3608)	2:38:B:ASP:HA	2:40:B:ILE:HD11	2	0.86
(1,3573)	2:33:C:LEU:HD21	2:19:C:ILE:HB	5	0.86
(1,3557)	2:25:C:ILE:HD12	2:5:B:LYS:HD2	1	0.86
(1,3552)	2:25:B:ILE:HD11	2:24:B:GLU:HB3	6	0.86
(1,3324)	2:27:B:GLU:HG3	2:27:B:GLU:H	10	0.86
(1,3132)	2:1:B:ASP:H	2:2:B:SER:H	1	0.86
(1,2951)	2:60:C:PHE:HD2	2:54:C:ILE:HB	7	0.86
(1,2950)	2:60:B:PHE:HD1	2:54:B:ILE:HB	7	0.86
(1,2720)	2:54:B:ILE:HD12	2:6:B:GLU:HG3	1	0.86
(1,2251)	2:11:C:LEU:HA	2:55:C:LEU:HB3	4	0.86
(1,2243)	2:11:C:LEU:HA	2:54:C:ILE:HB	3	0.86
(1,2193)	2:25:C:ILE:HD11	2:30:C:ALA:HA	6	0.86
(1,2044)	2:5:B:LYS:HD2	2:44:B:PHE:HZ	9	0.86
(1,1670)	1:136:A:LYS:HA	1:136:A:LYS:HE3	4	0.86
(1,1663)	1:85:A:LYS:HG2	1:85:A:LYS:HE3	1	0.86
(1,1175)	1:153:A:GLU:H	1:152:A:LEU:HD23	5	0.86
(1,790)	1:126:A:LEU:HG	1:124:A:LYS:HE3	10	0.86
(1,697)	1:79:A:LYS:HE3	1:79:A:LYS:HG3	5	0.86
(1,162)	1:78:A:LEU:HD23	1:92:A:PHE:HZ	9	0.86
(1,54)	1:81:A:ILE:HD12	1:82:A:GLN:H	1	0.86
(1,54)	1:81:A:ILE:HD11	1:82:A:GLN:H	3	0.86
(1,36)	1:106:A:ILE:HD11	1:106:A:ILE:HA	7	0.86
(1,35)	1:106:A:ILE:HD13	1:113:A:HIS:HA	4	0.86
(1,3971)	2:8:C:ILE:HD11	2:60:C:PHE:HE1	2	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3962)	2:36:B:ALA:HB2	2:40:C:ILE:HA	4	0.85
(1,3830)	2:40:B:ILE:HD11	2:13:B:VAL:HB	7	0.85
(1,3795)	2:17:C:SER:HA	2:19:C:ILE:HG22	3	0.85
(1,3744)	2:40:B:ILE:HD13	2:36:B:ALA:HB2	10	0.85
(1,3608)	2:38:B:ASP:HA	2:40:B:ILE:HD11	8	0.85
(1,3555)	2:25:C:ILE:HD12	2:19:C:ILE:HB	5	0.85
(1,3324)	2:27:B:GLU:HG3	2:27:B:GLU:H	3	0.85
(1,3220)	2:34:B:ASN:HA	2:17:B:SER:H	4	0.85
(1,3182)	2:12:B:ILE:HD13	2:9:B:ALA:H	4	0.85
(1,3015)	2:5:C:LYS:HG2	2:5:C:LYS:H	10	0.85
(1,2954)	2:16:B:PHE:HZ	2:12:C:ILE:HD13	6	0.85
(1,2563)	2:11:C:LEU:HD22	2:55:C:LEU:HD23	1	0.85
(1,2545)	2:51:C:VAL:HG12	2:55:C:LEU:HG	5	0.85
(1,2534)	2:36:B:ALA:HB2	2:40:C:ILE:HG13	10	0.85
(1,2299)	2:19:C:ILE:HA	2:22:C:LYS:HD3	7	0.85
(1,2182)	2:9:B:ALA:HA	2:40:B:ILE:HG21	1	0.85
(1,1661)	1:149:A:LYS:HE3	1:149:A:LYS:HD3	3	0.85
(1,1594)	1:142:A:SER:HB2	1:121:A:LEU:HD13	3	0.85
(1,1545)	1:136:A:LYS:HA	1:136:A:LYS:HE3	4	0.85
(1,1338)	1:99:A:LEU:HD11	1:103:A:GLN:HE21	10	0.85
(1,785)	1:122:A:LYS:HD3	1:121:A:LEU:HD11	9	0.85
(1,762)	1:119:A:LEU:HA	1:144:A:ILE:HG23	2	0.85
(1,703)	1:122:A:LYS:HE3	1:141:A:ASN:HD22	7	0.85
(1,672)	1:121:A:LEU:HD23	1:144:A:ILE:HA	1	0.85
(1,460)	1:126:A:LEU:HD13	1:120:A:LEU:HA	6	0.85
(1,132)	1:138:A:THR:HG22	1:141:A:ASN:HB3	6	0.85
(1,54)	1:81:A:ILE:HD13	1:82:A:GLN:H	4	0.85
(1,4090)	2:16:B:PHE:H	2:12:C:ILE:HD12	7	0.84
(1,3962)	2:36:B:ALA:HB1	2:40:C:ILE:HA	7	0.84
(1,3818)	2:6:B:GLU:HB3	2:46:B:PHE:HD1	7	0.84
(1,3794)	2:17:B:SER:HA	2:19:B:ILE:HG22	7	0.84
(1,3609)	2:38:C:ASP:HA	2:13:C:VAL:HG23	9	0.84
(1,3542)	2:51:B:VAL:HG23	2:49:B:GLU:HG3	1	0.84
(1,3325)	2:27:C:GLU:HG3	2:27:C:GLU:H	5	0.84
(1,3312)	2:26:B:SER:H	2:44:C:PHE:HD1	8	0.84
(1,3132)	2:1:B:ASP:H	2:2:B:SER:H	10	0.84
(1,2552)	2:35:B:VAL:HG12	2:37:B:MET:HB3	6	0.84
(1,2533)	2:36:C:ALA:HB2	2:35:C:VAL:HB	10	0.84
(1,2357)	2:49:C:GLU:HG2	2:49:C:GLU:H	5	0.84
(1,1794)	1:138:A:THR:H	1:121:A:LEU:HD22	2	0.84
(1,1594)	1:142:A:SER:HB2	1:121:A:LEU:HD13	10	0.84
(1,1159)	1:152:A:LEU:HG	1:152:A:LEU:H	6	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1123)	1:87:A:SER:H	1:79:A:LYS:HD3	5	0.84
(1,867)	1:145:A:THR:HG22	1:145:A:THR:H	6	0.84
(1,735)	1:79:A:LYS:HD3	1:79:A:LYS:HA	4	0.84
(1,669)	1:103:A:GLN:HG3	1:99:A:LEU:HD11	5	0.84
(1,511)	1:139:A:PRO:HD2	1:138:A:THR:HB	5	0.84
(1,25)	1:144:A:ILE:HD11	1:120:A:LEU:H	4	0.84
(1,4081)	2:13:C:VAL:H	2:41:C:SER:HA	9	0.83
(1,4080)	2:13:B:VAL:H	2:41:B:SER:HA	2	0.83
(1,3954)	2:5:B:LYS:HD3	2:19:C:ILE:HG21	8	0.83
(1,3929)	2:39:C:CYS:HB3	2:35:B:VAL:HB	6	0.83
(1,3664)	2:33:B:LEU:HD21	2:16:B:PHE:HD2	7	0.83
(1,3575)	2:33:C:LEU:HB2	2:33:C:LEU:HD23	5	0.83
(1,3574)	2:33:B:LEU:HB2	2:33:B:LEU:HD23	7	0.83
(1,3183)	2:12:C:ILE:HD11	2:9:C:ALA:H	1	0.83
(1,3183)	2:12:C:ILE:HD12	2:9:C:ALA:H	5	0.83
(1,3182)	2:12:B:ILE:HD13	2:9:B:ALA:H	10	0.83
(1,3118)	2:48:B:ARG:HB3	2:49:B:GLU:H	9	0.83
(1,2694)	2:54:B:ILE:HG23	2:46:B:PHE:HB2	10	0.83
(1,2490)	2:54:B:ILE:HG21	2:7:B:GLU:HG2	6	0.83
(1,2422)	2:25:B:ILE:HD13	2:44:C:PHE:HZ	2	0.83
(1,2299)	2:19:C:ILE:HA	2:22:C:LYS:HD3	4	0.83
(1,2182)	2:9:B:ALA:HA	2:40:B:ILE:HG23	6	0.83
(1,2127)	2:54:C:ILE:HB	2:13:C:VAL:HG23	2	0.83
(1,2043)	2:5:C:LYS:HD3	2:44:C:PHE:HZ	4	0.83
(1,2038)	2:5:B:LYS:HB3	2:44:B:PHE:HZ	7	0.83
(1,1441)	1:77:A:THR:HG22	1:143:A:THR:HA	5	0.83
(1,1441)	1:77:A:THR:HG23	1:79:A:LYS:HA	8	0.83
(1,1133)	1:126:A:LEU:HD11	1:126:A:LEU:H	2	0.83
(1,1071)	1:138:A:THR:H	1:138:A:THR:HG21	5	0.83
(1,697)	1:79:A:LYS:HE3	1:79:A:LYS:HG3	7	0.83
(1,535)	1:150:A:PRO:HA	1:116:A:GLU:HG3	10	0.83
(1,247)	1:103:A:GLN:HG2	1:100:A:GLN:HE22	7	0.83
(1,13)	1:119:A:LEU:HD21	1:98:A:ILE:HA	6	0.83
(3,33)	1:149:A:LYS:H	1:116:A:GLU:O	3	0.82
(1,4188)	1:79:A:LYS:HE2	2:35:C:VAL:H	3	0.82
(1,4183)	1:120:A:LEU:HD12	2:35:C:VAL:H	5	0.82
(1,4179)	1:147:A:MET:HE3	2:35:C:VAL:H	1	0.82
(1,4080)	2:13:B:VAL:H	2:41:B:SER:HA	9	0.82
(1,3971)	2:8:C:ILE:HD12	2:60:B:PHE:HE1	1	0.82
(1,3643)	2:68:C:ILE:HB	2:71:C:SER:H	10	0.82
(1,3629)	2:18:C:SER:HB3	2:19:C:ILE:HD13	2	0.82
(1,3629)	2:18:C:SER:HB3	2:19:C:ILE:HD13	3	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3622)	2:12:B:ILE:HA	2:13:B:VAL:HG13	9	0.82
(1,3620)	2:40:B:ILE:HA	2:36:C:ALA:HB3	4	0.82
(1,3549)	2:55:C:LEU:HD12	2:12:C:ILE:HA	3	0.82
(1,3547)	2:51:C:VAL:HG22	2:55:C:LEU:HG	8	0.82
(1,3221)	2:34:C:ASN:HA	2:17:C:SER:H	9	0.82
(1,3182)	2:12:B:ILE:HD11	2:9:B:ALA:H	1	0.82
(1,3044)	2:47:B:GLU:HB2	2:50:B:ALA:H	4	0.82
(1,2544)	2:51:B:VAL:HG12	2:55:B:LEU:HG	9	0.82
(1,2540)	2:36:B:ALA:HB3	2:33:B:LEU:HD11	2	0.82
(1,2483)	2:25:C:ILE:HB	2:19:C:ILE:HG22	6	0.82
(1,2483)	2:25:C:ILE:HB	2:19:C:ILE:HG22	8	0.82
(1,2472)	2:12:B:ILE:HG22	2:13:B:VAL:HG11	9	0.82
(1,2246)	2:11:B:LEU:HA	2:12:B:ILE:HD12	2	0.82
(1,2210)	2:22:B:LYS:HA	2:24:B:GLU:HB2	1	0.82
(1,2192)	2:25:B:ILE:HD11	2:30:B:ALA:HA	10	0.82
(1,2126)	2:54:B:ILE:HB	2:13:B:VAL:HG21	5	0.82
(1,2012)	2:47:B:GLU:HG3	2:47:B:GLU:H	4	0.82
(1,1801)	1:82:A:GLN:HE22	1:81:A:ILE:HG22	1	0.82
(1,1699)	1:98:A:ILE:HG23	1:128:A:ASP:H	10	0.82
(1,1041)	1:108:A:GLU:HG3	1:108:A:GLU:H	3	0.82
(1,958)	1:121:A:LEU:H	1:126:A:LEU:HB3	1	0.82
(1,669)	1:103:A:GLN:HG3	1:99:A:LEU:HD11	10	0.82
(1,229)	1:118:A:LYS:HB2	1:118:A:LYS:HE3	9	0.82
(1,36)	1:106:A:ILE:HD11	1:106:A:ILE:HA	5	0.82
(1,3934)	2:55:B:LEU:HD12	2:7:B:GLU:HG2	4	0.81
(1,3818)	2:6:B:GLU:HB3	2:46:B:PHE:HD2	8	0.81
(1,3795)	2:17:C:SER:HA	2:19:C:ILE:HG22	2	0.81
(1,3795)	2:17:C:SER:HA	2:19:C:ILE:HG22	7	0.81
(1,3770)	2:20:B:VAL:HG23	2:19:B:ILE:HA	9	0.81
(1,3730)	2:12:B:ILE:HD12	2:13:B:VAL:HG11	3	0.81
(1,3421)	2:51:C:VAL:H	2:54:C:ILE:HG12	8	0.81
(1,3133)	2:1:C:ASP:H	2:2:C:SER:H	10	0.81
(1,3069)	2:39:C:CYS:H	2:35:C:VAL:HB	1	0.81
(1,2949)	2:60:C:PHE:HD1	2:7:C:GLU:HB3	4	0.81
(1,2564)	2:33:B:LEU:HD12	2:19:B:ILE:HG21	4	0.81
(1,2251)	2:11:C:LEU:HA	2:55:C:LEU:HB3	2	0.81
(1,2242)	2:11:B:LEU:HA	2:54:B:ILE:HB	2	0.81
(1,2242)	2:11:B:LEU:HA	2:54:B:ILE:HB	7	0.81
(1,2062)	2:55:B:LEU:HD21	2:14:B:ASN:HB2	2	0.81
(1,1663)	1:85:A:LYS:HG2	1:85:A:LYS:HE3	6	0.81
(1,1594)	1:142:A:SER:HB2	1:121:A:LEU:HD13	1	0.81
(1,1455)	1:132:A:LEU:HD21	1:94:A:PRO:HA	1	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1435)	1:98:A:ILE:HG23	1:128:A:ASP:H	4	0.81
(1,804)	1:121:A:LEU:HD21	1:141:A:ASN:HD21	8	0.81
(1,804)	1:121:A:LEU:HD21	1:141:A:ASN:HD21	10	0.81
(1,717)	1:120:A:LEU:HG	1:125:A:VAL:HA	10	0.81
(1,703)	1:122:A:LYS:HE3	1:141:A:ASN:HD22	9	0.81
(1,183)	1:99:A:LEU:HD11	1:100:A:GLN:HE22	8	0.81
(1,85)	1:73:A:MET:HE1	1:73:A:MET:HA	10	0.81
(1,36)	1:106:A:ILE:HD12	1:106:A:ILE:HA	9	0.81
(1,4080)	2:13:B:VAL:H	2:41:B:SER:HA	3	0.8
(1,4080)	2:13:B:VAL:H	2:41:B:SER:HA	10	0.8
(1,4053)	2:55:C:LEU:HD22	2:8:C:ILE:H	4	0.8
(1,3794)	2:17:B:SER:HA	2:19:B:ILE:HG22	3	0.8
(1,3771)	2:20:C:VAL:HG23	2:19:C:ILE:HA	5	0.8
(1,3745)	2:40:C:ILE:HD12	2:36:B:ALA:HB2	3	0.8
(1,3642)	2:68:B:ILE:HB	2:71:B:SER:H	10	0.8
(1,3552)	2:25:B:ILE:HD11	2:24:B:GLU:HB3	7	0.8
(1,3069)	2:39:C:CYS:H	2:35:C:VAL:HB	7	0.8
(1,3069)	2:39:C:CYS:H	2:35:C:VAL:HB	10	0.8
(1,2950)	2:60:B:PHE:HD1	2:54:B:ILE:HB	4	0.8
(1,2693)	2:50:C:ALA:HB1	2:47:C:GLU:HB2	9	0.8
(1,2691)	2:50:C:ALA:HB1	2:47:C:GLU:HB3	1	0.8
(1,2552)	2:35:B:VAL:HG11	2:37:B:MET:HB3	8	0.8
(1,2552)	2:35:B:VAL:HG11	2:37:B:MET:HB3	9	0.8
(1,2532)	2:36:B:ALA:HB1	2:35:B:VAL:HB	1	0.8
(1,2491)	2:54:C:ILE:HG22	2:7:C:GLU:HG2	10	0.8
(1,2482)	2:25:B:ILE:HB	2:19:B:ILE:HG22	3	0.8
(1,2211)	2:22:C:LYS:HA	2:24:C:GLU:HB2	5	0.8
(1,2182)	2:9:B:ALA:HA	2:40:B:ILE:HG21	9	0.8
(1,2179)	2:9:C:ALA:HA	2:12:C:ILE:HD11	9	0.8
(1,2159)	2:13:C:VAL:HG21	2:48:C:ARG:HD3	2	0.8
(1,1457)	1:120:A:LEU:HD22	1:118:A:LYS:HE3	3	0.8
(1,1435)	1:98:A:ILE:HG23	1:128:A:ASP:H	6	0.8
(1,1435)	1:98:A:ILE:HG23	1:128:A:ASP:H	7	0.8
(1,1423)	1:119:A:LEU:HD23	1:117:A:ILE:HB	9	0.8
(1,1272)	1:111:A:ALA:H	1:106:A:ILE:HD11	5	0.8
(1,867)	1:145:A:THR:HG22	1:145:A:THR:H	3	0.8
(1,732)	1:81:A:ILE:HA	1:79:A:LYS:HD3	8	0.8
(1,396)	1:80:A:LYS:HD2	1:86:A:PHE:HZ	10	0.8
(1,180)	1:132:A:LEU:HD12	1:96:A:ASP:HB2	6	0.8
(1,176)	1:132:A:LEU:HD22	1:96:A:ASP:HB2	3	0.8
(1,47)	1:88:A:ILE:HD13	1:105:A:LEU:HA	6	0.8
(1,4188)	1:79:A:LYS:HE2	2:35:C:VAL:H	4	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4084)	2:14:B:ASN:H	2:12:B:ILE:HG21	6	0.79
(1,3819)	2:6:C:GLU:HB3	2:46:C:PHE:HD2	3	0.79
(1,3739)	2:68:C:ILE:HD12	2:11:B:LEU:HD23	5	0.79
(1,3672)	2:12:B:ILE:HG21	2:11:B:LEU:H	10	0.79
(1,3575)	2:33:C:LEU:HB2	2:33:C:LEU:HD22	8	0.79
(1,3571)	2:13:C:VAL:HG21	2:48:C:ARG:HG3	8	0.79
(1,2775)	2:71:C:SER:HB3	2:68:C:ILE:H	10	0.79
(1,2640)	2:33:B:LEU:HD12	2:20:B:VAL:HG11	3	0.79
(1,2639)	2:35:C:VAL:HG21	2:37:C:MET:HB3	5	0.79
(1,2534)	2:36:B:ALA:HB1	2:40:C:ILE:HG13	3	0.79
(1,2423)	2:25:C:ILE:HD12	2:44:B:PHE:HZ	6	0.79
(1,1809)	1:103:A:GLN:HE22	1:114:A:ILE:HG21	1	0.79
(1,1454)	1:105:A:LEU:HD22	1:105:A:LEU:HB2	1	0.79
(1,1452)	1:78:A:LEU:HD21	1:90:A:HIS:HE1	1	0.79
(1,791)	1:136:A:LYS:HG3	1:136:A:LYS:HE3	10	0.79
(1,101)	1:77:A:THR:HG23	1:87:A:SER:HB3	4	0.79
(1,67)	1:83:A:ALA:HB2	1:85:A:LYS:H	5	0.79
(1,36)	1:106:A:ILE:HD11	1:106:A:ILE:HA	8	0.79
(1,4188)	1:79:A:LYS:HE2	2:35:C:VAL:H	2	0.78
(1,4188)	1:79:A:LYS:HE2	2:35:C:VAL:H	9	0.78
(1,4186)	1:120:A:LEU:HG	2:35:B:VAL:H	8	0.78
(1,4185)	1:120:A:LEU:HG	2:35:B:VAL:H	8	0.78
(1,3771)	2:30:C:ALA:HA	2:20:C:VAL:HG22	8	0.78
(1,3738)	2:68:B:ILE:HD13	2:11:C:LEU:HD22	1	0.78
(1,3723)	2:25:C:ILE:HG21	2:5:B:LYS:HE3	2	0.78
(1,3575)	2:33:C:LEU:HD22	2:43:B:ALA:HB1	9	0.78
(1,3553)	2:25:C:ILE:HD12	2:24:C:GLU:HB3	7	0.78
(1,3221)	2:34:C:ASN:HA	2:17:C:SER:H	10	0.78
(1,2950)	2:60:B:PHE:HD1	2:54:B:ILE:HB	8	0.78
(1,2640)	2:33:B:LEU:HD12	2:20:B:VAL:HG13	8	0.78
(1,2595)	2:57:C:LYS:HB3	2:68:B:ILE:HG13	8	0.78
(1,2565)	2:33:C:LEU:HD11	2:19:C:ILE:HG23	6	0.78
(1,2533)	2:36:C:ALA:HB2	2:35:C:VAL:HB	1	0.78
(1,2483)	2:25:C:ILE:HB	2:19:C:ILE:HG23	7	0.78
(1,2357)	2:49:C:GLU:HG2	2:49:C:GLU:H	10	0.78
(1,2127)	2:54:C:ILE:HB	2:13:C:VAL:HG23	10	0.78
(1,1760)	1:152:A:LEU:HB3	1:153:A:GLU:H	10	0.78
(1,1683)	1:77:A:THR:H	1:76:A:LEU:HD11	2	0.78
(1,1648)	1:136:A:LYS:HA	1:135:A:LEU:HD11	5	0.78
(1,1594)	1:142:A:SER:HB2	1:121:A:LEU:HD13	7	0.78
(1,736)	1:114:A:ILE:HG12	1:102:A:LYS:HB3	2	0.78
(1,734)	1:87:A:SER:HA	1:79:A:LYS:HD3	3	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,695)	1:79:A:LYS:HE3	1:81:A:ILE:HB	2	0.78
(1,229)	1:118:A:LYS:HB2	1:118:A:LYS:HE3	7	0.78
(1,80)	1:148:A:ILE:HG22	1:112:A:SER:HA	10	0.78
(3,33)	1:149:A:LYS:H	1:116:A:GLU:O	7	0.77
(1,4188)	1:79:A:LYS:HE2	2:35:C:VAL:H	1	0.77
(1,4085)	2:14:C:ASN:H	2:12:C:ILE:HG23	4	0.77
(1,4008)	2:16:B:PHE:HZ	2:12:C:ILE:HG23	9	0.77
(1,3770)	2:20:B:VAL:HG23	2:19:B:ILE:HA	10	0.77
(1,3621)	2:40:C:ILE:HA	2:36:B:ALA:HB1	10	0.77
(1,3557)	2:25:C:ILE:HD12	2:5:B:LYS:HD2	8	0.77
(1,3546)	2:51:B:VAL:HG21	2:50:B:ALA:HB2	7	0.77
(1,3313)	2:26:C:SER:H	2:44:B:PHE:HD1	6	0.77
(1,2594)	2:57:B:LYS:HB3	2:68:C:ILE:HG13	8	0.77
(1,2553)	2:35:C:VAL:HG11	2:37:C:MET:HB3	9	0.77
(1,2535)	2:36:C:ALA:HB3	2:40:B:ILE:HG13	10	0.77
(1,2242)	2:11:B:LEU:HA	2:54:B:ILE:HB	8	0.77
(1,2205)	2:22:C:LYS:HG2	2:22:C:LYS:HA	5	0.77
(1,2182)	2:9:B:ALA:HA	2:40:B:ILE:HG22	7	0.77
(1,2127)	2:54:C:ILE:HB	2:13:C:VAL:HG23	7	0.77
(1,2126)	2:54:B:ILE:HB	2:13:B:VAL:HG21	9	0.77
(1,1663)	1:85:A:LYS:HG2	1:85:A:LYS:HE3	10	0.77
(1,1467)	1:145:A:THR:HG23	1:82:A:GLN:HE22	6	0.77
(1,1441)	1:77:A:THR:HG23	1:143:A:THR:HA	10	0.77
(1,1440)	1:74:A:VAL:HG11	1:96:A:ASP:H	5	0.77
(1,898)	1:85:A:LYS:HB3	1:86:A:PHE:H	3	0.77
(1,642)	1:97:A:THR:HG21	1:100:A:GLN:HG3	8	0.77
(1,176)	1:132:A:LEU:HD22	1:96:A:ASP:HB2	9	0.77
(1,173)	1:78:A:LEU:HD21	1:90:A:HIS:HB3	7	0.77
(1,113)	1:77:A:THR:HG22	1:88:A:ILE:H	1	0.77
(1,80)	1:148:A:ILE:HG22	1:112:A:SER:HA	1	0.77
(1,36)	1:106:A:ILE:HD13	1:106:A:ILE:HA	6	0.77
(1,3771)	2:20:C:VAL:HG23	2:19:C:ILE:HA	10	0.76
(1,3693)	2:9:C:ALA:HA	2:16:B:PHE:HZ	7	0.76
(1,3673)	2:12:C:ILE:HG22	2:11:C:LEU:H	3	0.76
(1,3620)	2:40:B:ILE:HA	2:36:C:ALA:HB2	9	0.76
(1,3546)	2:51:B:VAL:HG21	2:50:B:ALA:HB2	6	0.76
(1,3119)	2:48:C:ARG:HB3	2:49:C:GLU:H	10	0.76
(1,2553)	2:35:C:VAL:HG12	2:37:C:MET:HB3	5	0.76
(1,2545)	2:51:C:VAL:HG12	2:55:C:LEU:HG	4	0.76
(1,2482)	2:25:B:ILE:HB	2:19:B:ILE:HG23	4	0.76
(1,2473)	2:12:C:ILE:HG23	2:13:C:VAL:HG11	5	0.76
(1,2246)	2:11:B:LEU:HA	2:12:B:ILE:HD12	1	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1784)	1:105:A:LEU:H	1:117:A:ILE:HD13	1	0.76
(1,1697)	1:90:A:HIS:H	1:76:A:LEU:HD11	1	0.76
(1,1623)	1:126:A:LEU:HG	1:127:A:HIS:HB2	10	0.76
(1,1593)	1:142:A:SER:HB2	1:137:A:VAL:HB	8	0.76
(1,1593)	1:142:A:SER:HB2	1:137:A:VAL:HB	10	0.76
(1,1441)	1:77:A:THR:HG23	1:143:A:THR:HA	1	0.76
(1,1198)	1:113:A:HIS:H	1:116:A:GLU:HB3	10	0.76
(1,734)	1:87:A:SER:HA	1:79:A:LYS:HD3	8	0.76
(1,669)	1:103:A:GLN:HG3	1:99:A:LEU:HD11	7	0.76
(1,36)	1:106:A:ILE:HD11	1:106:A:ILE:HA	2	0.76
(1,36)	1:106:A:ILE:HD13	1:106:A:ILE:HA	3	0.76
(1,25)	1:144:A:ILE:HD12	1:120:A:LEU:H	9	0.76
(1,4188)	1:79:A:LYS:HE2	2:35:C:VAL:H	10	0.75
(1,4051)	2:54:C:ILE:HB	2:50:C:ALA:H	5	0.75
(1,3954)	2:5:B:LYS:HD3	2:19:C:ILE:HD11	9	0.75
(1,3937)	2:13:C:VAL:HG21	2:48:C:ARG:HG3	3	0.75
(1,3794)	2:17:B:SER:HA	2:19:B:ILE:HG21	4	0.75
(1,3620)	2:40:B:ILE:HA	2:36:C:ALA:HB2	5	0.75
(1,3544)	2:51:B:VAL:HG21	2:48:B:ARG:HB3	6	0.75
(1,3317)	2:26:C:SER:H	2:33:C:LEU:HD11	7	0.75
(1,3317)	2:26:C:SER:H	2:33:C:LEU:HD11	8	0.75
(1,3317)	2:26:C:SER:H	2:33:C:LEU:HD11	10	0.75
(1,3069)	2:39:C:CYS:H	2:35:C:VAL:HB	8	0.75
(1,3049)	2:50:C:ALA:H	2:13:C:VAL:HG11	7	0.75
(1,2694)	2:54:B:ILE:HG22	2:46:B:PHE:HB2	3	0.75
(1,2639)	2:35:C:VAL:HG21	2:37:C:MET:HB3	8	0.75
(1,2243)	2:11:C:LEU:HA	2:54:C:ILE:HB	10	0.75
(1,2210)	2:22:B:LYS:HA	2:24:B:GLU:HB2	9	0.75
(1,2193)	2:25:C:ILE:HD11	2:30:C:ALA:HA	8	0.75
(1,2090)	2:8:B:ILE:HD12	2:3:B:ALA:HB3	10	0.75
(1,1994)	2:36:B:ALA:HB3	2:33:B:LEU:HD23	2	0.75
(1,1699)	1:98:A:ILE:HG23	1:128:A:ASP:H	3	0.75
(1,1623)	1:126:A:LEU:HG	1:127:A:HIS:HB2	2	0.75
(1,1454)	1:105:A:LEU:HD23	1:105:A:LEU:HB2	5	0.75
(1,1441)	1:77:A:THR:HG23	1:79:A:LYS:HA	6	0.75
(1,1338)	1:99:A:LEU:HD11	1:103:A:GLN:HE21	3	0.75
(1,695)	1:79:A:LYS:HE3	1:81:A:ILE:HB	7	0.75
(1,4098)	2:17:B:SER:H	2:12:B:ILE:HG21	5	0.74
(1,4081)	2:13:C:VAL:H	2:41:C:SER:HA	1	0.74
(1,3888)	2:18:B:SER:HB3	2:22:B:LYS:HD3	9	0.74
(1,3801)	2:8:C:ILE:HG23	2:16:B:PHE:HD1	5	0.74
(1,3547)	2:51:C:VAL:HG22	2:55:C:LEU:HG	2	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3524)	2:6:B:GLU:HG3	2:46:B:PHE:HD1	1	0.74
(1,3220)	2:34:B:ASN:HA	2:17:B:SER:H	3	0.74
(1,3182)	2:12:B:ILE:HD11	2:9:B:ALA:H	2	0.74
(1,3069)	2:39:C:CYS:H	2:35:C:VAL:HB	4	0.74
(1,2951)	2:60:C:PHE:HD2	2:54:C:ILE:HB	8	0.74
(1,2597)	2:51:C:VAL:HB	2:55:C:LEU:HD13	9	0.74
(1,2545)	2:51:C:VAL:HG12	2:55:C:LEU:HG	8	0.74
(1,2308)	2:52:B:SER:HA	2:55:B:LEU:HD11	1	0.74
(1,2243)	2:11:C:LEU:HA	2:54:C:ILE:HB	1	0.74
(1,2242)	2:11:B:LEU:HA	2:54:B:ILE:HB	3	0.74
(1,2084)	2:25:B:ILE:HD13	2:25:B:ILE:HG22	8	0.74
(1,2065)	2:55:C:LEU:HD21	2:51:C:VAL:HB	1	0.74
(1,1603)	1:141:A:ASN:HB2	1:121:A:LEU:HD13	2	0.74
(1,1528)	1:121:A:LEU:HA	1:122:A:LYS:HB3	5	0.74
(1,1452)	1:78:A:LEU:HD21	1:90:A:HIS:HE1	7	0.74
(1,1399)	1:80:A:LYS:HE3	1:148:A:ILE:H	5	0.74
(1,1338)	1:99:A:LEU:HD11	1:103:A:GLN:HE21	7	0.74
(1,1169)	1:125:A:VAL:HG22	1:125:A:VAL:H	8	0.74
(1,1140)	1:82:A:GLN:HG2	1:82:A:GLN:H	4	0.74
(1,1140)	1:82:A:GLN:HG2	1:82:A:GLN:H	7	0.74
(1,535)	1:150:A:PRO:HA	1:116:A:GLU:HG3	1	0.74
(1,183)	1:99:A:LEU:HD11	1:100:A:GLN:HE22	7	0.74
(1,177)	1:132:A:LEU:HD23	1:97:A:THR:HA	1	0.74
(1,80)	1:148:A:ILE:HG22	1:112:A:SER:HA	6	0.74
(1,36)	1:106:A:ILE:HD13	1:106:A:ILE:HA	10	0.74
(1,35)	1:106:A:ILE:HD13	1:113:A:HIS:HA	10	0.74
(1,4181)	1:120:A:LEU:HD12	2:38:C:ASP:H	5	0.73
(1,4175)	1:125:A:VAL:HB	2:39:C:CYS:HG	10	0.73
(1,4051)	2:54:C:ILE:HB	2:50:C:ALA:H	1	0.73
(1,4051)	2:54:C:ILE:HB	2:50:C:ALA:H	8	0.73
(1,3933)	2:18:C:SER:HB3	2:22:C:LYS:HE3	5	0.73
(1,3665)	2:33:C:LEU:HD23	2:44:B:PHE:HZ	4	0.73
(1,3553)	2:25:C:ILE:HD12	2:24:C:GLU:HB3	3	0.73
(1,3549)	2:55:C:LEU:HD12	2:12:C:ILE:HA	8	0.73
(1,3183)	2:12:C:ILE:HD12	2:9:C:ALA:H	4	0.73
(1,3133)	2:1:C:ASP:H	2:2:C:SER:H	1	0.73
(1,3133)	2:1:C:ASP:H	2:2:C:SER:H	5	0.73
(1,3133)	2:1:C:ASP:H	2:2:C:SER:H	9	0.73
(1,3132)	2:1:B:ASP:H	2:2:B:SER:H	5	0.73
(1,2641)	2:33:C:LEU:HD11	2:20:C:VAL:HG12	4	0.73
(1,2630)	2:51:B:VAL:HB	2:55:B:LEU:HG	4	0.73
(1,2595)	2:57:C:LYS:HB3	2:68:B:ILE:HG13	3	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2565)	2:33:C:LEU:HD13	2:19:C:ILE:HG22	3	0.73
(1,2541)	2:36:C:ALA:HB1	2:33:C:LEU:HD12	7	0.73
(1,2535)	2:36:C:ALA:HB2	2:40:B:ILE:HG13	8	0.73
(1,2426)	2:68:B:ILE:HD13	2:60:C:PHE:HD2	2	0.73
(1,2251)	2:11:C:LEU:HA	2:55:C:LEU:HB3	6	0.73
(1,2247)	2:11:C:LEU:HA	2:12:C:ILE:HD11	8	0.73
(1,2193)	2:25:C:ILE:HD11	2:30:C:ALA:HA	3	0.73
(1,2065)	2:55:C:LEU:HD21	2:51:C:VAL:HB	5	0.73
(1,2064)	2:55:B:LEU:HD22	2:51:B:VAL:HB	9	0.73
(1,1801)	1:82:A:GLN:HE22	1:81:A:ILE:HG22	9	0.73
(1,1683)	1:77:A:THR:H	1:76:A:LEU:HD12	9	0.73
(1,1670)	1:136:A:LYS:HA	1:136:A:LYS:HE3	8	0.73
(1,1623)	1:126:A:LEU:HG	1:127:A:HIS:HB2	3	0.73
(1,1423)	1:119:A:LEU:HD21	1:126:A:LEU:HB3	2	0.73
(1,1169)	1:125:A:VAL:HG23	1:125:A:VAL:H	10	0.73
(1,53)	1:114:A:ILE:HD11	1:103:A:GLN:H	3	0.73
(1,35)	1:106:A:ILE:HD11	1:113:A:HIS:HA	5	0.73
(1,25)	1:144:A:ILE:HD12	1:120:A:LEU:H	5	0.73
(1,2)	1:120:A:LEU:HD11	1:120:A:LEU:H	5	0.73
(3,33)	1:149:A:LYS:H	1:116:A:GLU:O	2	0.72
(1,4099)	2:17:C:SER:H	2:12:C:ILE:HG22	10	0.72
(1,4080)	2:13:B:VAL:H	2:41:B:SER:HA	1	0.72
(1,4080)	2:13:B:VAL:H	2:41:B:SER:HA	4	0.72
(1,4051)	2:54:C:ILE:HB	2:50:C:ALA:H	6	0.72
(1,4051)	2:54:C:ILE:HB	2:50:C:ALA:H	10	0.72
(1,3937)	2:13:C:VAL:HG21	2:48:C:ARG:HG3	10	0.72
(1,3420)	2:51:B:VAL:H	2:54:B:ILE:HG12	6	0.72
(1,3317)	2:26:C:SER:H	2:33:C:LEU:HD13	2	0.72
(1,3312)	2:26:B:SER:H	2:44:C:PHE:HD1	5	0.72
(1,2594)	2:57:B:LYS:HB3	2:68:C:ILE:HG13	10	0.72
(1,2251)	2:11:C:LEU:HA	2:55:C:LEU:HB3	3	0.72
(1,2146)	2:23:B:LYS:HE3	2:23:B:LYS:HG3	2	0.72
(1,2061)	2:55:C:LEU:HD23	2:14:C:ASN:H	6	0.72
(1,2042)	2:5:B:LYS:HD3	2:44:B:PHE:HZ	7	0.72
(1,1809)	1:103:A:GLN:HE22	1:99:A:LEU:HD12	6	0.72
(1,1662)	1:149:A:LYS:HG3	1:149:A:LYS:HE3	8	0.72
(1,1648)	1:136:A:LYS:HA	1:135:A:LEU:HD12	6	0.72
(1,1454)	1:78:A:LEU:HD22	1:78:A:LEU:HB3	6	0.72
(1,1454)	1:78:A:LEU:HD21	1:78:A:LEU:HB3	9	0.72
(1,1169)	1:125:A:VAL:HG22	1:125:A:VAL:H	7	0.72
(1,1169)	1:125:A:VAL:HG23	1:125:A:VAL:H	9	0.72
(1,1037)	1:107:A:SER:HB3	1:107:A:SER:H	3	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1010)	1:98:A:ILE:H	1:98:A:ILE:HG13	5	0.72
(1,1010)	1:98:A:ILE:H	1:98:A:ILE:HG13	9	0.72
(1,791)	1:136:A:LYS:HG3	1:136:A:LYS:HE3	1	0.72
(1,735)	1:79:A:LYS:HD3	1:79:A:LYS:HA	7	0.72
(1,461)	1:96:A:ASP:HA	1:97:A:THR:HG22	8	0.72
(1,73)	1:88:A:ILE:HG22	1:90:A:HIS:HE1	3	0.72
(1,47)	1:88:A:ILE:HD13	1:105:A:LEU:HA	8	0.72
(1,4085)	2:14:C:ASN:H	2:12:C:ILE:HG23	7	0.71
(1,4014)	2:60:B:PHE:HD2	2:68:C:ILE:HD11	5	0.71
(1,3830)	2:40:B:ILE:HD13	2:13:B:VAL:HB	10	0.71
(1,3770)	2:20:B:VAL:HG23	2:19:B:ILE:HA	5	0.71
(1,3770)	2:30:B:ALA:HA	2:20:B:VAL:HG22	6	0.71
(1,3745)	2:40:C:ILE:HD13	2:36:C:ALA:HB3	9	0.71
(1,3673)	2:12:C:ILE:HG21	2:11:C:LEU:H	7	0.71
(1,3622)	2:12:B:ILE:HA	2:13:B:VAL:HG13	5	0.71
(1,3571)	2:13:C:VAL:HG21	2:48:C:ARG:HG3	3	0.71
(1,3556)	2:25:B:ILE:HD12	2:5:C:LYS:HD2	10	0.71
(1,3220)	2:34:B:ASN:HA	2:17:B:SER:H	5	0.71
(1,3068)	2:39:B:CYS:H	2:35:B:VAL:HB	2	0.71
(1,2955)	2:16:C:PHE:HZ	2:12:B:ILE:HD13	10	0.71
(1,2694)	2:54:B:ILE:HG23	2:46:B:PHE:HB2	1	0.71
(1,2628)	2:37:B:MET:HB3	2:17:B:SER:HB3	7	0.71
(1,2594)	2:57:B:LYS:HB3	2:68:C:ILE:HG13	7	0.71
(1,2541)	2:36:C:ALA:HB1	2:33:C:LEU:HD12	5	0.71
(1,2534)	2:36:B:ALA:HB2	2:40:C:ILE:HG13	5	0.71
(1,2251)	2:11:C:LEU:HA	2:55:C:LEU:HB3	7	0.71
(1,2251)	2:11:C:LEU:HA	2:55:C:LEU:HB3	10	0.71
(1,2091)	2:8:C:ILE:HD11	2:3:C:ALA:HB1	6	0.71
(1,2090)	2:8:B:ILE:HD13	2:3:B:ALA:HB3	8	0.71
(1,1648)	1:136:A:LYS:HA	1:135:A:LEU:HD12	2	0.71
(1,1648)	1:136:A:LYS:HA	1:135:A:LEU:HD12	3	0.71
(1,1632)	1:147:A:MET:HG3	1:120:A:LEU:HB2	7	0.71
(1,1545)	1:136:A:LYS:HA	1:136:A:LYS:HE3	8	0.71
(1,1272)	1:111:A:ALA:H	1:106:A:ILE:HD11	7	0.71
(1,1037)	1:107:A:SER:HB3	1:107:A:SER:H	1	0.71
(1,1037)	1:107:A:SER:HB3	1:107:A:SER:H	4	0.71
(1,1010)	1:98:A:ILE:H	1:98:A:ILE:HG13	2	0.71
(1,736)	1:114:A:ILE:HG12	1:102:A:LYS:HB3	7	0.71
(1,732)	1:81:A:ILE:HA	1:79:A:LYS:HD3	3	0.71
(1,535)	1:150:A:PRO:HA	1:116:A:GLU:HG3	7	0.71
(1,4169)	1:81:A:ILE:HD13	2:31:C:ASP:OD2	7	0.7
(1,4080)	2:13:B:VAL:H	2:41:B:SER:HA	5	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4050)	2:54:B:ILE:HB	2:50:B:ALA:H	4	0.7
(1,3889)	2:18:C:SER:HB3	2:22:C:LYS:HG2	10	0.7
(1,3549)	2:55:C:LEU:HD13	2:12:C:ILE:HA	6	0.7
(1,3547)	2:51:C:VAL:HG22	2:55:C:LEU:HG	7	0.7
(1,3542)	2:51:B:VAL:HG23	2:49:B:GLU:HG3	10	0.7
(1,3476)	2:55:B:LEU:HD21	2:14:B:ASN:HD21	3	0.7
(1,3316)	2:26:B:SER:H	2:33:B:LEU:HD13	4	0.7
(1,3316)	2:26:B:SER:H	2:33:B:LEU:HD13	7	0.7
(1,3196)	2:14:B:ASN:H	2:48:B:ARG:HA	5	0.7
(1,3118)	2:48:B:ARG:HB3	2:49:B:GLU:H	10	0.7
(1,3069)	2:39:C:CYS:H	2:35:C:VAL:HB	9	0.7
(1,3023)	2:48:C:ARG:HG2	2:48:C:ARG:H	3	0.7
(1,2702)	2:13:B:VAL:HA	2:40:B:ILE:HD11	2	0.7
(1,2551)	2:20:C:VAL:HG12	2:19:C:ILE:HB	9	0.7
(1,2534)	2:36:B:ALA:HB2	2:40:C:ILE:HG13	1	0.7
(1,2534)	2:36:B:ALA:HB2	2:40:C:ILE:HG13	6	0.7
(1,2423)	2:25:C:ILE:HD12	2:44:B:PHE:HZ	8	0.7
(1,2246)	2:11:B:LEU:HA	2:12:B:ILE:HD11	10	0.7
(1,2245)	2:55:C:LEU:HD21	2:11:C:LEU:HA	10	0.7
(1,2242)	2:11:B:LEU:HA	2:54:B:ILE:HB	9	0.7
(1,2210)	2:22:B:LYS:HA	2:24:B:GLU:HB2	10	0.7
(1,2126)	2:54:B:ILE:HB	2:13:B:VAL:HG21	1	0.7
(1,1994)	2:36:B:ALA:HB3	2:33:B:LEU:HD21	1	0.7
(1,1809)	1:103:A:GLN:HE22	1:99:A:LEU:HD12	10	0.7
(1,1467)	1:145:A:THR:HG23	1:82:A:GLN:HE22	2	0.7
(1,1457)	1:120:A:LEU:HD23	1:118:A:LYS:HE3	2	0.7
(1,1454)	1:105:A:LEU:HD23	1:105:A:LEU:HB2	2	0.7
(1,1169)	1:125:A:VAL:HG23	1:125:A:VAL:H	6	0.7
(1,1037)	1:107:A:SER:HB3	1:107:A:SER:H	6	0.7
(1,1037)	1:107:A:SER:HB3	1:107:A:SER:H	10	0.7
(1,672)	1:121:A:LEU:HD23	1:144:A:ILE:HA	5	0.7
(1,638)	1:132:A:LEU:HB3	1:135:A:LEU:HD13	7	0.7
(1,410)	1:122:A:LYS:HD3	1:122:A:LYS:H	5	0.7
(1,180)	1:132:A:LEU:HD11	1:96:A:ASP:HB2	2	0.7
(1,179)	1:120:A:LEU:HD22	1:147:A:MET:HG3	2	0.7
(1,147)	1:132:A:LEU:HD23	1:98:A:ILE:H	9	0.7
(1,113)	1:77:A:THR:HG23	1:88:A:ILE:H	6	0.7
(1,58)	1:114:A:ILE:HD11	1:99:A:LEU:HA	3	0.7
(1,44)	1:88:A:ILE:HD13	1:78:A:LEU:HB3	9	0.7
(1,28)	1:144:A:ILE:HD11	1:121:A:LEU:HA	7	0.7
(1,13)	1:119:A:LEU:HD21	1:98:A:ILE:HA	1	0.7
(1,4053)	2:55:C:LEU:HD21	2:8:C:ILE:H	5	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3936)	2:13:B:VAL:HG23	2:48:B:ARG:HG3	9	0.69
(1,3643)	2:68:C:ILE:HB	2:71:C:SER:H	1	0.69
(1,3609)	2:38:C:ASP:HA	2:40:C:ILE:HD12	1	0.69
(1,3571)	2:13:C:VAL:HG21	2:48:C:ARG:HG3	10	0.69
(1,3552)	2:25:B:ILE:HD11	2:24:B:GLU:HB3	3	0.69
(1,3420)	2:51:B:VAL:H	2:54:B:ILE:HG12	4	0.69
(1,3324)	2:27:B:GLU:HG3	2:27:B:GLU:H	5	0.69
(1,3143)	2:6:C:GLU:HG2	2:6:C:GLU:H	6	0.69
(1,3118)	2:48:B:ARG:HB3	2:49:B:GLU:H	2	0.69
(1,2694)	2:54:B:ILE:HG21	2:46:B:PHE:HB2	4	0.69
(1,2563)	2:11:C:LEU:HD21	2:55:C:LEU:HD23	10	0.69
(1,2562)	2:11:B:LEU:HD22	2:55:B:LEU:HD21	9	0.69
(1,2541)	2:36:C:ALA:HB1	2:33:C:LEU:HD12	8	0.69
(1,2501)	2:25:C:ILE:HG23	2:20:C:VAL:HB	4	0.69
(1,2501)	2:25:C:ILE:HG22	2:20:C:VAL:HB	5	0.69
(1,2482)	2:25:B:ILE:HB	2:19:B:ILE:HG21	1	0.69
(1,2408)	2:19:B:ILE:HG21	2:44:C:PHE:HZ	1	0.69
(1,2243)	2:11:C:LEU:HA	2:54:C:ILE:HB	2	0.69
(1,2243)	2:11:C:LEU:HA	2:54:C:ILE:HB	8	0.69
(1,2182)	2:9:B:ALA:HA	2:40:B:ILE:HG22	3	0.69
(1,2065)	2:55:C:LEU:HD23	2:51:C:VAL:HB	3	0.69
(1,2042)	2:5:B:LYS:HD3	2:44:B:PHE:HZ	2	0.69
(1,1809)	1:103:A:GLN:HE22	1:99:A:LEU:HD12	7	0.69
(1,1733)	1:129:A:ASN:H	1:97:A:THR:HG21	3	0.69
(1,1662)	1:149:A:LYS:HG3	1:149:A:LYS:HE3	3	0.69
(1,1648)	1:136:A:LYS:HA	1:135:A:LEU:HD12	8	0.69
(1,1454)	1:78:A:LEU:HD21	1:78:A:LEU:HB3	10	0.69
(1,1442)	1:143:A:THR:HG21	1:77:A:THR:H	2	0.69
(1,1441)	1:77:A:THR:HG23	1:143:A:THR:HA	4	0.69
(1,1272)	1:111:A:ALA:H	1:106:A:ILE:HD12	6	0.69
(1,1037)	1:107:A:SER:HB3	1:107:A:SER:H	5	0.69
(1,979)	1:101:A:ILE:HG12	1:101:A:ILE:H	3	0.69
(1,728)	1:99:A:LEU:HG	1:103:A:GLN:HE22	8	0.69
(1,697)	1:79:A:LYS:HE3	1:79:A:LYS:HG3	4	0.69
(1,247)	1:103:A:GLN:HG2	1:100:A:GLN:HE22	8	0.69
(1,3963)	2:36:C:ALA:HB2	2:40:B:ILE:HA	3	0.68
(1,3803)	2:3:C:ALA:HB1	2:7:C:GLU:H	9	0.68
(1,3628)	2:18:B:SER:HB3	2:19:B:ILE:HD11	2	0.68
(1,3476)	2:55:B:LEU:HD21	2:14:B:ASN:HD21	8	0.68
(1,3312)	2:26:B:SER:H	2:44:C:PHE:HD1	6	0.68
(1,3221)	2:34:C:ASN:HA	2:17:C:SER:H	8	0.68
(1,3119)	2:48:C:ARG:HB3	2:49:C:GLU:H	4	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3118)	2:48:B:ARG:HB3	2:49:B:GLU:H	1	0.68
(1,2890)	2:21:B:GLU:HA	2:23:B:LYS:HE3	9	0.68
(1,2545)	2:51:C:VAL:HG12	2:55:C:LEU:HG	3	0.68
(1,2539)	2:12:C:ILE:HG21	2:12:C:ILE:HG13	10	0.68
(1,2538)	2:12:B:ILE:HG22	2:12:B:ILE:HG13	6	0.68
(1,2501)	2:25:C:ILE:HG22	2:20:C:VAL:HB	9	0.68
(1,2251)	2:11:C:LEU:HA	2:55:C:LEU:HB3	8	0.68
(1,2246)	2:11:B:LEU:HA	2:12:B:ILE:HD13	5	0.68
(1,2242)	2:11:B:LEU:HA	2:54:B:ILE:HB	10	0.68
(1,2091)	2:8:C:ILE:HD11	2:3:C:ALA:HB3	2	0.68
(1,1809)	1:103:A:GLN:HE22	1:99:A:LEU:HD12	4	0.68
(1,1457)	1:120:A:LEU:HD22	1:118:A:LYS:HE3	6	0.68
(1,1411)	1:116:A:GLU:HG3	1:151:A:ASN:H	9	0.68
(1,1338)	1:99:A:LEU:HD11	1:103:A:GLN:HE21	2	0.68
(1,1328)	1:100:A:GLN:HE21	1:99:A:LEU:HD11	1	0.68
(1,1175)	1:153:A:GLU:H	1:152:A:LEU:HD21	10	0.68
(1,1169)	1:125:A:VAL:HG21	1:125:A:VAL:H	2	0.68
(1,1159)	1:152:A:LEU:HG	1:152:A:LEU:H	1	0.68
(1,1140)	1:82:A:GLN:HG2	1:82:A:GLN:H	5	0.68
(1,785)	1:122:A:LYS:HD3	1:121:A:LEU:HD12	1	0.68
(1,176)	1:132:A:LEU:HD22	1:96:A:ASP:HB2	7	0.68
(1,85)	1:73:A:MET:HE1	1:73:A:MET:HA	8	0.68
(1,13)	1:119:A:LEU:HD21	1:98:A:ILE:HA	2	0.68
(1,4080)	2:13:B:VAL:H	2:41:B:SER:HA	7	0.67
(1,3818)	2:6:B:GLU:HB3	2:46:B:PHE:HD2	3	0.67
(1,3816)	2:6:B:GLU:HB2	2:46:B:PHE:HD2	1	0.67
(1,3739)	2:68:C:ILE:HD12	2:11:B:LEU:HD23	9	0.67
(1,3704)	2:6:B:GLU:HA	2:46:B:PHE:HE1	8	0.67
(1,3679)	2:54:C:ILE:HG21	2:55:C:LEU:H	9	0.67
(1,3671)	2:3:C:ALA:HB3	2:60:B:PHE:HD2	9	0.67
(1,3658)	2:51:B:VAL:HG23	2:46:B:PHE:HE2	4	0.67
(1,3642)	2:68:B:ILE:HB	2:71:B:SER:H	5	0.67
(1,3221)	2:34:C:ASN:HA	2:17:C:SER:H	2	0.67
(1,3118)	2:48:B:ARG:HB3	2:49:B:GLU:H	7	0.67
(1,3068)	2:39:B:CYS:H	2:35:B:VAL:HB	4	0.67
(1,2695)	2:54:C:ILE:HG23	2:46:C:PHE:HB2	5	0.67
(1,2539)	2:12:C:ILE:HG22	2:12:C:ILE:HG13	1	0.67
(1,2243)	2:11:C:LEU:HA	2:54:C:ILE:HB	7	0.67
(1,2211)	2:22:C:LYS:HA	2:24:C:GLU:HB2	4	0.67
(1,2091)	2:8:C:ILE:HD11	2:3:C:ALA:HB3	7	0.67
(1,1793)	1:141:A:ASN:HB2	1:140:A:ALA:H	2	0.67
(1,1736)	1:110:A:LYS:H	1:105:A:LEU:HB3	3	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1435)	1:98:A:ILE:HG23	1:128:A:ASP:H	1	0.67
(1,1314)	1:137:A:VAL:HB	1:142:A:SER:H	2	0.67
(1,1270)	1:108:A:GLU:H	1:106:A:ILE:HG21	5	0.67
(1,1010)	1:98:A:ILE:H	1:98:A:ILE:HG13	3	0.67
(1,769)	1:132:A:LEU:HA	1:135:A:LEU:HD13	7	0.67
(1,672)	1:121:A:LEU:HD23	1:144:A:ILE:HA	3	0.67
(1,661)	1:76:A:LEU:HD23	1:76:A:LEU:HA	7	0.67
(1,25)	1:144:A:ILE:HD12	1:120:A:LEU:H	1	0.67
(3,34)	1:149:A:LYS:N	1:116:A:GLU:O	10	0.66
(3,33)	1:149:A:LYS:H	1:116:A:GLU:O	4	0.66
(1,4108)	2:21:B:GLU:H	2:22:B:LYS:HG3	4	0.66
(1,3722)	2:25:B:ILE:HG21	2:5:C:LYS:HE3	6	0.66
(1,3705)	2:6:C:GLU:HA	2:46:C:PHE:HE1	8	0.66
(1,3664)	2:33:B:LEU:HD23	2:16:B:PHE:HD1	4	0.66
(1,3623)	2:12:C:ILE:HA	2:13:C:VAL:HG11	5	0.66
(1,3623)	2:40:C:ILE:HA	2:33:B:LEU:HG	9	0.66
(1,3622)	2:40:B:ILE:HA	2:33:C:LEU:HG	10	0.66
(1,3570)	2:13:B:VAL:HG23	2:48:B:ARG:HG3	9	0.66
(1,3220)	2:34:B:ASN:HA	2:17:B:SER:H	7	0.66
(1,3162)	2:6:B:GLU:HB2	2:7:B:GLU:H	7	0.66
(1,3048)	2:50:B:ALA:H	2:13:B:VAL:HG12	5	0.66
(1,2594)	2:57:B:LYS:HB3	2:68:C:ILE:HG13	1	0.66
(1,2298)	2:19:B:ILE:HA	2:22:B:LYS:HD3	6	0.66
(1,2127)	2:54:C:ILE:HB	2:13:C:VAL:HG23	3	0.66
(1,2127)	2:54:C:ILE:HB	2:13:C:VAL:HG23	8	0.66
(1,2090)	2:8:B:ILE:HD12	2:3:B:ALA:HB1	2	0.66
(1,2065)	2:55:C:LEU:HD22	2:51:C:VAL:HB	4	0.66
(1,2065)	2:55:C:LEU:HD21	2:51:C:VAL:HB	10	0.66
(1,2012)	2:47:B:GLU:HG3	2:47:B:GLU:H	6	0.66
(1,1663)	1:85:A:LYS:HG2	1:85:A:LYS:HE3	3	0.66
(1,1648)	1:136:A:LYS:HA	1:135:A:LEU:HD12	4	0.66
(1,1623)	1:126:A:LEU:HG	1:127:A:HIS:HB2	8	0.66
(1,1272)	1:111:A:ALA:H	1:106:A:ILE:HD11	8	0.66
(1,1169)	1:125:A:VAL:HG23	1:125:A:VAL:H	3	0.66
(1,979)	1:101:A:ILE:HG12	1:101:A:ILE:H	5	0.66
(1,960)	1:121:A:LEU:H	1:124:A:LYS:H	6	0.66
(1,860)	1:80:A:LYS:H	1:79:A:LYS:HD3	6	0.66
(1,709)	1:122:A:LYS:HE3	1:141:A:ASN:HA	2	0.66
(1,201)	1:144:A:ILE:HG23	1:120:A:LEU:H	4	0.66
(1,54)	1:81:A:ILE:HD12	1:82:A:GLN:H	2	0.66
(1,47)	1:88:A:ILE:HD13	1:105:A:LEU:HA	1	0.66
(1,13)	1:119:A:LEU:HD21	1:98:A:ILE:HA	3	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4186)	1:120:A:LEU:HG	2:35:B:VAL:H	7	0.65
(1,4185)	1:120:A:LEU:HG	2:35:B:VAL:H	7	0.65
(1,4184)	1:120:A:LEU:HD23	2:35:B:VAL:H	1	0.65
(1,4087)	2:15:C:TYR:H	2:12:B:ILE:HD13	1	0.65
(1,4087)	2:15:C:TYR:H	2:12:B:ILE:HD11	4	0.65
(1,4081)	2:13:C:VAL:H	2:41:C:SER:HA	10	0.65
(1,3850)	2:40:B:ILE:HG22	2:13:B:VAL:HB	6	0.65
(1,3744)	2:40:B:ILE:HD12	2:36:C:ALA:HB3	8	0.65
(1,3744)	2:40:B:ILE:HD11	2:36:C:ALA:HB3	9	0.65
(1,3722)	2:25:B:ILE:HG21	2:5:C:LYS:HE3	3	0.65
(1,3621)	2:40:C:ILE:HA	2:36:B:ALA:HB1	9	0.65
(1,3183)	2:12:C:ILE:HD11	2:9:C:ALA:H	10	0.65
(1,3118)	2:48:B:ARG:HB3	2:49:B:GLU:H	8	0.65
(1,3023)	2:48:C:ARG:HG2	2:48:C:ARG:H	10	0.65
(1,2552)	2:35:B:VAL:HG12	2:37:B:MET:HB3	7	0.65
(1,2540)	2:36:B:ALA:HB3	2:33:B:LEU:HD11	8	0.65
(1,2538)	2:12:B:ILE:HG23	2:12:B:ILE:HG13	4	0.65
(1,2499)	2:25:C:ILE:HG23	2:20:C:VAL:HG13	5	0.65
(1,2298)	2:19:B:ILE:HA	2:22:B:LYS:HD3	8	0.65
(1,2251)	2:11:C:LEU:HA	2:55:C:LEU:HB3	5	0.65
(1,2090)	2:8:B:ILE:HD12	2:3:B:ALA:HB1	7	0.65
(1,2043)	2:5:C:LYS:HD3	2:44:C:PHE:HZ	10	0.65
(1,1831)	1:148:A:ILE:HG23	1:148:A:ILE:H	4	0.65
(1,1808)	1:99:A:LEU:HG	1:103:A:GLN:HE22	3	0.65
(1,1803)	1:82:A:GLN:HE21	1:81:A:ILE:HG22	6	0.65
(1,1787)	1:111:A:ALA:H	1:106:A:ILE:HG22	2	0.65
(1,1707)	1:120:A:LEU:H	1:119:A:LEU:HD11	4	0.65
(1,1704)	1:121:A:LEU:H	1:121:A:LEU:HD23	10	0.65
(1,1632)	1:147:A:MET:HG3	1:120:A:LEU:HB2	8	0.65
(1,1623)	1:126:A:LEU:HG	1:127:A:HIS:HB2	7	0.65
(1,1455)	1:132:A:LEU:HD21	1:94:A:PRO:HA	9	0.65
(1,1454)	1:78:A:LEU:HD21	1:78:A:LEU:HB3	7	0.65
(1,1351)	1:141:A:ASN:HD21	1:121:A:LEU:HG	6	0.65
(1,1272)	1:111:A:ALA:H	1:106:A:ILE:HD13	10	0.65
(1,1270)	1:108:A:GLU:H	1:106:A:ILE:HG21	3	0.65
(1,1270)	1:108:A:GLU:H	1:106:A:ILE:HG21	8	0.65
(1,1010)	1:98:A:ILE:H	1:98:A:ILE:HG13	7	0.65
(1,1010)	1:98:A:ILE:H	1:98:A:ILE:HG13	10	0.65
(1,786)	1:126:A:LEU:HD11	1:124:A:LYS:HD3	3	0.65
(1,720)	1:148:A:ILE:HD11	1:86:A:PHE:HZ	4	0.65
(1,717)	1:120:A:LEU:HG	1:125:A:VAL:HA	8	0.65
(1,661)	1:76:A:LEU:HD23	1:76:A:LEU:HA	3	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,655)	1:81:A:ILE:HG12	1:145:A:THR:HA	7	0.65
(1,533)	1:114:A:ILE:HA	1:114:A:ILE:HG12	1	0.65
(1,177)	1:132:A:LEU:HD23	1:97:A:THR:HA	6	0.65
(1,162)	1:78:A:LEU:HD21	1:92:A:PHE:HZ	6	0.65
(1,132)	1:138:A:THR:HG22	1:141:A:ASN:HB3	4	0.65
(1,67)	1:83:A:ALA:HB2	1:85:A:LYS:H	4	0.65
(1,4085)	2:14:C:ASN:H	2:12:C:ILE:HG22	8	0.64
(1,4051)	2:54:C:ILE:HB	2:50:C:ALA:H	7	0.64
(1,4014)	2:60:B:PHE:HD1	2:8:B:ILE:HD13	6	0.64
(1,3525)	2:6:C:GLU:HG3	2:46:C:PHE:HD1	4	0.64
(1,3220)	2:34:B:ASN:HA	2:17:B:SER:H	6	0.64
(1,3186)	2:40:B:ILE:H	2:13:B:VAL:HG11	6	0.64
(1,3182)	2:12:B:ILE:HD12	2:9:B:ALA:H	9	0.64
(1,3162)	2:6:B:GLU:HB2	2:7:B:GLU:H	3	0.64
(1,2595)	2:57:C:LYS:HB3	2:68:B:ILE:HG13	2	0.64
(1,2552)	2:35:B:VAL:HG12	2:37:B:MET:HB3	5	0.64
(1,2544)	2:51:B:VAL:HG11	2:55:B:LEU:HG	7	0.64
(1,2538)	2:12:B:ILE:HG21	2:12:B:ILE:HG13	9	0.64
(1,2499)	2:25:C:ILE:HG21	2:20:C:VAL:HG13	4	0.64
(1,2422)	2:25:B:ILE:HD13	2:44:C:PHE:HZ	8	0.64
(1,2242)	2:11:B:LEU:HA	2:54:B:ILE:HB	5	0.64
(1,2065)	2:55:C:LEU:HD22	2:51:C:VAL:HB	9	0.64
(1,1831)	1:148:A:ILE:HG21	1:148:A:ILE:H	3	0.64
(1,1784)	1:105:A:LEU:H	1:117:A:ILE:HD13	4	0.64
(1,1454)	1:78:A:LEU:HD21	1:78:A:LEU:HB3	3	0.64
(1,1417)	1:73:A:MET:HB3	1:74:A:VAL:H	5	0.64
(1,1328)	1:100:A:GLN:HE21	1:99:A:LEU:HD11	3	0.64
(1,1169)	1:125:A:VAL:HG22	1:125:A:VAL:H	4	0.64
(1,1010)	1:98:A:ILE:H	1:98:A:ILE:HG13	1	0.64
(1,719)	1:148:A:ILE:HD12	1:112:A:SER:H	3	0.64
(1,717)	1:120:A:LEU:HG	1:125:A:VAL:HA	4	0.64
(1,717)	1:120:A:LEU:HG	1:125:A:VAL:HA	7	0.64
(1,372)	1:151:A:ASN:HA	1:151:A:ASN:HD21	5	0.64
(1,80)	1:148:A:ILE:HG22	1:112:A:SER:HA	9	0.64
(1,75)	1:98:A:ILE:HG23	1:128:A:ASP:HA	7	0.64
(1,2)	1:120:A:LEU:HD13	1:120:A:LEU:H	9	0.64
(1,4087)	2:15:C:TYR:H	2:12:B:ILE:HD12	5	0.63
(1,4080)	2:13:B:VAL:H	2:41:B:SER:HA	6	0.63
(1,3932)	2:18:B:SER:HB3	2:22:B:LYS:HE3	1	0.63
(1,3888)	2:18:B:SER:HB3	2:22:B:LYS:HD3	10	0.63
(1,3823)	2:40:C:ILE:HD11	2:36:C:ALA:HA	7	0.63
(1,3588)	2:5:B:LYS:HE2	2:19:C:ILE:HD11	2	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3420)	2:51:B:VAL:H	2:54:B:ILE:HG12	7	0.63
(1,3317)	2:26:C:SER:H	2:33:C:LEU:HD11	6	0.63
(1,3312)	2:26:B:SER:H	2:44:C:PHE:HD1	1	0.63
(1,3252)	2:21:B:GLU:HB3	2:21:B:GLU:H	3	0.63
(1,3220)	2:34:B:ASN:HA	2:17:B:SER:H	10	0.63
(1,3182)	2:12:B:ILE:HD11	2:9:B:ALA:H	7	0.63
(1,3069)	2:39:C:CYS:H	2:35:C:VAL:HB	2	0.63
(1,3049)	2:50:C:ALA:H	2:13:C:VAL:HG13	10	0.63
(1,2703)	2:13:C:VAL:HA	2:40:C:ILE:HD13	2	0.63
(1,2699)	2:54:C:ILE:HG23	2:6:C:GLU:HG3	9	0.63
(1,2559)	2:55:C:LEU:HD22	2:13:C:VAL:HG23	4	0.63
(1,2544)	2:51:B:VAL:HG12	2:55:B:LEU:HG	5	0.63
(1,2427)	2:68:C:ILE:HD11	2:60:B:PHE:HD2	10	0.63
(1,2408)	2:19:B:ILE:HG21	2:44:C:PHE:HZ	10	0.63
(1,2299)	2:19:C:ILE:HA	2:22:C:LYS:HD3	2	0.63
(1,2270)	2:20:B:VAL:HA	2:25:B:ILE:HG23	1	0.63
(1,2126)	2:54:B:ILE:HB	2:13:B:VAL:HG23	7	0.63
(1,2091)	2:8:C:ILE:HD12	2:3:C:ALA:HB1	1	0.63
(1,2063)	2:55:C:LEU:HD23	2:14:C:ASN:HB2	9	0.63
(1,1831)	1:148:A:ILE:HG21	1:148:A:ILE:H	7	0.63
(1,1784)	1:105:A:LEU:H	1:117:A:ILE:HD13	8	0.63
(1,1697)	1:78:A:LEU:HD11	1:90:A:HIS:H	6	0.63
(1,1270)	1:108:A:GLU:H	1:106:A:ILE:HG21	4	0.63
(1,1141)	1:82:A:GLN:H	1:80:A:LYS:HG2	2	0.63
(1,791)	1:136:A:LYS:HG3	1:136:A:LYS:HE3	6	0.63
(1,661)	1:76:A:LEU:HD23	1:76:A:LEU:HA	1	0.63
(1,642)	1:97:A:THR:HG21	1:100:A:GLN:HG3	1	0.63
(1,147)	1:132:A:LEU:HD23	1:98:A:ILE:H	1	0.63
(1,113)	1:77:A:THR:HG23	1:88:A:ILE:H	10	0.63
(1,58)	1:114:A:ILE:HD13	1:99:A:LEU:HA	2	0.63
(1,4085)	2:14:C:ASN:H	2:12:C:ILE:HG22	9	0.62
(1,4052)	2:55:B:LEU:HD22	2:8:B:ILE:H	1	0.62
(1,4051)	2:54:C:ILE:HB	2:50:C:ALA:H	2	0.62
(1,3744)	2:40:B:ILE:HD12	2:36:B:ALA:HB2	3	0.62
(1,3723)	2:25:C:ILE:HG23	2:5:B:LYS:HE3	4	0.62
(1,3692)	2:9:B:ALA:HA	2:16:C:PHE:HZ	4	0.62
(1,3672)	2:12:B:ILE:HG21	2:11:B:LEU:H	2	0.62
(1,2978)	2:25:B:ILE:HD12	2:30:B:ALA:H	2	0.62
(1,2964)	2:48:B:ARG:HB3	2:48:B:ARG:H	8	0.62
(1,2937)	2:6:C:GLU:HG2	2:44:C:PHE:HD1	3	0.62
(1,2551)	2:20:C:VAL:HG12	2:19:C:ILE:HB	6	0.62
(1,2539)	2:12:C:ILE:HG22	2:12:C:ILE:HG13	4	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2534)	2:36:B:ALA:HB2	2:40:C:ILE:HG13	9	0.62
(1,2408)	2:19:B:ILE:HG23	2:44:C:PHE:HZ	7	0.62
(1,2251)	2:11:C:LEU:HA	2:55:C:LEU:HB3	1	0.62
(1,1635)	1:122:A:LYS:HE3	1:122:A:LYS:HG2	2	0.62
(1,1454)	1:78:A:LEU:HD21	1:78:A:LEU:HB3	4	0.62
(1,1449)	1:78:A:LEU:HD11	1:90:A:HIS:H	5	0.62
(1,1353)	1:121:A:LEU:HD13	1:141:A:ASN:HD21	2	0.62
(1,1270)	1:108:A:GLU:H	1:106:A:ILE:HG23	2	0.62
(1,979)	1:101:A:ILE:HG12	1:101:A:ILE:H	9	0.62
(1,791)	1:136:A:LYS:HG3	1:136:A:LYS:HE3	4	0.62
(1,762)	1:119:A:LEU:HA	1:144:A:ILE:HG23	7	0.62
(1,704)	1:122:A:LYS:HE3	1:141:A:ASN:HD21	10	0.62
(1,186)	1:120:A:LEU:HD23	1:120:A:LEU:H	2	0.62
(1,47)	1:88:A:ILE:HD11	1:105:A:LEU:HA	5	0.62
(1,47)	1:88:A:ILE:HD13	1:105:A:LEU:HA	7	0.62
(1,33)	1:106:A:ILE:HD12	1:113:A:HIS:HB3	9	0.62
(1,2)	1:120:A:LEU:HD13	1:120:A:LEU:H	1	0.62
(3,33)	1:149:A:LYS:H	1:116:A:GLU:O	9	0.61
(1,4099)	2:17:C:SER:H	2:12:C:ILE:HG23	5	0.61
(1,4087)	2:15:C:TYR:H	2:12:B:ILE:HD12	10	0.61
(1,4053)	2:55:C:LEU:HD21	2:8:C:ILE:H	10	0.61
(1,4051)	2:54:C:ILE:HB	2:50:C:ALA:H	4	0.61
(1,3874)	2:15:B:TYR:HA	2:12:C:ILE:HD12	2	0.61
(1,3851)	2:40:C:ILE:HG23	2:13:C:VAL:HB	1	0.61
(1,3816)	2:6:B:GLU:HB2	2:46:B:PHE:HD2	6	0.61
(1,3771)	2:30:C:ALA:HA	2:20:C:VAL:HG22	7	0.61
(1,3715)	2:19:C:ILE:HG22	2:24:C:GLU:HB3	4	0.61
(1,3664)	2:33:B:LEU:HD22	2:44:C:PHE:HZ	2	0.61
(1,3259)	2:22:C:LYS:HG3	2:22:C:LYS:H	5	0.61
(1,3162)	2:6:B:GLU:HB2	2:7:B:GLU:H	9	0.61
(1,3119)	2:48:C:ARG:HB3	2:49:C:GLU:H	9	0.61
(1,3118)	2:48:B:ARG:HB3	2:49:B:GLU:H	3	0.61
(1,3069)	2:39:C:CYS:H	2:35:C:VAL:HB	3	0.61
(1,3068)	2:39:B:CYS:H	2:35:B:VAL:HB	6	0.61
(1,2965)	2:48:C:ARG:HB3	2:48:C:ARG:H	2	0.61
(1,2965)	2:48:C:ARG:HB3	2:48:C:ARG:H	5	0.61
(1,2964)	2:48:B:ARG:HB3	2:48:B:ARG:H	3	0.61
(1,2631)	2:51:C:VAL:HB	2:55:C:LEU:HG	1	0.61
(1,2541)	2:36:C:ALA:HB1	2:33:C:LEU:HD12	3	0.61
(1,2539)	2:12:C:ILE:HG22	2:12:C:ILE:HG13	5	0.61
(1,2482)	2:25:B:ILE:HB	2:19:B:ILE:HG22	7	0.61
(1,2112)	2:13:B:VAL:HG22	2:51:B:VAL:HB	8	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1995)	2:36:C:ALA:HB1	2:33:C:LEU:HD23	9	0.61
(1,1454)	1:78:A:LEU:HD21	1:78:A:LEU:HB3	8	0.61
(1,1411)	1:116:A:GLU:HG3	1:151:A:ASN:H	5	0.61
(1,1270)	1:108:A:GLU:H	1:106:A:ILE:HG21	1	0.61
(1,889)	1:130:A:LEU:HB3	1:130:A:LEU:H	5	0.61
(1,703)	1:122:A:LYS:HE3	1:141:A:ASN:HD22	1	0.61
(1,229)	1:118:A:LYS:HB2	1:118:A:LYS:HE3	4	0.61
(1,107)	1:126:A:LEU:HD11	1:127:A:HIS:H	1	0.61
(1,55)	1:114:A:ILE:HD11	1:103:A:GLN:HE22	6	0.61
(1,4098)	2:17:B:SER:H	2:12:B:ILE:HG22	9	0.6
(1,4091)	2:16:C:PHE:H	2:12:B:ILE:HD12	5	0.6
(1,4086)	2:15:B:TYR:H	2:12:C:ILE:HD12	7	0.6
(1,3551)	2:25:C:ILE:HD12	2:5:B:LYS:HE3	2	0.6
(1,3162)	2:6:B:GLU:HB2	2:7:B:GLU:H	2	0.6
(1,2965)	2:48:C:ARG:HB3	2:48:C:ARG:H	4	0.6
(1,2965)	2:48:C:ARG:HB3	2:48:C:ARG:H	6	0.6
(1,2965)	2:48:C:ARG:HB3	2:48:C:ARG:H	7	0.6
(1,2965)	2:48:C:ARG:HB3	2:48:C:ARG:H	9	0.6
(1,2964)	2:48:B:ARG:HB3	2:48:B:ARG:H	2	0.6
(1,2550)	2:20:B:VAL:HG11	2:19:B:ILE:HB	9	0.6
(1,2541)	2:36:C:ALA:HB1	2:33:C:LEU:HD12	9	0.6
(1,2535)	2:36:C:ALA:HB3	2:40:B:ILE:HG13	1	0.6
(1,2482)	2:25:B:ILE:HB	2:19:B:ILE:HG21	9	0.6
(1,2472)	2:12:B:ILE:HG23	2:13:B:VAL:HG12	7	0.6
(1,2389)	2:20:C:VAL:HG21	2:34:C:ASN:HD22	1	0.6
(1,2250)	2:11:B:LEU:HA	2:55:B:LEU:HB3	10	0.6
(1,2192)	2:25:B:ILE:HD13	2:30:B:ALA:HA	3	0.6
(1,2064)	2:55:B:LEU:HD21	2:51:B:VAL:HB	6	0.6
(1,1995)	2:36:C:ALA:HB1	2:33:C:LEU:HD23	5	0.6
(1,1818)	1:129:A:ASN:HD22	1:130:A:LEU:HD21	2	0.6
(1,1704)	1:121:A:LEU:H	1:121:A:LEU:HD22	4	0.6
(1,1417)	1:73:A:MET:HB3	1:74:A:VAL:H	6	0.6
(1,1392)	1:144:A:ILE:HG12	1:144:A:ILE:H	7	0.6
(1,1272)	1:111:A:ALA:H	1:106:A:ILE:HD11	4	0.6
(1,1041)	1:108:A:GLU:HG3	1:108:A:GLU:H	8	0.6
(1,979)	1:101:A:ILE:HG12	1:101:A:ILE:H	2	0.6
(1,717)	1:120:A:LEU:HG	1:125:A:VAL:HA	3	0.6
(1,669)	1:103:A:GLN:HG3	1:99:A:LEU:HD11	3	0.6
(1,308)	1:129:A:ASN:HA	1:129:A:ASN:HD21	8	0.6
(1,147)	1:132:A:LEU:HD23	1:98:A:ILE:H	6	0.6
(1,89)	1:101:A:ILE:HG22	1:119:A:LEU:HA	5	0.6
(3,34)	1:149:A:LYS:N	1:116:A:GLU:O	3	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4176)	1:145:A:THR:HG21	2:35:C:VAL:HG11	7	0.59
(1,4169)	1:81:A:ILE:HD12	2:35:C:VAL:HG11	6	0.59
(1,4169)	1:81:A:ILE:HD12	2:39:B:CYS:HG	9	0.59
(1,3738)	2:68:B:ILE:HD13	2:11:C:LEU:HD21	5	0.59
(1,3722)	2:25:B:ILE:HG23	2:5:C:LYS:HE3	5	0.59
(1,3550)	2:25:B:ILE:HD13	2:5:C:LYS:HE3	1	0.59
(1,3420)	2:51:B:VAL:H	2:54:B:ILE:HG12	3	0.59
(1,3325)	2:27:C:GLU:HG3	2:27:C:GLU:H	9	0.59
(1,3317)	2:26:C:SER:H	2:33:C:LEU:HD11	3	0.59
(1,3313)	2:26:C:SER:H	2:44:B:PHE:HD1	2	0.59
(1,3118)	2:48:B:ARG:HB3	2:49:B:GLU:H	6	0.59
(1,3069)	2:39:C:CYS:H	2:35:C:VAL:HB	5	0.59
(1,3049)	2:50:C:ALA:H	2:13:C:VAL:HG11	2	0.59
(1,3049)	2:50:C:ALA:H	2:13:C:VAL:HG11	8	0.59
(1,2964)	2:48:B:ARG:HB3	2:48:B:ARG:H	4	0.59
(1,2964)	2:48:B:ARG:HB3	2:48:B:ARG:H	5	0.59
(1,2964)	2:48:B:ARG:HB3	2:48:B:ARG:H	6	0.59
(1,2964)	2:48:B:ARG:HB3	2:48:B:ARG:H	10	0.59
(1,2247)	2:11:C:LEU:HA	2:12:C:ILE:HD11	7	0.59
(1,2064)	2:55:B:LEU:HD21	2:51:B:VAL:HB	7	0.59
(1,2039)	2:5:C:LYS:HB3	2:44:C:PHE:HZ	5	0.59
(1,1803)	1:82:A:GLN:HE21	1:81:A:ILE:HG22	7	0.59
(1,1784)	1:105:A:LEU:H	1:117:A:ILE:HD13	9	0.59
(1,1704)	1:121:A:LEU:H	1:121:A:LEU:HD22	9	0.59
(1,1567)	1:143:A:THR:HB	1:144:A:ILE:HB	5	0.59
(1,1461)	1:126:A:LEU:HD21	1:145:A:THR:H	9	0.59
(1,1441)	1:77:A:THR:HG23	1:143:A:THR:HA	9	0.59
(1,1423)	1:119:A:LEU:HD23	1:117:A:ILE:HB	3	0.59
(1,1211)	1:81:A:ILE:H	1:82:A:GLN:HG2	3	0.59
(1,1211)	1:81:A:ILE:H	1:82:A:GLN:HG2	4	0.59
(1,1037)	1:107:A:SER:HB3	1:107:A:SER:H	2	0.59
(1,1010)	1:98:A:ILE:H	1:98:A:ILE:HG13	4	0.59
(1,980)	1:101:A:ILE:HG13	1:101:A:ILE:H	8	0.59
(1,979)	1:101:A:ILE:HG12	1:101:A:ILE:H	1	0.59
(1,785)	1:122:A:LYS:HD3	1:121:A:LEU:HD12	2	0.59
(1,700)	1:79:A:LYS:HE3	1:81:A:ILE:HA	6	0.59
(1,511)	1:139:A:PRO:HD2	1:138:A:THR:HB	9	0.59
(1,247)	1:103:A:GLN:HG2	1:100:A:GLN:HE22	6	0.59
(1,55)	1:114:A:ILE:HD11	1:103:A:GLN:HE22	9	0.59
(1,4090)	2:16:B:PHE:H	2:12:C:ILE:HD12	8	0.58
(1,3795)	2:17:C:SER:HA	2:19:C:ILE:HG23	4	0.58
(1,3623)	2:40:C:ILE:HA	2:33:B:LEU:HG	10	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3622)	2:40:B:ILE:HA	2:33:C:LEU:HG	6	0.58
(1,3476)	2:55:B:LEU:HD21	2:14:B:ASN:HD21	1	0.58
(1,3421)	2:51:C:VAL:H	2:54:C:ILE:HG12	3	0.58
(1,3320)	2:19:B:ILE:HG22	2:26:B:SER:H	3	0.58
(1,3312)	2:26:B:SER:H	2:44:C:PHE:HD1	2	0.58
(1,3222)	2:17:B:SER:HB3	2:17:B:SER:H	4	0.58
(1,3197)	2:14:C:ASN:H	2:48:C:ARG:HA	8	0.58
(1,3118)	2:48:B:ARG:HB3	2:49:B:GLU:H	4	0.58
(1,2640)	2:33:B:LEU:HD12	2:20:B:VAL:HG13	2	0.58
(1,2565)	2:33:C:LEU:HD11	2:19:C:ILE:HG23	5	0.58
(1,2552)	2:35:B:VAL:HG13	2:37:B:MET:HB3	10	0.58
(1,2280)	2:12:B:ILE:HA	2:12:B:ILE:HG13	5	0.58
(1,2193)	2:25:C:ILE:HD11	2:30:C:ALA:HA	7	0.58
(1,2083)	2:25:C:ILE:HD12	2:19:C:ILE:HG21	4	0.58
(1,1704)	1:121:A:LEU:H	1:121:A:LEU:HD22	8	0.58
(1,1167)	1:124:A:LYS:HG2	1:125:A:VAL:H	1	0.58
(1,1010)	1:98:A:ILE:H	1:98:A:ILE:HG13	8	0.58
(1,979)	1:101:A:ILE:HG12	1:101:A:ILE:H	7	0.58
(1,979)	1:101:A:ILE:HG12	1:101:A:ILE:H	10	0.58
(1,759)	1:114:A:ILE:HA	1:114:A:ILE:HG23	2	0.58
(1,725)	1:148:A:ILE:HD13	1:80:A:LYS:HD3	2	0.58
(1,704)	1:122:A:LYS:HE3	1:141:A:ASN:HD21	6	0.58
(1,672)	1:121:A:LEU:HD23	1:144:A:ILE:HA	6	0.58
(1,201)	1:144:A:ILE:HG23	1:120:A:LEU:H	6	0.58
(1,183)	1:99:A:LEU:HD12	1:100:A:GLN:HE22	5	0.58
(1,177)	1:132:A:LEU:HD22	1:97:A:THR:HA	2	0.58
(1,177)	1:132:A:LEU:HD23	1:97:A:THR:HA	9	0.58
(1,142)	1:140:A:ALA:HB3	1:141:A:ASN:HD22	5	0.58
(1,119)	1:97:A:THR:HG22	1:131:A:PHE:HD1	6	0.58
(1,113)	1:77:A:THR:HG23	1:88:A:ILE:H	9	0.58
(1,80)	1:148:A:ILE:HG23	1:112:A:SER:HA	2	0.58
(1,80)	1:148:A:ILE:HG22	1:112:A:SER:HA	8	0.58
(1,4177)	1:147:A:MET:HB3	2:35:B:VAL:HG21	3	0.57
(1,4169)	1:81:A:ILE:HD11	2:39:B:CYS:HG	1	0.57
(1,4098)	2:17:B:SER:H	2:12:B:ILE:HG21	10	0.57
(1,3770)	2:30:B:ALA:HA	2:20:B:VAL:HG22	3	0.57
(1,3692)	2:9:B:ALA:HA	2:46:B:PHE:HE1	5	0.57
(1,3685)	2:12:C:ILE:HD12	2:15:C:TYR:HD2	9	0.57
(1,3622)	2:40:B:ILE:HA	2:33:C:LEU:HG	4	0.57
(1,3548)	2:55:B:LEU:HD11	2:8:B:ILE:HA	3	0.57
(1,3321)	2:19:C:ILE:HG22	2:26:C:SER:H	6	0.57
(1,3320)	2:19:B:ILE:HG21	2:26:B:SER:H	4	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3223)	2:17:C:SER:HB3	2:17:C:SER:H	1	0.57
(1,3223)	2:17:C:SER:HB3	2:17:C:SER:H	4	0.57
(1,3222)	2:17:B:SER:HB3	2:17:B:SER:H	1	0.57
(1,3163)	2:6:C:GLU:HB2	2:7:C:GLU:H	1	0.57
(1,3119)	2:48:C:ARG:HB3	2:49:C:GLU:H	5	0.57
(1,3069)	2:39:C:CYS:H	2:35:C:VAL:HB	6	0.57
(1,2965)	2:48:C:ARG:HB3	2:48:C:ARG:H	1	0.57
(1,2964)	2:48:B:ARG:HB3	2:48:B:ARG:H	7	0.57
(1,2940)	2:44:B:PHE:HZ	2:33:C:LEU:HD23	4	0.57
(1,2790)	2:33:B:LEU:HD11	2:19:B:ILE:HB	7	0.57
(1,2629)	2:37:C:MET:HB3	2:17:C:SER:HB3	6	0.57
(1,2564)	2:33:B:LEU:HD12	2:19:B:ILE:HG21	5	0.57
(1,2551)	2:20:C:VAL:HG12	2:19:C:ILE:HB	4	0.57
(1,2551)	2:20:C:VAL:HG12	2:19:C:ILE:HB	5	0.57
(1,2550)	2:20:B:VAL:HG13	2:19:B:ILE:HB	2	0.57
(1,2541)	2:36:C:ALA:HB1	2:33:C:LEU:HD12	10	0.57
(1,2520)	2:51:B:VAL:HA	2:54:B:ILE:HD12	2	0.57
(1,2114)	2:13:B:VAL:HG21	2:48:B:ARG:HG2	6	0.57
(1,2091)	2:8:C:ILE:HD12	2:3:C:ALA:HB2	4	0.57
(1,2038)	2:5:B:LYS:HB3	2:44:B:PHE:HZ	3	0.57
(1,1787)	1:111:A:ALA:H	1:106:A:ILE:HG23	4	0.57
(1,1784)	1:105:A:LEU:H	1:117:A:ILE:HD13	7	0.57
(1,1704)	1:121:A:LEU:H	1:121:A:LEU:HD12	1	0.57
(1,1697)	1:90:A:HIS:H	1:76:A:LEU:HD12	3	0.57
(1,1654)	1:121:A:LEU:HG	1:121:A:LEU:HD22	7	0.57
(1,1428)	1:106:A:ILE:HD13	1:102:A:LYS:HB3	1	0.57
(1,1346)	1:141:A:ASN:HD22	1:138:A:THR:HG22	2	0.57
(1,1071)	1:138:A:THR:H	1:138:A:THR:HG23	7	0.57
(1,791)	1:136:A:LYS:HG3	1:136:A:LYS:HE3	5	0.57
(1,695)	1:79:A:LYS:HE3	1:81:A:ILE:HB	8	0.57
(1,661)	1:76:A:LEU:HD23	1:76:A:LEU:HA	6	0.57
(1,460)	1:126:A:LEU:HD13	1:120:A:LEU:HA	4	0.57
(1,231)	1:149:A:LYS:HB3	1:149:A:LYS:HE3	5	0.57
(1,183)	1:99:A:LEU:HD11	1:100:A:GLN:HE22	9	0.57
(1,75)	1:98:A:ILE:HG22	1:128:A:ASP:HA	6	0.57
(1,47)	1:88:A:ILE:HD13	1:105:A:LEU:HA	4	0.57
(1,11)	1:119:A:LEU:HD22	1:102:A:LYS:HB3	5	0.57
(1,4098)	2:17:B:SER:H	2:12:B:ILE:HG21	2	0.56
(1,4086)	2:15:B:TYR:H	2:12:C:ILE:HD12	3	0.56
(1,4009)	2:44:C:PHE:HZ	2:19:B:ILE:HG21	1	0.56
(1,3996)	2:5:B:LYS:HG3	2:44:B:PHE:HZ	9	0.56
(1,3928)	2:39:B:CYS:HB2	2:35:B:VAL:HB	1	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3831)	2:40:C:ILE:HD11	2:13:C:VAL:HB	3	0.56
(1,3818)	2:6:B:GLU:HB3	2:46:B:PHE:HD2	5	0.56
(1,3723)	2:25:C:ILE:HG22	2:5:B:LYS:HE3	5	0.56
(1,3704)	2:6:B:GLU:HA	2:46:B:PHE:HE1	1	0.56
(1,3682)	2:12:B:ILE:HD13	2:16:C:PHE:HD1	1	0.56
(1,3665)	2:33:C:LEU:HD21	2:44:B:PHE:HZ	1	0.56
(1,3588)	2:5:B:LYS:HE2	2:19:C:ILE:HG21	8	0.56
(1,3553)	2:25:C:ILE:HD12	2:24:C:GLU:HB3	6	0.56
(1,3477)	2:55:C:LEU:HD23	2:14:C:ASN:HD21	7	0.56
(1,3476)	2:55:B:LEU:HD21	2:14:B:ASN:HD21	7	0.56
(1,3312)	2:26:B:SER:H	2:44:C:PHE:HD1	3	0.56
(1,3223)	2:17:C:SER:HB3	2:17:C:SER:H	10	0.56
(1,3222)	2:17:B:SER:HB3	2:17:B:SER:H	9	0.56
(1,3222)	2:17:B:SER:HB3	2:17:B:SER:H	10	0.56
(1,3162)	2:6:B:GLU:HB2	2:7:B:GLU:H	4	0.56
(1,3147)	2:6:C:GLU:H	2:6:C:GLU:HB3	4	0.56
(1,3146)	2:6:B:GLU:H	2:6:B:GLU:HB3	10	0.56
(1,3119)	2:48:C:ARG:HB3	2:49:C:GLU:H	2	0.56
(1,2540)	2:36:B:ALA:HB3	2:33:B:LEU:HD11	3	0.56
(1,2538)	2:12:B:ILE:HG21	2:12:B:ILE:HG13	7	0.56
(1,2538)	2:12:B:ILE:HG23	2:12:B:ILE:HG13	8	0.56
(1,2499)	2:25:C:ILE:HG22	2:20:C:VAL:HG13	9	0.56
(1,2309)	2:52:C:SER:HA	2:55:C:LEU:HD11	5	0.56
(1,2182)	2:9:B:ALA:HA	2:40:B:ILE:HG22	8	0.56
(1,2126)	2:54:B:ILE:HB	2:13:B:VAL:HG23	6	0.56
(1,2060)	2:55:B:LEU:HD21	2:14:B:ASN:H	3	0.56
(1,1995)	2:36:C:ALA:HB1	2:33:C:LEU:HD23	10	0.56
(1,1801)	1:82:A:GLN:HE22	1:81:A:ILE:HG22	8	0.56
(1,1704)	1:121:A:LEU:H	1:121:A:LEU:HD23	2	0.56
(1,1704)	1:121:A:LEU:H	1:121:A:LEU:HD22	5	0.56
(1,1654)	1:121:A:LEU:HG	1:121:A:LEU:HD13	1	0.56
(1,1654)	1:121:A:LEU:HG	1:121:A:LEU:HD12	4	0.56
(1,1654)	1:121:A:LEU:HG	1:121:A:LEU:HD21	9	0.56
(1,1428)	1:106:A:ILE:HD13	1:102:A:LYS:HB3	8	0.56
(1,1272)	1:111:A:ALA:H	1:106:A:ILE:HD12	9	0.56
(1,1133)	1:126:A:LEU:HD11	1:126:A:LEU:H	8	0.56
(1,738)	1:115:A:SER:HA	1:114:A:ILE:HG13	7	0.56
(1,717)	1:120:A:LEU:HG	1:125:A:VAL:HA	5	0.56
(1,655)	1:81:A:ILE:HG12	1:145:A:THR:HA	6	0.56
(1,461)	1:96:A:ASP:HA	1:97:A:THR:HG22	1	0.56
(1,147)	1:132:A:LEU:HD22	1:98:A:ILE:H	2	0.56
(1,118)	1:97:A:THR:HG22	1:97:A:THR:H	7	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:106:A:ILE:HD11	1:106:A:ILE:HA	1	0.56
(1,3970)	2:8:B:ILE:HD12	2:60:C:PHE:HE1	1	0.55
(1,3947)	2:5:C:LYS:HB3	2:19:B:ILE:HD12	10	0.55
(1,3939)	2:33:C:LEU:HD11	2:5:B:LYS:HE3	9	0.55
(1,3875)	2:15:C:TYR:HA	2:12:C:ILE:HD11	6	0.55
(1,3741)	2:25:C:ILE:HD12	2:19:C:ILE:HD11	4	0.55
(1,3673)	2:12:C:ILE:HG22	2:11:C:LEU:H	8	0.55
(1,3622)	2:40:B:ILE:HA	2:33:C:LEU:HG	7	0.55
(1,3556)	2:25:B:ILE:HD13	2:5:C:LYS:HD2	5	0.55
(1,3324)	2:27:B:GLU:HG3	2:27:B:GLU:H	1	0.55
(1,3321)	2:19:C:ILE:HG21	2:26:C:SER:H	10	0.55
(1,3223)	2:17:C:SER:HB3	2:17:C:SER:H	5	0.55
(1,3223)	2:17:C:SER:HB3	2:17:C:SER:H	9	0.55
(1,3222)	2:17:B:SER:HB3	2:17:B:SER:H	5	0.55
(1,3147)	2:6:C:GLU:H	2:6:C:GLU:HB3	2	0.55
(1,3147)	2:6:C:GLU:H	2:6:C:GLU:HB3	9	0.55
(1,3146)	2:6:B:GLU:H	2:6:B:GLU:HB3	1	0.55
(1,3071)	2:40:C:ILE:HG13	2:40:C:ILE:H	2	0.55
(1,3068)	2:39:B:CYS:H	2:35:B:VAL:HB	8	0.55
(1,3029)	2:55:C:LEU:HB3	2:56:C:GLY:H	9	0.55
(1,2964)	2:48:B:ARG:HB3	2:48:B:ARG:H	1	0.55
(1,2544)	2:51:B:VAL:HG11	2:55:B:LEU:HG	3	0.55
(1,2491)	2:54:C:ILE:HG23	2:7:C:GLU:HG2	2	0.55
(1,2193)	2:25:C:ILE:HD11	2:30:C:ALA:HA	10	0.55
(1,2091)	2:8:C:ILE:HD13	2:3:C:ALA:HB1	8	0.55
(1,2090)	2:8:B:ILE:HD11	2:3:B:ALA:HB2	4	0.55
(1,2038)	2:5:B:LYS:HB3	2:44:B:PHE:HZ	6	0.55
(1,1787)	1:111:A:ALA:H	1:106:A:ILE:HG23	6	0.55
(1,1784)	1:105:A:LEU:H	1:117:A:ILE:HD11	2	0.55
(1,1704)	1:121:A:LEU:H	1:144:A:ILE:HG23	7	0.55
(1,1699)	1:98:A:ILE:HG23	1:128:A:ASP:H	4	0.55
(1,1697)	1:90:A:HIS:H	1:76:A:LEU:HD11	7	0.55
(1,1670)	1:136:A:LYS:HA	1:136:A:LYS:HE3	3	0.55
(1,1656)	1:124:A:LYS:HD3	1:121:A:LEU:HD23	2	0.55
(1,1419)	1:107:A:SER:HB3	1:108:A:GLU:H	10	0.55
(1,1198)	1:113:A:HIS:H	1:116:A:GLU:HB3	8	0.55
(1,1010)	1:98:A:ILE:H	1:98:A:ILE:HG13	6	0.55
(1,980)	1:101:A:ILE:HG13	1:101:A:ILE:H	9	0.55
(1,979)	1:101:A:ILE:HG12	1:101:A:ILE:H	4	0.55
(1,759)	1:114:A:ILE:HA	1:114:A:ILE:HG22	8	0.55
(1,759)	1:114:A:ILE:HA	1:114:A:ILE:HG21	10	0.55
(1,720)	1:148:A:ILE:HD13	1:86:A:PHE:HZ	1	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,703)	1:122:A:LYS:HE3	1:141:A:ASN:HD22	6	0.55
(1,437)	1:94:A:PRO:HD2	1:74:A:VAL:HG11	10	0.55
(1,36)	1:106:A:ILE:HD11	1:106:A:ILE:HA	4	0.55
(1,2)	1:120:A:LEU:HD13	1:120:A:LEU:H	3	0.55
(1,4180)	1:147:A:MET:HE1	2:38:B:ASP:H	5	0.54
(1,4177)	1:147:A:MET:HG3	2:35:B:VAL:HG21	2	0.54
(1,4177)	1:147:A:MET:HE3	2:39:B:CYS:HB2	10	0.54
(1,4081)	2:13:C:VAL:H	2:41:C:SER:HA	5	0.54
(1,3937)	2:51:C:VAL:HG22	2:55:C:LEU:HG	8	0.54
(1,3823)	2:40:C:ILE:HD12	2:36:C:ALA:HA	10	0.54
(1,3818)	2:6:B:GLU:HB3	2:46:B:PHE:HD1	4	0.54
(1,3692)	2:9:B:ALA:HA	2:16:C:PHE:HZ	3	0.54
(1,3622)	2:12:B:ILE:HA	2:13:B:VAL:HG13	1	0.54
(1,3609)	2:38:C:ASP:HA	2:40:C:ILE:HD13	8	0.54
(1,3547)	2:51:C:VAL:HG23	2:55:C:LEU:HG	6	0.54
(1,3163)	2:6:C:GLU:HB2	2:7:C:GLU:H	7	0.54
(1,3163)	2:6:C:GLU:HB2	2:7:C:GLU:H	8	0.54
(1,2690)	2:50:B:ALA:HB1	2:47:B:GLU:HB3	4	0.54
(1,2565)	2:33:C:LEU:HD13	2:19:C:ILE:HG21	1	0.54
(1,2245)	2:55:C:LEU:HD21	2:11:C:LEU:HA	5	0.54
(1,2193)	2:25:C:ILE:HD11	2:30:C:ALA:HA	9	0.54
(1,2182)	2:9:B:ALA:HA	2:40:B:ILE:HG21	10	0.54
(1,2112)	2:13:B:VAL:HG22	2:51:B:VAL:HB	7	0.54
(1,2043)	2:5:C:LYS:HD3	2:44:C:PHE:HZ	5	0.54
(1,1831)	1:148:A:ILE:HG21	1:148:A:ILE:H	8	0.54
(1,1707)	1:144:A:ILE:HG23	1:120:A:LEU:H	8	0.54
(1,1654)	1:99:A:LEU:HG	1:99:A:LEU:HD11	8	0.54
(1,1567)	1:143:A:THR:HB	1:144:A:ILE:HB	1	0.54
(1,1545)	1:136:A:LYS:HA	1:136:A:LYS:HE3	3	0.54
(1,1435)	1:98:A:ILE:HG22	1:128:A:ASP:H	9	0.54
(1,979)	1:101:A:ILE:HG12	1:101:A:ILE:H	8	0.54
(1,867)	1:145:A:THR:HG21	1:145:A:THR:H	5	0.54
(1,724)	1:148:A:ILE:HD13	1:80:A:LYS:HE3	3	0.54
(1,461)	1:96:A:ASP:HA	1:97:A:THR:HG22	9	0.54
(1,460)	1:126:A:LEU:HD13	1:120:A:LEU:HA	8	0.54
(1,372)	1:151:A:ASN:HA	1:151:A:ASN:HD21	1	0.54
(1,201)	1:144:A:ILE:HG23	1:120:A:LEU:H	8	0.54
(1,186)	1:120:A:LEU:HD23	1:120:A:LEU:H	7	0.54
(1,118)	1:97:A:THR:HG22	1:97:A:THR:H	10	0.54
(1,116)	1:125:A:VAL:HG22	1:120:A:LEU:H	3	0.54
(1,35)	1:106:A:ILE:HD12	1:113:A:HIS:HA	6	0.54
(1,4050)	2:54:B:ILE:HB	2:50:B:ALA:H	2	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4012)	2:44:B:PHE:HZ	2:5:B:LYS:HE2	9	0.53
(1,3831)	2:40:C:ILE:HD12	2:13:C:VAL:HB	8	0.53
(1,3744)	2:40:B:ILE:HD11	2:36:C:ALA:HB3	5	0.53
(1,3664)	2:33:B:LEU:HD22	2:44:C:PHE:HZ	6	0.53
(1,3556)	2:25:B:ILE:HD11	2:5:C:LYS:HD2	6	0.53
(1,3550)	2:25:B:ILE:HD13	2:5:C:LYS:HE3	9	0.53
(1,3527)	2:6:C:GLU:HG2	2:46:C:PHE:HD1	2	0.53
(1,3146)	2:6:B:GLU:H	2:6:B:GLU:HB3	6	0.53
(1,2694)	2:54:B:ILE:HG23	2:46:B:PHE:HB2	9	0.53
(1,2641)	2:33:C:LEU:HD13	2:20:C:VAL:HG12	8	0.53
(1,2380)	2:55:B:LEU:HD12	2:60:B:PHE:HD2	8	0.53
(1,2250)	2:11:B:LEU:HA	2:55:B:LEU:HB3	9	0.53
(1,2211)	2:22:C:LYS:HA	2:24:C:GLU:HB2	9	0.53
(1,2159)	2:13:C:VAL:HG23	2:48:C:ARG:HD3	1	0.53
(1,2112)	2:13:B:VAL:HG22	2:51:B:VAL:HB	6	0.53
(1,2061)	2:55:C:LEU:HD23	2:14:C:ASN:H	3	0.53
(1,2061)	2:55:C:LEU:HD23	2:14:C:ASN:H	7	0.53
(1,2060)	2:55:B:LEU:HD22	2:14:B:ASN:H	5	0.53
(1,2043)	2:5:C:LYS:HD3	2:44:C:PHE:HZ	3	0.53
(1,1994)	2:36:B:ALA:HB3	2:33:B:LEU:HD23	3	0.53
(1,1831)	1:148:A:ILE:HD11	1:148:A:ILE:H	10	0.53
(1,1699)	1:98:A:ILE:HG23	1:128:A:ASP:H	6	0.53
(1,1699)	1:98:A:ILE:HG23	1:128:A:ASP:H	7	0.53
(1,1663)	1:85:A:LYS:HG2	1:85:A:LYS:HE3	8	0.53
(1,1622)	1:128:A:ASP:HB2	1:99:A:LEU:HG	5	0.53
(1,1350)	1:141:A:ASN:HB3	1:141:A:ASN:HD21	4	0.53
(1,1140)	1:82:A:GLN:HG2	1:82:A:GLN:H	9	0.53
(1,1011)	1:98:A:ILE:H	1:98:A:ILE:HG12	6	0.53
(1,749)	1:124:A:LYS:HG2	1:125:A:VAL:HA	8	0.53
(1,683)	1:106:A:ILE:HG12	1:106:A:ILE:H	2	0.53
(1,535)	1:150:A:PRO:HA	1:116:A:GLU:HG3	4	0.53
(1,535)	1:150:A:PRO:HA	1:116:A:GLU:HG3	8	0.53
(1,113)	1:77:A:THR:HG23	1:88:A:ILE:H	7	0.53
(1,101)	1:77:A:THR:HG23	1:87:A:SER:HB3	9	0.53
(1,4086)	2:15:B:TYR:H	2:12:C:ILE:HD12	8	0.52
(1,3851)	2:40:C:ILE:HG23	2:13:C:VAL:HB	9	0.52
(1,3745)	2:40:C:ILE:HD13	2:36:C:ALA:HB3	8	0.52
(1,3744)	2:40:B:ILE:HD12	2:36:C:ALA:HB3	6	0.52
(1,3692)	2:9:B:ALA:HA	2:46:B:PHE:HE1	2	0.52
(1,3642)	2:68:B:ILE:HB	2:71:B:SER:H	1	0.52
(1,3556)	2:25:B:ILE:HD13	2:5:C:LYS:HD2	1	0.52
(1,3548)	2:55:B:LEU:HD12	2:8:B:ILE:HA	5	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3068)	2:39:B:CYS:H	2:35:B:VAL:HB	1	0.52
(1,3049)	2:50:C:ALA:H	2:13:C:VAL:HG11	3	0.52
(1,2564)	2:33:B:LEU:HD13	2:19:B:ILE:HG21	1	0.52
(1,2559)	2:55:C:LEU:HD21	2:13:C:VAL:HG22	5	0.52
(1,2544)	2:51:B:VAL:HG11	2:55:B:LEU:HG	2	0.52
(1,2499)	2:25:C:ILE:HG21	2:20:C:VAL:HG11	2	0.52
(1,2482)	2:25:B:ILE:HB	2:19:B:ILE:HG22	6	0.52
(1,2482)	2:25:B:ILE:HB	2:19:B:ILE:HG21	10	0.52
(1,2298)	2:19:B:ILE:HA	2:22:B:LYS:HD3	2	0.52
(1,2247)	2:11:C:LEU:HA	2:12:C:ILE:HD11	6	0.52
(1,1803)	1:82:A:GLN:HE21	1:81:A:ILE:HG22	1	0.52
(1,1654)	1:121:A:LEU:HG	1:121:A:LEU:HD13	3	0.52
(1,1622)	1:128:A:ASP:HB2	1:99:A:LEU:HG	7	0.52
(1,1462)	1:76:A:LEU:HD21	1:92:A:PHE:HE2	8	0.52
(1,1458)	1:126:A:LEU:HD21	1:126:A:LEU:HA	6	0.52
(1,1455)	1:132:A:LEU:HD21	1:94:A:PRO:HA	3	0.52
(1,1455)	1:132:A:LEU:HD21	1:94:A:PRO:HA	4	0.52
(1,1419)	1:107:A:SER:HB3	1:108:A:GLU:H	1	0.52
(1,1419)	1:107:A:SER:HB3	1:108:A:GLU:H	3	0.52
(1,1270)	1:108:A:GLU:H	1:106:A:ILE:HG21	7	0.52
(1,1133)	1:126:A:LEU:HD13	1:126:A:LEU:H	4	0.52
(1,980)	1:101:A:ILE:HG13	1:101:A:ILE:H	4	0.52
(1,980)	1:101:A:ILE:HG13	1:101:A:ILE:H	6	0.52
(1,979)	1:101:A:ILE:HG12	1:101:A:ILE:H	6	0.52
(1,786)	1:126:A:LEU:HD12	1:124:A:LYS:HD3	7	0.52
(1,759)	1:114:A:ILE:HA	1:114:A:ILE:HG22	4	0.52
(1,717)	1:120:A:LEU:HG	1:125:A:VAL:HA	6	0.52
(1,531)	1:137:A:VAL:HA	1:138:A:THR:HG23	9	0.52
(1,511)	1:139:A:PRO:HD2	1:138:A:THR:HB	8	0.52
(1,155)	1:135:A:LEU:HD12	1:137:A:VAL:H	1	0.52
(1,54)	1:81:A:ILE:HD12	1:82:A:GLN:H	6	0.52
(1,26)	1:144:A:ILE:HD13	1:121:A:LEU:H	2	0.52
(1,26)	1:144:A:ILE:HD12	1:121:A:LEU:H	10	0.52
(1,3771)	2:30:C:ALA:HA	2:20:C:VAL:HG22	2	0.51
(1,3744)	2:40:B:ILE:HD11	2:36:C:ALA:HB3	1	0.51
(1,3705)	2:6:C:GLU:HA	2:46:C:PHE:HE1	2	0.51
(1,3628)	2:18:B:SER:HB3	2:19:B:ILE:HD11	3	0.51
(1,3622)	2:40:B:ILE:HA	2:33:C:LEU:HG	3	0.51
(1,3609)	2:38:C:ASP:HA	2:40:C:ILE:HD13	4	0.51
(1,3593)	2:9:C:ALA:HA	2:12:C:ILE:HG23	10	0.51
(1,3316)	2:26:B:SER:H	2:33:B:LEU:HD12	2	0.51
(1,3163)	2:6:C:GLU:HB2	2:7:C:GLU:H	5	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3119)	2:48:C:ARG:HB3	2:49:C:GLU:H	6	0.51
(1,3092)	2:13:B:VAL:HG12	2:41:B:SER:H	2	0.51
(1,2941)	2:44:C:PHE:HZ	2:33:B:LEU:HD23	1	0.51
(1,2790)	2:33:B:LEU:HD11	2:19:B:ILE:HB	3	0.51
(1,2790)	2:33:B:LEU:HD11	2:19:B:ILE:HB	4	0.51
(1,2695)	2:54:C:ILE:HG22	2:46:C:PHE:HB2	4	0.51
(1,2521)	2:51:C:VAL:HA	2:54:C:ILE:HD11	3	0.51
(1,2483)	2:25:C:ILE:HB	2:19:C:ILE:HG22	1	0.51
(1,2470)	2:12:B:ILE:HG22	2:12:B:ILE:HG12	5	0.51
(1,2423)	2:25:C:ILE:HD12	2:44:B:PHE:HZ	9	0.51
(1,2388)	2:20:B:VAL:HG21	2:34:B:ASN:HD22	10	0.51
(1,2183)	2:9:C:ALA:HA	2:40:C:ILE:HG23	5	0.51
(1,2179)	2:9:C:ALA:HA	2:12:C:ILE:HD13	2	0.51
(1,2179)	2:9:C:ALA:HA	2:12:C:ILE:HD13	3	0.51
(1,2112)	2:13:B:VAL:HG22	2:51:B:VAL:HB	2	0.51
(1,2060)	2:55:B:LEU:HD21	2:14:B:ASN:H	7	0.51
(1,1831)	1:148:A:ILE:HG21	1:148:A:ILE:H	9	0.51
(1,1802)	1:82:A:GLN:HE21	1:82:A:GLN:HB3	5	0.51
(1,1622)	1:128:A:ASP:HB2	1:99:A:LEU:HG	1	0.51
(1,1594)	1:142:A:SER:HB2	1:74:A:VAL:HG21	2	0.51
(1,1461)	1:126:A:LEU:HD21	1:145:A:THR:H	7	0.51
(1,1458)	1:126:A:LEU:HD23	1:126:A:LEU:HA	4	0.51
(1,1458)	1:126:A:LEU:HD23	1:126:A:LEU:HA	7	0.51
(1,1458)	1:126:A:LEU:HD23	1:126:A:LEU:HA	10	0.51
(1,1450)	1:99:A:LEU:HD21	1:102:A:LYS:H	10	0.51
(1,1411)	1:116:A:GLU:HG3	1:151:A:ASN:H	4	0.51
(1,1350)	1:141:A:ASN:HB3	1:141:A:ASN:HD21	5	0.51
(1,1270)	1:108:A:GLU:H	1:106:A:ILE:HG21	6	0.51
(1,1011)	1:98:A:ILE:H	1:98:A:ILE:HG12	8	0.51
(1,759)	1:114:A:ILE:HA	1:114:A:ILE:HG22	5	0.51
(1,702)	1:122:A:LYS:HE3	1:122:A:LYS:H	7	0.51
(1,697)	1:79:A:LYS:HE3	1:79:A:LYS:HG3	1	0.51
(1,669)	1:103:A:GLN:HG3	1:99:A:LEU:HD11	4	0.51
(1,661)	1:76:A:LEU:HD23	1:76:A:LEU:HA	4	0.51
(1,661)	1:76:A:LEU:HD23	1:76:A:LEU:HA	10	0.51
(1,655)	1:81:A:ILE:HG12	1:145:A:THR:HA	8	0.51
(1,176)	1:132:A:LEU:HD22	1:96:A:ASP:HB2	10	0.51
(1,150)	1:78:A:LEU:HD13	1:92:A:PHE:HZ	3	0.51
(1,101)	1:77:A:THR:HG23	1:87:A:SER:HB3	8	0.51
(1,54)	1:81:A:ILE:HD12	1:82:A:GLN:H	10	0.51
(3,34)	1:149:A:LYS:N	1:116:A:GLU:O	7	0.5
(1,4186)	1:120:A:LEU:HG	2:35:B:VAL:H	2	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4185)	1:120:A:LEU:HG	2:35:B:VAL:H	2	0.5
(1,4182)	1:120:A:LEU:HD22	2:38:C:ASP:H	10	0.5
(1,4098)	2:17:B:SER:H	2:12:B:ILE:HG23	7	0.5
(1,4085)	2:14:C:ASN:H	2:12:C:ILE:HG23	6	0.5
(1,4050)	2:54:B:ILE:HB	2:50:B:ALA:H	6	0.5
(1,4009)	2:44:C:PHE:HZ	2:19:B:ILE:HG21	10	0.5
(1,3693)	2:9:C:ALA:HA	2:16:B:PHE:HZ	4	0.5
(1,3693)	2:9:C:ALA:HA	2:46:C:PHE:HE1	6	0.5
(1,3693)	2:9:C:ALA:HA	2:16:B:PHE:HZ	10	0.5
(1,3664)	2:33:B:LEU:HD22	2:44:C:PHE:HZ	3	0.5
(1,3321)	2:19:C:ILE:HG22	2:26:C:SER:H	7	0.5
(1,2951)	2:60:C:PHE:HD1	2:54:C:ILE:HB	4	0.5
(1,2836)	2:40:B:ILE:HB	2:13:B:VAL:HG11	6	0.5
(1,2694)	2:54:B:ILE:HG23	2:46:B:PHE:HB2	5	0.5
(1,2595)	2:57:C:LYS:HB3	2:68:B:ILE:HG13	6	0.5
(1,2594)	2:57:B:LYS:HB3	2:68:C:ILE:HG13	6	0.5
(1,2562)	2:11:B:LEU:HD22	2:55:B:LEU:HD21	10	0.5
(1,2427)	2:68:C:ILE:HD13	2:60:B:PHE:HD2	6	0.5
(1,2426)	2:68:B:ILE:HD13	2:60:C:PHE:HD2	8	0.5
(1,2409)	2:19:C:ILE:HG21	2:44:B:PHE:HZ	5	0.5
(1,1995)	2:36:C:ALA:HB1	2:33:C:LEU:HD21	7	0.5
(1,1994)	2:36:B:ALA:HB3	2:33:B:LEU:HD23	8	0.5
(1,1813)	1:141:A:ASN:HD22	1:122:A:LYS:HG2	5	0.5
(1,1802)	1:82:A:GLN:HE21	1:82:A:GLN:HB3	4	0.5
(1,1707)	1:120:A:LEU:H	1:119:A:LEU:HD13	6	0.5
(1,1661)	1:149:A:LYS:HE3	1:149:A:LYS:HD3	8	0.5
(1,1654)	1:121:A:LEU:HG	1:121:A:LEU:HD21	5	0.5
(1,1654)	1:121:A:LEU:HG	1:121:A:LEU:HD13	6	0.5
(1,1567)	1:145:A:THR:HB	1:144:A:ILE:HB	3	0.5
(1,1557)	1:81:A:ILE:HA	1:85:A:LYS:HD3	2	0.5
(1,1423)	1:119:A:LEU:HD23	1:117:A:ILE:HB	8	0.5
(1,1338)	1:99:A:LEU:HD11	1:103:A:GLN:HE21	9	0.5
(1,1313)	1:142:A:SER:H	1:141:A:ASN:HB3	5	0.5
(1,1272)	1:111:A:ALA:H	1:106:A:ILE:HD13	2	0.5
(1,1270)	1:108:A:GLU:H	1:106:A:ILE:HG21	9	0.5
(1,1266)	1:107:A:SER:H	1:106:A:ILE:HG21	3	0.5
(1,1159)	1:152:A:LEU:HG	1:152:A:LEU:H	5	0.5
(1,759)	1:114:A:ILE:HA	1:114:A:ILE:HG22	6	0.5
(1,759)	1:114:A:ILE:HA	1:114:A:ILE:HG21	7	0.5
(1,700)	1:79:A:LYS:HE3	1:81:A:ILE:HA	9	0.5
(1,638)	1:132:A:LEU:HB3	1:135:A:LEU:HD13	10	0.5
(1,460)	1:126:A:LEU:HD13	1:120:A:LEU:HA	9	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:77:A:THR:HG23	1:88:A:ILE:H	8	0.5
(1,44)	1:88:A:ILE:HD13	1:78:A:LEU:HB3	10	0.5
(1,35)	1:106:A:ILE:HD11	1:113:A:HIS:HA	2	0.5
(1,4099)	2:17:C:SER:H	2:12:C:ILE:HG23	2	0.49
(1,4099)	2:17:C:SER:H	2:12:C:ILE:HG23	4	0.49
(1,3954)	2:5:B:LYS:HD3	2:19:C:ILE:HD11	2	0.49
(1,3888)	2:18:B:SER:HB3	2:22:B:LYS:HD3	3	0.49
(1,3745)	2:40:C:ILE:HD13	2:36:C:ALA:HB3	5	0.49
(1,3683)	2:12:C:ILE:HD13	2:16:B:PHE:HD1	7	0.49
(1,3628)	2:18:B:SER:HB3	2:19:B:ILE:HD11	7	0.49
(1,3609)	2:38:C:ASP:HA	2:40:C:ILE:HD13	7	0.49
(1,3589)	2:5:C:LYS:HE2	2:19:B:ILE:HG21	3	0.49
(1,3477)	2:55:C:LEU:HD23	2:14:C:ASN:HD21	3	0.49
(1,3119)	2:48:C:ARG:HB3	2:49:C:GLU:H	7	0.49
(1,2694)	2:54:B:ILE:HG22	2:46:B:PHE:HB2	2	0.49
(1,2551)	2:20:C:VAL:HG12	2:19:C:ILE:HB	3	0.49
(1,2550)	2:20:B:VAL:HG12	2:19:B:ILE:HB	4	0.49
(1,2540)	2:36:B:ALA:HB3	2:33:B:LEU:HD11	7	0.49
(1,2501)	2:25:C:ILE:HG21	2:20:C:VAL:HB	7	0.49
(1,2091)	2:8:C:ILE:HD12	2:3:C:ALA:HB1	9	0.49
(1,2064)	2:55:B:LEU:HD21	2:51:B:VAL:HB	2	0.49
(1,1654)	1:121:A:LEU:HG	1:121:A:LEU:HD22	2	0.49
(1,1623)	1:126:A:LEU:HG	1:127:A:HIS:HB2	4	0.49
(1,1465)	1:117:A:ILE:HG22	1:102:A:LYS:HB3	8	0.49
(1,1458)	1:126:A:LEU:HD23	1:126:A:LEU:HA	3	0.49
(1,1455)	1:132:A:LEU:HD21	1:94:A:PRO:HA	6	0.49
(1,1452)	1:78:A:LEU:HD21	1:90:A:HIS:HE1	5	0.49
(1,1198)	1:113:A:HIS:H	1:116:A:GLU:HB3	2	0.49
(1,1198)	1:113:A:HIS:H	1:116:A:GLU:HB3	3	0.49
(1,980)	1:101:A:ILE:HG13	1:101:A:ILE:H	7	0.49
(1,791)	1:136:A:LYS:HG3	1:136:A:LYS:HE3	7	0.49
(1,769)	1:132:A:LEU:HA	1:135:A:LEU:HD13	10	0.49
(1,535)	1:150:A:PRO:HA	1:116:A:GLU:HG3	9	0.49
(1,494)	1:98:A:ILE:HA	1:101:A:ILE:HG12	3	0.49
(1,109)	1:126:A:LEU:HD11	1:126:A:LEU:HA	1	0.49
(1,101)	1:77:A:THR:HG23	1:87:A:SER:HB3	7	0.49
(1,90)	1:101:A:ILE:HG22	1:78:A:LEU:HA	5	0.49
(1,8)	1:120:A:LEU:HD13	1:147:A:MET:HG3	1	0.49
(1,4169)	1:81:A:ILE:HD12	2:31:C:ASP:OD2	8	0.48
(1,4099)	2:17:C:SER:H	2:12:C:ILE:HG22	6	0.48
(1,4099)	2:17:C:SER:H	2:12:C:ILE:HG21	8	0.48
(1,4099)	2:17:C:SER:H	2:12:C:ILE:HG21	9	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3830)	2:40:B:ILE:HD11	2:13:B:VAL:HB	4	0.48
(1,3683)	2:12:C:ILE:HD12	2:16:B:PHE:HD1	8	0.48
(1,3566)	2:19:B:ILE:HD13	2:5:C:LYS:HG2	3	0.48
(1,3557)	2:25:C:ILE:HD12	2:5:B:LYS:HD2	7	0.48
(1,3139)	2:2:C:SER:H	2:3:C:ALA:H	7	0.48
(1,2790)	2:33:B:LEU:HD11	2:19:B:ILE:HB	2	0.48
(1,2550)	2:20:B:VAL:HG13	2:19:B:ILE:HB	3	0.48
(1,2483)	2:25:C:ILE:HB	2:19:C:ILE:HG22	2	0.48
(1,2427)	2:68:C:ILE:HD13	2:60:B:PHE:HD2	8	0.48
(1,2247)	2:11:C:LEU:HA	2:12:C:ILE:HD11	2	0.48
(1,2247)	2:11:C:LEU:HA	2:12:C:ILE:HD12	9	0.48
(1,2245)	2:55:C:LEU:HD22	2:11:C:LEU:HA	4	0.48
(1,2126)	2:54:B:ILE:HB	2:13:B:VAL:HG23	8	0.48
(1,2112)	2:13:B:VAL:HG23	2:51:B:VAL:HB	10	0.48
(1,1994)	2:36:B:ALA:HB3	2:33:B:LEU:HD21	5	0.48
(1,1831)	1:148:A:ILE:HD12	1:148:A:ILE:H	1	0.48
(1,1723)	1:102:A:LYS:H	1:117:A:ILE:HD13	10	0.48
(1,1663)	1:85:A:LYS:HG2	1:85:A:LYS:HE3	7	0.48
(1,1661)	1:149:A:LYS:HB3	1:149:A:LYS:HE3	9	0.48
(1,1659)	1:124:A:LYS:HE2	1:124:A:LYS:HD3	5	0.48
(1,1479)	1:82:A:GLN:HG3	1:82:A:GLN:H	8	0.48
(1,1458)	1:126:A:LEU:HD22	1:126:A:LEU:HA	5	0.48
(1,1458)	1:126:A:LEU:HD23	1:126:A:LEU:HA	8	0.48
(1,1435)	1:98:A:ILE:HG23	1:128:A:ASP:H	8	0.48
(1,1272)	1:111:A:ALA:H	1:106:A:ILE:HD13	3	0.48
(1,1270)	1:108:A:GLU:H	1:106:A:ILE:HG21	10	0.48
(1,1132)	1:126:A:LEU:H	1:126:A:LEU:HB3	1	0.48
(1,1055)	1:115:A:SER:H	1:114:A:ILE:HG22	1	0.48
(1,1011)	1:98:A:ILE:H	1:98:A:ILE:HG12	4	0.48
(1,980)	1:101:A:ILE:HG13	1:101:A:ILE:H	1	0.48
(1,791)	1:136:A:LYS:HG3	1:136:A:LYS:HE3	8	0.48
(1,759)	1:114:A:ILE:HA	1:114:A:ILE:HG22	9	0.48
(1,494)	1:98:A:ILE:HA	1:101:A:ILE:HG12	9	0.48
(1,283)	1:120:A:LEU:HB3	1:145:A:THR:HB	1	0.48
(1,186)	1:120:A:LEU:HD21	1:120:A:LEU:H	8	0.48
(1,113)	1:77:A:THR:HG23	1:88:A:ILE:H	4	0.48
(1,105)	1:143:A:THR:HG22	1:79:A:LYS:H	2	0.48
(1,75)	1:98:A:ILE:HG22	1:128:A:ASP:HA	4	0.48
(1,67)	1:83:A:ALA:HB1	1:85:A:LYS:H	2	0.48
(3,139)	2:38:C:ASP:H	2:34:C:ASN:O	8	0.47
(1,4147)	2:48:C:ARG:HA	2:51:C:VAL:H	9	0.47
(1,3770)	2:30:B:ALA:HA	2:20:B:VAL:HG22	2	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3692)	2:9:B:ALA:HA	2:46:B:PHE:HE1	10	0.47
(1,3593)	2:9:C:ALA:HA	2:12:C:ILE:HG21	5	0.47
(1,3552)	2:25:B:ILE:HD11	2:24:B:GLU:HB3	8	0.47
(1,3544)	2:51:B:VAL:HG21	2:48:B:ARG:HB3	7	0.47
(1,3320)	2:19:B:ILE:HG22	2:26:B:SER:H	7	0.47
(1,3233)	2:72:C:ALA:H	2:72:C:ALA:HB2	4	0.47
(1,3232)	2:72:B:ALA:H	2:72:B:ALA:HB2	7	0.47
(1,3221)	2:34:C:ASN:HA	2:17:C:SER:H	3	0.47
(1,3220)	2:34:B:ASN:HA	2:17:B:SER:H	2	0.47
(1,3092)	2:13:B:VAL:HG12	2:41:B:SER:H	8	0.47
(1,3068)	2:39:B:CYS:H	2:35:B:VAL:HB	3	0.47
(1,2790)	2:33:B:LEU:HD11	2:19:B:ILE:HB	6	0.47
(1,2551)	2:20:C:VAL:HG12	2:19:C:ILE:HB	10	0.47
(1,2550)	2:20:B:VAL:HG11	2:19:B:ILE:HB	5	0.47
(1,2550)	2:20:B:VAL:HG13	2:19:B:ILE:HB	6	0.47
(1,2540)	2:36:B:ALA:HB3	2:33:B:LEU:HD11	6	0.47
(1,2535)	2:36:C:ALA:HB3	2:40:B:ILE:HG13	6	0.47
(1,2535)	2:36:C:ALA:HB2	2:40:B:ILE:HG13	9	0.47
(1,2270)	2:20:B:VAL:HA	2:25:B:ILE:HG23	9	0.47
(1,2039)	2:5:C:LYS:HB3	2:44:C:PHE:HZ	4	0.47
(1,1995)	2:36:C:ALA:HB1	2:33:C:LEU:HD21	6	0.47
(1,1995)	2:36:C:ALA:HB1	2:33:C:LEU:HD21	8	0.47
(1,1994)	2:36:B:ALA:HB3	2:33:B:LEU:HD21	9	0.47
(1,1808)	1:103:A:GLN:HE22	1:114:A:ILE:HG13	5	0.47
(1,1784)	1:105:A:LEU:H	1:117:A:ILE:HD13	5	0.47
(1,1659)	1:124:A:LYS:HE2	1:124:A:LYS:HD3	3	0.47
(1,1659)	1:124:A:LYS:HE2	1:124:A:LYS:HD3	8	0.47
(1,1654)	1:121:A:LEU:HG	1:121:A:LEU:HD22	10	0.47
(1,1461)	1:126:A:LEU:HD21	1:145:A:THR:H	6	0.47
(1,1460)	1:132:A:LEU:HD13	1:132:A:LEU:HA	6	0.47
(1,1450)	1:99:A:LEU:HD21	1:102:A:LYS:H	6	0.47
(1,1435)	1:98:A:ILE:HG22	1:128:A:ASP:H	5	0.47
(1,1295)	1:129:A:ASN:H	1:97:A:THR:HB	2	0.47
(1,1159)	1:152:A:LEU:HG	1:152:A:LEU:H	8	0.47
(1,756)	1:146:A:VAL:HG21	1:119:A:LEU:HA	5	0.47
(1,734)	1:87:A:SER:HA	1:79:A:LYS:HD3	10	0.47
(1,683)	1:106:A:ILE:HG12	1:106:A:ILE:H	1	0.47
(1,669)	1:103:A:GLN:HG3	1:99:A:LEU:HD11	1	0.47
(1,669)	1:103:A:GLN:HG3	1:99:A:LEU:HD12	2	0.47
(1,669)	1:103:A:GLN:HG3	1:99:A:LEU:HD11	9	0.47
(1,511)	1:139:A:PRO:HD2	1:138:A:THR:HB	3	0.47
(1,411)	1:122:A:LYS:HD3	1:123:A:GLY:H	9	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,235)	1:118:A:LYS:HB3	1:118:A:LYS:HE3	2	0.47
(1,180)	1:132:A:LEU:HD11	1:96:A:ASP:HB2	9	0.47
(1,119)	1:97:A:THR:HG22	1:131:A:PHE:HD1	8	0.47
(3,139)	2:38:C:ASP:H	2:34:C:ASN:O	6	0.46
(3,89)	2:38:B:ASP:H	2:34:B:ASN:O	4	0.46
(1,4186)	1:120:A:LEU:HG	2:35:B:VAL:H	4	0.46
(1,4185)	1:120:A:LEU:HG	2:35:B:VAL:H	4	0.46
(1,4099)	2:17:C:SER:H	2:12:C:ILE:HG23	1	0.46
(1,4084)	2:14:B:ASN:H	2:12:B:ILE:HG21	10	0.46
(1,3936)	2:13:B:VAL:HG22	2:48:B:ARG:HG3	1	0.46
(1,3796)	2:8:B:ILE:HG21	2:9:B:ALA:HB2	5	0.46
(1,3724)	2:25:B:ILE:HG21	2:19:B:ILE:HB	4	0.46
(1,3704)	2:6:B:GLU:HA	2:46:B:PHE:HE1	6	0.46
(1,3659)	2:51:C:VAL:HG23	2:46:C:PHE:HE2	10	0.46
(1,3622)	2:40:B:ILE:HA	2:33:C:LEU:HG	2	0.46
(1,3549)	2:55:C:LEU:HD11	2:8:C:ILE:HA	4	0.46
(1,3186)	2:40:B:ILE:H	2:13:B:VAL:HG12	8	0.46
(1,3182)	2:12:B:ILE:HD12	2:9:B:ALA:H	3	0.46
(1,2804)	2:52:B:SER:HB3	2:68:C:ILE:HG22	2	0.46
(1,2550)	2:20:B:VAL:HG13	2:19:B:ILE:HB	8	0.46
(1,2550)	2:20:B:VAL:HG11	2:19:B:ILE:HB	10	0.46
(1,2545)	2:51:C:VAL:HG12	2:55:C:LEU:HG	7	0.46
(1,2535)	2:36:C:ALA:HB2	2:40:B:ILE:HG13	7	0.46
(1,2426)	2:68:B:ILE:HD13	2:60:C:PHE:HD2	7	0.46
(1,2422)	2:25:B:ILE:HD11	2:44:C:PHE:HZ	3	0.46
(1,2346)	2:44:B:PHE:HB2	2:46:B:PHE:HD1	1	0.46
(1,2250)	2:11:B:LEU:HA	2:55:B:LEU:HB3	5	0.46
(1,2126)	2:54:B:ILE:HB	2:13:B:VAL:HG22	3	0.46
(1,2113)	2:13:C:VAL:HG22	2:51:C:VAL:HB	7	0.46
(1,2039)	2:5:C:LYS:HB3	2:44:C:PHE:HZ	3	0.46
(1,1994)	2:36:B:ALA:HB2	2:33:B:LEU:HD22	4	0.46
(1,1994)	2:36:B:ALA:HB3	2:33:B:LEU:HD21	10	0.46
(1,1831)	1:148:A:ILE:HD13	1:148:A:ILE:H	2	0.46
(1,1801)	1:82:A:GLN:HE22	1:81:A:ILE:HG22	7	0.46
(1,1758)	1:83:A:ALA:H	1:85:A:LYS:HG2	7	0.46
(1,1704)	1:121:A:LEU:H	1:121:A:LEU:HD22	3	0.46
(1,1620)	1:149:A:LYS:HB2	1:148:A:ILE:HG22	2	0.46
(1,1461)	1:120:A:LEU:HD23	1:145:A:THR:H	10	0.46
(1,1460)	1:132:A:LEU:HD13	1:132:A:LEU:HA	2	0.46
(1,1455)	1:132:A:LEU:HD21	1:94:A:PRO:HA	7	0.46
(1,1449)	1:78:A:LEU:HD11	1:90:A:HIS:H	4	0.46
(1,1440)	1:74:A:VAL:HG12	1:137:A:VAL:H	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:121:A:LEU:HD12	1:141:A:ASN:HD21	9	0.46
(1,1338)	1:99:A:LEU:HD11	1:103:A:GLN:HE21	1	0.46
(1,1211)	1:81:A:ILE:H	1:82:A:GLN:HG2	7	0.46
(1,1159)	1:152:A:LEU:HG	1:152:A:LEU:H	3	0.46
(1,704)	1:122:A:LYS:HE3	1:141:A:ASN:HD21	7	0.46
(1,683)	1:106:A:ILE:HG12	1:106:A:ILE:H	6	0.46
(1,531)	1:137:A:VAL:HA	1:138:A:THR:HG21	3	0.46
(1,494)	1:98:A:ILE:HA	1:101:A:ILE:HG12	6	0.46
(1,154)	1:135:A:LEU:HD12	1:136:A:LYS:H	7	0.46
(1,149)	1:78:A:LEU:HD11	1:92:A:PHE:HE1	2	0.46
(1,75)	1:98:A:ILE:HG22	1:128:A:ASP:HA	10	0.46
(1,72)	1:88:A:ILE:HG21	1:86:A:PHE:HD1	2	0.46
(1,29)	1:144:A:ILE:HD11	1:144:A:ILE:HA	7	0.46
(1,4176)	1:145:A:THR:HG21	2:35:C:VAL:HG11	2	0.45
(1,3963)	2:36:C:ALA:HB2	2:40:B:ILE:HA	10	0.45
(1,3955)	2:5:C:LYS:HD3	2:19:B:ILE:HG23	3	0.45
(1,3955)	2:5:C:LYS:HD3	2:19:B:ILE:HD13	4	0.45
(1,3744)	2:40:B:ILE:HD12	2:36:C:ALA:HB1	4	0.45
(1,3545)	2:51:C:VAL:HG23	2:48:C:ARG:HB3	5	0.45
(1,3316)	2:26:B:SER:H	2:33:B:LEU:HD13	8	0.45
(1,3186)	2:40:B:ILE:H	2:13:B:VAL:HG12	3	0.45
(1,3186)	2:40:B:ILE:H	2:13:B:VAL:HG12	7	0.45
(1,2951)	2:60:C:PHE:HD1	2:54:C:ILE:HB	6	0.45
(1,2937)	2:6:C:GLU:HG2	2:44:C:PHE:HD1	8	0.45
(1,2880)	2:33:B:LEU:HD11	2:19:B:ILE:HD12	7	0.45
(1,2836)	2:40:B:ILE:HB	2:13:B:VAL:HG12	2	0.45
(1,2810)	2:25:B:ILE:HA	2:33:B:LEU:HD13	4	0.45
(1,2559)	2:55:C:LEU:HD21	2:13:C:VAL:HG22	1	0.45
(1,2545)	2:51:C:VAL:HG12	2:55:C:LEU:HG	6	0.45
(1,2540)	2:36:B:ALA:HB2	2:33:B:LEU:HD11	4	0.45
(1,2482)	2:25:B:ILE:HB	2:19:B:ILE:HG22	8	0.45
(1,2426)	2:68:B:ILE:HD13	2:60:C:PHE:HD2	3	0.45
(1,2115)	2:13:C:VAL:HG23	2:48:C:ARG:HG2	9	0.45
(1,2113)	2:13:C:VAL:HG22	2:51:C:VAL:HB	6	0.45
(1,2060)	2:55:B:LEU:HD21	2:14:B:ASN:H	6	0.45
(1,2044)	2:5:B:LYS:HD2	2:44:B:PHE:HZ	8	0.45
(1,2012)	2:47:B:GLU:HG3	2:47:B:GLU:H	5	0.45
(1,1995)	2:36:C:ALA:HB1	2:33:C:LEU:HD21	3	0.45
(1,1802)	1:82:A:GLN:HE21	1:82:A:GLN:HB3	2	0.45
(1,1787)	1:111:A:ALA:H	1:106:A:ILE:HG23	7	0.45
(1,1683)	1:77:A:THR:H	1:76:A:LEU:HD12	10	0.45
(1,1661)	1:149:A:LYS:HB3	1:149:A:LYS:HE3	2	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1659)	1:124:A:LYS:HE2	1:124:A:LYS:HD3	7	0.45
(1,1623)	1:126:A:LEU:HG	1:127:A:HIS:HB2	6	0.45
(1,1450)	1:99:A:LEU:HD21	1:102:A:LYS:H	7	0.45
(1,1392)	1:144:A:ILE:HG12	1:144:A:ILE:H	10	0.45
(1,1033)	1:106:A:ILE:HG13	1:106:A:ILE:H	10	0.45
(1,769)	1:132:A:LEU:HA	1:135:A:LEU:HD13	8	0.45
(1,725)	1:148:A:ILE:HD13	1:80:A:LYS:HD3	8	0.45
(1,684)	1:105:A:LEU:HD12	1:86:A:PHE:HZ	10	0.45
(1,683)	1:106:A:ILE:HG12	1:106:A:ILE:H	7	0.45
(1,610)	1:108:A:GLU:HG3	1:107:A:SER:HB3	1	0.45
(1,137)	1:125:A:VAL:HG22	1:127:A:HIS:HA	1	0.45
(1,44)	1:88:A:ILE:HD13	1:78:A:LEU:HB3	2	0.45
(1,31)	1:106:A:ILE:HD12	1:112:A:SER:H	9	0.45
(1,4176)	1:145:A:THR:HG21	2:35:C:VAL:HG13	4	0.44
(1,4050)	2:54:B:ILE:HB	2:50:B:ALA:H	8	0.44
(1,3936)	2:13:B:VAL:HG22	2:48:B:ARG:HG3	5	0.44
(1,3850)	2:40:B:ILE:HG21	2:13:B:VAL:HB	5	0.44
(1,3738)	2:68:B:ILE:HD13	2:11:C:LEU:HD23	6	0.44
(1,3705)	2:6:C:GLU:HA	2:46:C:PHE:HE1	3	0.44
(1,3704)	2:6:B:GLU:HA	2:46:B:PHE:HE1	9	0.44
(1,3548)	2:55:B:LEU:HD12	2:8:B:ILE:HA	4	0.44
(1,3317)	2:26:C:SER:H	2:33:C:LEU:HD12	4	0.44
(1,3253)	2:21:C:GLU:HB3	2:21:C:GLU:H	7	0.44
(1,3092)	2:13:B:VAL:HG13	2:41:B:SER:H	7	0.44
(1,3048)	2:50:B:ALA:H	2:13:B:VAL:HG12	1	0.44
(1,2941)	2:44:C:PHE:HZ	2:33:B:LEU:HD22	2	0.44
(1,2646)	2:55:B:LEU:HD13	2:11:B:LEU:HD23	5	0.44
(1,2599)	2:13:C:VAL:HG11	2:41:C:SER:HA	7	0.44
(1,2562)	2:11:B:LEU:HD22	2:55:B:LEU:HD21	1	0.44
(1,2499)	2:25:C:ILE:HG22	2:20:C:VAL:HG13	7	0.44
(1,2472)	2:12:B:ILE:HG21	2:13:B:VAL:HG13	5	0.44
(1,2427)	2:68:C:ILE:HD12	2:60:B:PHE:HD1	9	0.44
(1,2422)	2:25:B:ILE:HD13	2:44:C:PHE:HZ	4	0.44
(1,2210)	2:22:B:LYS:HA	2:24:B:GLU:HB2	4	0.44
(1,2210)	2:22:B:LYS:HA	2:24:B:GLU:HB2	5	0.44
(1,2044)	2:5:B:LYS:HD2	2:44:B:PHE:HZ	4	0.44
(1,1889)	2:22:C:LYS:HD3	2:22:C:LYS:H	7	0.44
(1,1793)	1:141:A:ASN:HB2	1:140:A:ALA:H	7	0.44
(1,1784)	1:105:A:LEU:H	1:117:A:ILE:HD13	3	0.44
(1,1450)	1:99:A:LEU:HD22	1:102:A:LYS:H	4	0.44
(1,1428)	1:106:A:ILE:HD11	1:102:A:LYS:HB3	6	0.44
(1,1328)	1:100:A:GLN:HE21	1:99:A:LEU:HD11	9	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1166)	1:125:A:VAL:HB	1:125:A:VAL:H	1	0.44
(1,997)	1:93:A:SER:HB3	1:96:A:ASP:H	2	0.44
(1,949)	1:100:A:GLN:H	1:99:A:LEU:HD11	3	0.44
(1,785)	1:122:A:LYS:HD3	1:121:A:LEU:HD12	4	0.44
(1,757)	1:78:A:LEU:HA	1:144:A:ILE:HG23	7	0.44
(1,707)	1:122:A:LYS:HE3	1:143:A:THR:HG21	3	0.44
(1,358)	1:95:A:SER:HB2	1:131:A:PHE:HD2	10	0.44
(1,186)	1:120:A:LEU:HD22	1:120:A:LEU:H	4	0.44
(1,155)	1:135:A:LEU:HD13	1:137:A:VAL:H	7	0.44
(1,150)	1:78:A:LEU:HD13	1:92:A:PHE:HZ	1	0.44
(1,101)	1:77:A:THR:HG21	1:87:A:SER:HB3	2	0.44
(1,4177)	1:147:A:MET:HG2	2:35:B:VAL:HG21	7	0.43
(1,4084)	2:14:B:ASN:H	2:12:B:ILE:HG21	8	0.43
(1,3929)	2:39:C:CYS:HB2	2:35:C:VAL:HB	10	0.43
(1,3890)	2:18:B:SER:HB3	2:19:B:ILE:HG12	4	0.43
(1,3889)	2:18:C:SER:HB3	2:22:C:LYS:HD3	1	0.43
(1,3831)	2:40:C:ILE:HD12	2:13:C:VAL:HB	5	0.43
(1,3819)	2:6:C:GLU:HB3	2:44:C:PHE:HZ	7	0.43
(1,3643)	2:68:C:ILE:HB	2:71:C:SER:H	9	0.43
(1,3609)	2:38:C:ASP:HA	2:40:C:ILE:HD11	2	0.43
(1,3588)	2:5:B:LYS:HE2	2:19:C:ILE:HG21	7	0.43
(1,3320)	2:19:B:ILE:HG23	2:26:B:SER:H	1	0.43
(1,3290)	2:19:B:ILE:HG22	2:25:B:ILE:H	3	0.43
(1,3232)	2:72:B:ALA:H	2:72:B:ALA:HB3	4	0.43
(1,3231)	2:20:C:VAL:H	2:25:C:ILE:HG22	1	0.43
(1,3162)	2:6:B:GLU:HB2	2:7:B:GLU:H	5	0.43
(1,2791)	2:33:C:LEU:HD12	2:19:C:ILE:HB	10	0.43
(1,2563)	2:11:C:LEU:HD23	2:55:C:LEU:HD23	5	0.43
(1,2551)	2:20:C:VAL:HG12	2:19:C:ILE:HB	1	0.43
(1,2551)	2:20:C:VAL:HG12	2:19:C:ILE:HB	7	0.43
(1,2541)	2:36:C:ALA:HB1	2:33:C:LEU:HD12	1	0.43
(1,2405)	2:8:C:ILE:HG21	2:15:B:TYR:H	9	0.43
(1,2271)	2:20:C:VAL:HA	2:25:C:ILE:HG22	1	0.43
(1,2192)	2:25:B:ILE:HD12	2:30:B:ALA:HA	1	0.43
(1,2183)	2:9:C:ALA:HA	2:40:C:ILE:HG23	1	0.43
(1,2112)	2:13:B:VAL:HG23	2:51:B:VAL:HB	5	0.43
(1,2090)	2:8:B:ILE:HD12	2:3:B:ALA:HB3	9	0.43
(1,2064)	2:55:B:LEU:HD22	2:51:B:VAL:HB	10	0.43
(1,2061)	2:55:C:LEU:HD23	2:14:C:ASN:H	2	0.43
(1,2013)	2:47:C:GLU:HG3	2:47:C:GLU:H	5	0.43
(1,1808)	1:99:A:LEU:HG	1:103:A:GLN:HE22	1	0.43
(1,1808)	1:99:A:LEU:HG	1:103:A:GLN:HE22	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1802)	1:82:A:GLN:HE21	1:82:A:GLN:HB2	3	0.43
(1,1794)	1:138:A:THR:H	1:121:A:LEU:HD21	6	0.43
(1,1793)	1:141:A:ASN:HB2	1:140:A:ALA:H	5	0.43
(1,1760)	1:152:A:LEU:HB3	1:153:A:GLU:H	4	0.43
(1,1723)	1:114:A:ILE:HD12	1:102:A:LYS:H	4	0.43
(1,1450)	1:99:A:LEU:HD21	1:102:A:LYS:H	8	0.43
(1,1440)	1:74:A:VAL:HG11	1:137:A:VAL:H	8	0.43
(1,1411)	1:116:A:GLU:HG3	1:151:A:ASN:H	1	0.43
(1,1338)	1:99:A:LEU:HD11	1:103:A:GLN:HE21	4	0.43
(1,1139)	1:82:A:GLN:HG3	1:82:A:GLN:H	8	0.43
(1,1011)	1:98:A:ILE:H	1:98:A:ILE:HG12	1	0.43
(1,897)	1:85:A:LYS:HB2	1:86:A:PHE:H	4	0.43
(1,889)	1:130:A:LEU:HB3	1:130:A:LEU:H	8	0.43
(1,889)	1:130:A:LEU:HB3	1:130:A:LEU:H	9	0.43
(1,749)	1:124:A:LYS:HG2	1:125:A:VAL:HA	6	0.43
(1,437)	1:94:A:PRO:HD2	1:74:A:VAL:HG11	3	0.43
(1,201)	1:144:A:ILE:HG23	1:120:A:LEU:H	7	0.43
(1,104)	1:143:A:THR:HG22	1:144:A:ILE:H	2	0.43
(1,67)	1:83:A:ALA:HB2	1:85:A:LYS:H	6	0.43
(1,47)	1:88:A:ILE:HD13	1:105:A:LEU:HA	3	0.43
(1,4189)	1:124:A:LYS:H	2:38:C:ASP:H	1	0.42
(1,4153)	2:54:C:ILE:H	2:55:C:LEU:HD11	9	0.42
(1,3962)	2:36:B:ALA:HB1	2:40:C:ILE:HA	3	0.42
(1,3816)	2:6:B:GLU:HB2	2:46:B:PHE:HD1	10	0.42
(1,3802)	2:3:B:ALA:HB3	2:7:B:GLU:H	9	0.42
(1,3771)	2:30:C:ALA:HA	2:20:C:VAL:HG22	3	0.42
(1,3722)	2:25:B:ILE:HG21	2:5:C:LYS:HE3	8	0.42
(1,3693)	2:9:C:ALA:HA	2:46:C:PHE:HE1	5	0.42
(1,3693)	2:9:C:ALA:HA	2:46:C:PHE:HE1	9	0.42
(1,3570)	2:13:B:VAL:HG22	2:48:B:ARG:HG3	1	0.42
(1,3420)	2:51:B:VAL:H	2:54:B:ILE:HG12	1	0.42
(1,3175)	2:7:C:GLU:H	2:4:C:SER:HB3	6	0.42
(1,3138)	2:2:B:SER:H	2:3:B:ALA:H	7	0.42
(1,3068)	2:39:B:CYS:H	2:35:B:VAL:HB	7	0.42
(1,2836)	2:40:B:ILE:HB	2:13:B:VAL:HG12	8	0.42
(1,2640)	2:33:B:LEU:HD12	2:20:B:VAL:HG11	7	0.42
(1,2535)	2:36:C:ALA:HB2	2:40:B:ILE:HG13	5	0.42
(1,2520)	2:51:B:VAL:HA	2:54:B:ILE:HD11	4	0.42
(1,2367)	2:33:C:LEU:HD11	2:44:B:PHE:HZ	5	0.42
(1,2270)	2:20:B:VAL:HA	2:25:B:ILE:HG23	10	0.42
(1,2243)	2:11:C:LEU:HA	2:54:C:ILE:HB	6	0.42
(1,2193)	2:25:C:ILE:HD11	2:30:C:ALA:HA	4	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2192)	2:25:B:ILE:HD13	2:30:B:ALA:HA	7	0.42
(1,2070)	2:51:B:VAL:HG22	2:14:B:ASN:HA	2	0.42
(1,2070)	2:51:B:VAL:HG22	2:14:B:ASN:HA	6	0.42
(1,2043)	2:5:C:LYS:HD3	2:44:C:PHE:HZ	8	0.42
(1,1707)	1:144:A:ILE:HG23	1:120:A:LEU:H	3	0.42
(1,1661)	1:149:A:LYS:HB3	1:149:A:LYS:HE3	4	0.42
(1,1458)	1:126:A:LEU:HD21	1:126:A:LEU:HA	2	0.42
(1,1350)	1:141:A:ASN:HB3	1:141:A:ASN:HD21	1	0.42
(1,1033)	1:106:A:ILE:HG13	1:106:A:ILE:H	5	0.42
(1,980)	1:101:A:ILE:HG13	1:101:A:ILE:H	10	0.42
(1,958)	1:121:A:LEU:H	1:126:A:LEU:HB3	9	0.42
(1,766)	1:76:A:LEU:HA	1:76:A:LEU:HD12	8	0.42
(1,247)	1:103:A:GLN:HG2	1:100:A:GLN:HE22	4	0.42
(1,201)	1:144:A:ILE:HG23	1:120:A:LEU:H	3	0.42
(1,184)	1:130:A:LEU:HD21	1:130:A:LEU:H	1	0.42
(1,90)	1:101:A:ILE:HG21	1:78:A:LEU:HA	2	0.42
(1,67)	1:83:A:ALA:HB2	1:85:A:LYS:H	7	0.42
(1,13)	1:119:A:LEU:HD21	1:98:A:ILE:HA	9	0.42
(1,4177)	1:147:A:MET:HG3	2:35:B:VAL:HG22	1	0.41
(1,4091)	2:16:C:PHE:H	2:12:B:ILE:HD13	1	0.41
(1,4004)	2:46:B:PHE:HE2	2:54:B:ILE:HG23	5	0.41
(1,3968)	2:25:B:ILE:HG22	2:44:C:PHE:HD1	6	0.41
(1,3963)	2:36:C:ALA:HB2	2:40:B:ILE:HA	8	0.41
(1,3771)	2:30:C:ALA:HA	2:20:C:VAL:HG22	6	0.41
(1,3760)	2:51:B:VAL:HG13	2:51:B:VAL:HB	10	0.41
(1,3750)	2:51:B:VAL:HG11	2:51:B:VAL:HB	6	0.41
(1,3750)	2:51:B:VAL:HG13	2:51:B:VAL:HB	10	0.41
(1,3727)	2:25:C:ILE:HG23	2:25:C:ILE:HG12	7	0.41
(1,3726)	2:25:B:ILE:HG22	2:25:B:ILE:HG12	5	0.41
(1,3554)	2:25:B:ILE:HD12	2:5:C:LYS:HB3	10	0.41
(1,3548)	2:55:B:LEU:HD12	2:8:B:ILE:HA	10	0.41
(1,3421)	2:51:C:VAL:H	2:54:C:ILE:HG12	5	0.41
(1,3312)	2:26:B:SER:H	2:44:C:PHE:HD1	9	0.41
(1,3163)	2:6:C:GLU:HB2	2:7:C:GLU:H	3	0.41
(1,2880)	2:33:B:LEU:HD11	2:19:B:ILE:HD12	2	0.41
(1,2699)	2:54:C:ILE:HG23	2:6:C:GLU:HG3	5	0.41
(1,2631)	2:51:C:VAL:HB	2:55:C:LEU:HG	5	0.41
(1,2615)	2:13:C:VAL:HG11	2:48:C:ARG:HG2	7	0.41
(1,2544)	2:51:B:VAL:HG11	2:55:B:LEU:HG	6	0.41
(1,2347)	2:44:C:PHE:HB2	2:46:C:PHE:HD1	1	0.41
(1,2227)	2:5:C:LYS:HA	2:8:C:ILE:HG13	9	0.41
(1,2204)	2:22:B:LYS:HG2	2:22:B:LYS:HA	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2178)	2:9:B:ALA:HA	2:12:B:ILE:HD13	10	0.41
(1,2115)	2:13:C:VAL:HG23	2:48:C:ARG:HG2	5	0.41
(1,2100)	2:19:B:ILE:HD12	2:24:B:GLU:HG3	6	0.41
(1,2100)	2:19:B:ILE:HD12	2:24:B:GLU:HG3	8	0.41
(1,2043)	2:5:C:LYS:HD3	2:44:C:PHE:HZ	6	0.41
(1,1994)	2:36:B:ALA:HB3	2:33:B:LEU:HD23	6	0.41
(1,1680)	1:145:A:THR:H	1:121:A:LEU:HG	2	0.41
(1,1659)	1:124:A:LYS:HE2	1:124:A:LYS:HD3	9	0.41
(1,1140)	1:82:A:GLN:HG2	1:82:A:GLN:H	6	0.41
(1,1077)	1:129:A:ASN:HB3	1:129:A:ASN:H	5	0.41
(1,1033)	1:106:A:ILE:HG13	1:106:A:ILE:H	3	0.41
(1,1011)	1:98:A:ILE:H	1:98:A:ILE:HG12	7	0.41
(1,1011)	1:98:A:ILE:H	1:98:A:ILE:HG12	10	0.41
(1,949)	1:100:A:GLN:H	1:99:A:LEU:HD11	1	0.41
(1,949)	1:100:A:GLN:H	1:99:A:LEU:HD13	9	0.41
(1,867)	1:145:A:THR:HG22	1:145:A:THR:H	4	0.41
(1,734)	1:87:A:SER:HA	1:79:A:LYS:HD3	1	0.41
(1,719)	1:148:A:ILE:HD12	1:112:A:SER:H	7	0.41
(1,686)	1:122:A:LYS:HA	1:122:A:LYS:HD3	2	0.41
(1,158)	1:99:A:LEU:HD21	1:103:A:GLN:H	3	0.41
(1,156)	1:99:A:LEU:HD22	1:103:A:GLN:HE21	3	0.41
(1,110)	1:126:A:LEU:HD13	1:125:A:VAL:HA	4	0.41
(3,140)	2:38:C:ASP:N	2:34:C:ASN:O	8	0.4
(3,34)	1:149:A:LYS:N	1:116:A:GLU:O	4	0.4
(1,4189)	1:124:A:LYS:H	2:38:C:ASP:H	2	0.4
(1,4181)	1:120:A:LEU:HD11	2:38:C:ASP:H	9	0.4
(1,4108)	2:21:B:GLU:H	2:22:B:LYS:HG3	5	0.4
(1,4085)	2:14:C:ASN:H	2:12:C:ILE:HG23	2	0.4
(1,3995)	2:5:C:LYS:HD3	2:44:C:PHE:HZ	10	0.4
(1,3760)	2:20:B:VAL:HG12	2:20:B:VAL:HB	6	0.4
(1,3750)	2:51:B:VAL:HG11	2:51:B:VAL:HB	3	0.4
(1,3745)	2:40:C:ILE:HD13	2:36:C:ALA:HB3	1	0.4
(1,3724)	2:25:B:ILE:HG22	2:19:B:ILE:HB	3	0.4
(1,3704)	2:6:B:GLU:HA	2:46:B:PHE:HE1	7	0.4
(1,3628)	2:18:B:SER:HB3	2:19:B:ILE:HD11	6	0.4
(1,3570)	2:13:B:VAL:HG22	2:48:B:ARG:HG3	5	0.4
(1,3421)	2:51:C:VAL:H	2:54:C:ILE:HG12	2	0.4
(1,3174)	2:7:B:GLU:H	2:4:B:SER:HB3	2	0.4
(1,3139)	2:2:C:SER:H	2:3:C:ALA:H	2	0.4
(1,2940)	2:44:B:PHE:HZ	2:33:C:LEU:HD21	1	0.4
(1,2940)	2:44:B:PHE:HZ	2:33:C:LEU:HD23	3	0.4
(1,2836)	2:40:B:ILE:HB	2:13:B:VAL:HG12	3	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2691)	2:50:C:ALA:HB3	2:47:C:GLU:HB3	3	0.4
(1,2650)	2:8:B:ILE:HG22	2:19:C:ILE:HG12	5	0.4
(1,2044)	2:5:B:LYS:HD2	2:44:B:PHE:HZ	1	0.4
(1,2043)	2:5:C:LYS:HD3	2:44:C:PHE:HZ	2	0.4
(1,1787)	1:111:A:ALA:H	1:106:A:ILE:HG23	1	0.4
(1,1761)	1:82:A:GLN:H	1:80:A:LYS:HD2	9	0.4
(1,1723)	1:102:A:LYS:H	1:117:A:ILE:HD11	9	0.4
(1,1699)	1:98:A:ILE:HG23	1:128:A:ASP:H	1	0.4
(1,1663)	1:85:A:LYS:HG2	1:85:A:LYS:HE3	4	0.4
(1,1659)	1:124:A:LYS:HE2	1:124:A:LYS:HD3	4	0.4
(1,1532)	1:151:A:ASN:HA	1:152:A:LEU:HG	8	0.4
(1,1458)	1:126:A:LEU:HD23	1:126:A:LEU:HA	9	0.4
(1,1266)	1:107:A:SER:H	1:106:A:ILE:HG21	8	0.4
(1,897)	1:85:A:LYS:HB2	1:86:A:PHE:H	9	0.4
(1,790)	1:126:A:LEU:HG	1:124:A:LYS:HE3	3	0.4
(1,790)	1:126:A:LEU:HG	1:124:A:LYS:HE3	8	0.4
(1,780)	1:148:A:ILE:HG21	1:148:A:ILE:HB	9	0.4
(1,780)	1:148:A:ILE:HG22	1:148:A:ILE:HB	10	0.4
(1,709)	1:122:A:LYS:HE3	1:141:A:ASN:HA	1	0.4
(1,638)	1:132:A:LEU:HB3	1:135:A:LEU:HD13	8	0.4
(1,494)	1:98:A:ILE:HA	1:101:A:ILE:HG12	4	0.4
(1,177)	1:132:A:LEU:HD23	1:97:A:THR:HA	8	0.4
(1,101)	1:77:A:THR:HG23	1:87:A:SER:HB3	3	0.4
(1,89)	1:101:A:ILE:HG21	1:119:A:LEU:HA	2	0.4
(1,67)	1:83:A:ALA:HB2	1:85:A:LYS:H	1	0.4
(1,44)	1:88:A:ILE:HD13	1:78:A:LEU:HB3	8	0.4
(3,139)	2:38:C:ASP:H	2:34:C:ASN:O	1	0.39
(1,4169)	1:81:A:ILE:HD11	2:31:C:ASP:OD2	2	0.39
(1,3829)	2:40:C:ILE:HD13	2:37:C:MET:HG3	2	0.39
(1,3817)	2:6:C:GLU:HB2	2:46:C:PHE:HD1	7	0.39
(1,3760)	2:20:B:VAL:HG11	2:20:B:VAL:HB	3	0.39
(1,3727)	2:25:C:ILE:HG23	2:30:C:ALA:HB2	8	0.39
(1,3727)	2:25:C:ILE:HG21	2:25:C:ILE:HG12	9	0.39
(1,3658)	2:51:B:VAL:HG21	2:46:B:PHE:HE2	7	0.39
(1,3252)	2:21:B:GLU:HB3	2:21:B:GLU:H	6	0.39
(1,3252)	2:21:B:GLU:HB3	2:21:B:GLU:H	8	0.39
(1,3186)	2:40:B:ILE:H	2:13:B:VAL:HG12	2	0.39
(1,3163)	2:6:C:GLU:HB2	2:7:C:GLU:H	6	0.39
(1,3139)	2:2:C:SER:H	2:3:C:ALA:H	3	0.39
(1,3049)	2:50:C:ALA:H	2:13:C:VAL:HG13	9	0.39
(1,2811)	2:25:C:ILE:HA	2:33:C:LEU:HD11	10	0.39
(1,2790)	2:33:B:LEU:HD11	2:19:B:ILE:HB	8	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2630)	2:51:B:VAL:HB	2:55:B:LEU:HG	3	0.39
(1,2614)	2:13:B:VAL:HG13	2:48:B:ARG:HG2	2	0.39
(1,2598)	2:13:B:VAL:HG13	2:41:B:SER:HA	8	0.39
(1,2595)	2:57:C:LYS:HB3	2:68:B:ILE:HG13	5	0.39
(1,2565)	2:33:C:LEU:HD11	2:19:C:ILE:HG21	9	0.39
(1,2492)	2:54:B:ILE:HB	2:54:B:ILE:HG22	1	0.39
(1,2409)	2:19:C:ILE:HG21	2:44:B:PHE:HZ	1	0.39
(1,2271)	2:20:C:VAL:HA	2:25:C:ILE:HG22	10	0.39
(1,2183)	2:9:C:ALA:HA	2:40:C:ILE:HG21	4	0.39
(1,2182)	2:9:B:ALA:HA	2:40:B:ILE:HG21	5	0.39
(1,2178)	2:9:B:ALA:HA	2:12:B:ILE:HD11	1	0.39
(1,2082)	2:25:B:ILE:HD13	2:19:B:ILE:HG21	5	0.39
(1,1831)	1:148:A:ILE:HD13	1:148:A:ILE:H	5	0.39
(1,1803)	1:82:A:GLN:HE21	1:81:A:ILE:HG22	4	0.39
(1,1802)	1:82:A:GLN:HE21	1:82:A:GLN:HB2	9	0.39
(1,1787)	1:111:A:ALA:H	1:106:A:ILE:HG23	9	0.39
(1,1723)	1:114:A:ILE:HD12	1:102:A:LYS:H	7	0.39
(1,1707)	1:144:A:ILE:HG21	1:120:A:LEU:H	5	0.39
(1,1680)	1:145:A:THR:H	1:121:A:LEU:HG	5	0.39
(1,1450)	1:99:A:LEU:HD21	1:102:A:LYS:H	3	0.39
(1,949)	1:100:A:GLN:H	1:99:A:LEU:HD11	6	0.39
(1,783)	1:106:A:ILE:HG21	1:106:A:ILE:HB	8	0.39
(1,783)	1:106:A:ILE:HG22	1:106:A:ILE:HB	10	0.39
(1,780)	1:148:A:ILE:HG22	1:148:A:ILE:HB	1	0.39
(1,780)	1:148:A:ILE:HG23	1:148:A:ILE:HB	2	0.39
(1,695)	1:79:A:LYS:HE3	1:81:A:ILE:HB	3	0.39
(1,382)	1:73:A:MET:HB2	1:74:A:VAL:H	2	0.39
(1,201)	1:144:A:ILE:HG21	1:120:A:LEU:H	5	0.39
(1,181)	1:132:A:LEU:HD13	1:92:A:PHE:HB2	2	0.39
(1,180)	1:132:A:LEU:HD11	1:96:A:ASP:HB2	4	0.39
(1,148)	1:132:A:LEU:HD21	1:92:A:PHE:HD2	2	0.39
(1,46)	1:88:A:ILE:HD11	1:88:A:ILE:HG12	3	0.39
(1,46)	1:88:A:ILE:HD11	1:88:A:ILE:HG12	6	0.39
(1,4189)	1:124:A:LYS:H	2:38:C:ASP:H	6	0.38
(1,4186)	1:120:A:LEU:HG	2:35:C:VAL:H	9	0.38
(1,4185)	1:120:A:LEU:HG	2:35:C:VAL:H	9	0.38
(1,3796)	2:8:B:ILE:HG21	2:9:B:ALA:HB2	1	0.38
(1,3761)	2:20:C:VAL:HG23	2:20:C:VAL:HB	3	0.38
(1,3665)	2:33:C:LEU:HD22	2:44:B:PHE:HZ	10	0.38
(1,3659)	2:51:C:VAL:HG23	2:46:C:PHE:HE2	7	0.38
(1,3628)	2:18:B:SER:HB3	2:19:B:ILE:HD11	8	0.38
(1,3595)	2:9:C:ALA:HA	2:12:C:ILE:HG13	7	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3549)	2:55:C:LEU:HD12	2:12:C:ILE:HA	9	0.38
(1,3545)	2:51:C:VAL:HG22	2:48:C:ARG:HB3	6	0.38
(1,2784)	2:51:B:VAL:HG22	2:14:B:ASN:H	2	0.38
(1,2692)	2:50:B:ALA:HB3	2:47:B:GLU:HB2	7	0.38
(1,2630)	2:51:B:VAL:HB	2:55:B:LEU:HG	9	0.38
(1,2550)	2:20:B:VAL:HG13	2:19:B:ILE:HB	7	0.38
(1,2493)	2:54:C:ILE:HB	2:54:C:ILE:HG22	4	0.38
(1,2493)	2:54:C:ILE:HB	2:54:C:ILE:HG23	6	0.38
(1,2492)	2:54:B:ILE:HB	2:54:B:ILE:HG21	2	0.38
(1,2492)	2:54:B:ILE:HB	2:54:B:ILE:HG21	3	0.38
(1,2492)	2:54:B:ILE:HB	2:54:B:ILE:HG23	4	0.38
(1,2492)	2:54:B:ILE:HB	2:54:B:ILE:HG23	5	0.38
(1,2492)	2:54:B:ILE:HB	2:54:B:ILE:HG21	7	0.38
(1,2380)	2:55:B:LEU:HD12	2:60:B:PHE:HD2	6	0.38
(1,2113)	2:13:C:VAL:HG22	2:51:C:VAL:HB	4	0.38
(1,1820)	1:129:A:ASN:HD21	1:99:A:LEU:HD12	6	0.38
(1,1802)	1:82:A:GLN:HE21	1:82:A:GLN:HB3	1	0.38
(1,1793)	1:141:A:ASN:HB2	1:138:A:THR:H	4	0.38
(1,1787)	1:111:A:ALA:H	1:148:A:ILE:HD12	5	0.38
(1,1659)	1:124:A:LYS:HE2	1:124:A:LYS:HD3	1	0.38
(1,1659)	1:118:A:LYS:HB2	1:118:A:LYS:HE3	10	0.38
(1,1461)	1:126:A:LEU:HD21	1:145:A:THR:H	8	0.38
(1,1140)	1:82:A:GLN:HG2	1:82:A:GLN:H	1	0.38
(1,980)	1:101:A:ILE:HG13	1:101:A:ILE:H	2	0.38
(1,980)	1:101:A:ILE:HG13	1:101:A:ILE:H	5	0.38
(1,783)	1:106:A:ILE:HG22	1:106:A:ILE:HB	4	0.38
(1,780)	1:148:A:ILE:HG21	1:148:A:ILE:HB	3	0.38
(1,780)	1:148:A:ILE:HG22	1:148:A:ILE:HB	8	0.38
(1,722)	1:148:A:ILE:HA	1:148:A:ILE:HD12	6	0.38
(1,720)	1:148:A:ILE:HD13	1:86:A:PHE:HZ	2	0.38
(1,440)	1:83:A:ALA:HA	1:85:A:LYS:HE3	4	0.38
(1,172)	1:78:A:LEU:HD21	1:78:A:LEU:HG	2	0.38
(1,172)	1:78:A:LEU:HD23	1:78:A:LEU:HG	4	0.38
(1,172)	1:78:A:LEU:HD23	1:78:A:LEU:HG	10	0.38
(1,162)	1:78:A:LEU:HD23	1:92:A:PHE:HZ	7	0.38
(1,46)	1:88:A:ILE:HD11	1:88:A:ILE:HG12	2	0.38
(1,46)	1:88:A:ILE:HD11	1:88:A:ILE:HG12	5	0.38
(1,46)	1:88:A:ILE:HD11	1:88:A:ILE:HG12	9	0.38
(3,139)	2:38:C:ASP:H	2:34:C:ASN:O	3	0.37
(3,90)	2:38:B:ASP:N	2:34:B:ASN:O	4	0.37
(3,34)	1:149:A:LYS:N	1:116:A:GLU:O	9	0.37
(1,4189)	1:124:A:LYS:H	2:38:C:ASP:H	4	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4099)	2:17:C:SER:H	2:12:C:ILE:HG23	7	0.37
(1,4098)	2:17:B:SER:H	2:12:B:ILE:HG22	4	0.37
(1,4090)	2:16:B:PHE:H	2:12:C:ILE:HD12	3	0.37
(1,4084)	2:14:B:ASN:H	2:12:B:ILE:HG23	1	0.37
(1,4084)	2:14:B:ASN:H	2:12:B:ILE:HG21	2	0.37
(1,4057)	2:17:C:SER:HA	2:18:C:SER:H	10	0.37
(1,4008)	2:44:B:PHE:HZ	2:19:C:ILE:HG21	5	0.37
(1,3875)	2:15:C:TYR:HA	2:12:C:ILE:HD12	9	0.37
(1,3823)	2:40:C:ILE:HD11	2:36:C:ALA:HA	4	0.37
(1,3819)	2:6:C:GLU:HB3	2:46:C:PHE:HD1	5	0.37
(1,3760)	2:51:B:VAL:HG12	2:51:B:VAL:HB	1	0.37
(1,3751)	2:20:C:VAL:HG23	2:20:C:VAL:HB	3	0.37
(1,3751)	2:20:C:VAL:HG23	2:20:C:VAL:HB	6	0.37
(1,3750)	2:51:B:VAL:HG12	2:51:B:VAL:HB	1	0.37
(1,3692)	2:9:B:ALA:HA	2:46:B:PHE:HE1	7	0.37
(1,3665)	2:33:C:LEU:HD22	2:16:C:PHE:HD1	3	0.37
(1,3659)	2:51:C:VAL:HG22	2:46:C:PHE:HE2	4	0.37
(1,3593)	2:9:C:ALA:HA	2:12:C:ILE:HG21	1	0.37
(1,3588)	2:5:B:LYS:HE2	2:19:C:ILE:HG22	9	0.37
(1,3556)	2:25:B:ILE:HD11	2:5:C:LYS:HD2	3	0.37
(1,3551)	2:25:C:ILE:HD12	2:5:B:LYS:HE3	4	0.37
(1,3545)	2:51:C:VAL:HG23	2:48:C:ARG:HB3	7	0.37
(1,3477)	2:55:C:LEU:HD23	2:14:C:ASN:HD21	5	0.37
(1,3321)	2:19:C:ILE:HG22	2:26:C:SER:H	8	0.37
(1,3233)	2:72:C:ALA:H	2:72:C:ALA:HB2	7	0.37
(1,3015)	2:5:C:LYS:HG2	2:5:C:LYS:H	9	0.37
(1,2941)	2:44:C:PHE:HZ	2:33:B:LEU:HD22	6	0.37
(1,2715)	2:54:C:ILE:HD12	2:47:C:GLU:H	2	0.37
(1,2651)	2:8:C:ILE:HG21	2:19:B:ILE:HG12	5	0.37
(1,2651)	2:8:C:ILE:HG21	2:19:B:ILE:HG12	9	0.37
(1,2641)	2:33:C:LEU:HD13	2:20:C:VAL:HG12	7	0.37
(1,2552)	2:35:B:VAL:HG12	2:37:B:MET:HB3	1	0.37
(1,2550)	2:20:B:VAL:HG11	2:19:B:ILE:HB	1	0.37
(1,2521)	2:51:C:VAL:HA	2:54:C:ILE:HD11	8	0.37
(1,2493)	2:54:C:ILE:HB	2:54:C:ILE:HG21	3	0.37
(1,2492)	2:54:B:ILE:HB	2:54:B:ILE:HG22	8	0.37
(1,2492)	2:54:B:ILE:HB	2:54:B:ILE:HG22	10	0.37
(1,2408)	2:19:B:ILE:HG21	2:44:C:PHE:HZ	5	0.37
(1,2347)	2:44:C:PHE:HB2	2:46:C:PHE:HD1	7	0.37
(1,2226)	2:5:B:LYS:HA	2:8:B:ILE:HG13	9	0.37
(1,2113)	2:13:C:VAL:HG22	2:51:C:VAL:HB	2	0.37
(1,2064)	2:55:B:LEU:HD22	2:51:B:VAL:HB	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1818)	1:99:A:LEU:HD23	1:129:A:ASN:HD22	7	0.37
(1,1808)	1:99:A:LEU:HG	1:103:A:GLN:HE22	4	0.37
(1,1683)	1:77:A:THR:H	1:76:A:LEU:HD12	3	0.37
(1,1659)	1:124:A:LYS:HE2	1:124:A:LYS:HD3	2	0.37
(1,1461)	1:126:A:LEU:HD21	1:145:A:THR:H	3	0.37
(1,1419)	1:107:A:SER:HB3	1:108:A:GLU:H	6	0.37
(1,1411)	1:116:A:GLU:HG3	1:151:A:ASN:H	2	0.37
(1,1132)	1:126:A:LEU:H	1:126:A:LEU:HB3	10	0.37
(1,1011)	1:98:A:ILE:H	1:98:A:ILE:HG12	3	0.37
(1,897)	1:85:A:LYS:HB2	1:86:A:PHE:H	5	0.37
(1,765)	1:152:A:LEU:HA	1:152:A:LEU:HD21	10	0.37
(1,759)	1:114:A:ILE:HA	1:114:A:ILE:HG22	3	0.37
(1,751)	1:149:A:LYS:HG2	1:149:A:LYS:HE3	3	0.37
(1,722)	1:148:A:ILE:HA	1:148:A:ILE:HD12	2	0.37
(1,683)	1:106:A:ILE:HG12	1:106:A:ILE:H	9	0.37
(1,535)	1:150:A:PRO:HA	1:116:A:GLU:HG3	6	0.37
(1,132)	1:138:A:THR:HG22	1:141:A:ASN:HB3	10	0.37
(1,46)	1:88:A:ILE:HD13	1:88:A:ILE:HG12	7	0.37
(3,140)	2:38:C:ASP:N	2:34:C:ASN:O	6	0.36
(3,139)	2:38:C:ASP:H	2:34:C:ASN:O	9	0.36
(1,4057)	2:17:C:SER:HA	2:18:C:SER:H	1	0.36
(1,4057)	2:17:C:SER:HA	2:18:C:SER:H	9	0.36
(1,4051)	2:54:C:ILE:HB	2:50:C:ALA:H	3	0.36
(1,4005)	2:44:C:PHE:HZ	2:25:B:ILE:HG21	5	0.36
(1,4005)	2:44:C:PHE:HZ	2:25:B:ILE:HG22	8	0.36
(1,3940)	2:33:B:LEU:HB2	2:19:B:ILE:HB	6	0.36
(1,3797)	2:8:C:ILE:HG23	2:9:C:ALA:HB1	5	0.36
(1,3761)	2:20:C:VAL:HG23	2:20:C:VAL:HB	7	0.36
(1,3761)	2:20:C:VAL:HG23	2:20:C:VAL:HB	8	0.36
(1,3760)	2:51:B:VAL:HG11	2:51:B:VAL:HB	4	0.36
(1,3760)	2:20:B:VAL:HG22	2:20:B:VAL:HB	8	0.36
(1,3751)	2:20:C:VAL:HG23	2:20:C:VAL:HB	8	0.36
(1,3750)	2:51:B:VAL:HG11	2:51:B:VAL:HB	4	0.36
(1,3750)	2:20:B:VAL:HG22	2:20:B:VAL:HB	8	0.36
(1,3705)	2:6:C:GLU:HA	2:46:C:PHE:HE1	10	0.36
(1,3658)	2:51:B:VAL:HG21	2:46:B:PHE:HE2	8	0.36
(1,3629)	2:18:C:SER:HB3	2:19:C:ILE:HD13	7	0.36
(1,3564)	2:19:B:ILE:HB	2:19:B:ILE:HD11	9	0.36
(1,3554)	2:25:B:ILE:HD13	2:19:B:ILE:HB	5	0.36
(1,3322)	2:25:B:ILE:HG12	2:26:B:SER:H	8	0.36
(1,3233)	2:72:C:ALA:H	2:72:C:ALA:HB2	3	0.36
(1,3232)	2:72:B:ALA:H	2:72:B:ALA:HB3	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3230)	2:20:B:VAL:H	2:25:B:ILE:HG23	1	0.36
(1,3048)	2:50:B:ALA:H	2:13:B:VAL:HG13	3	0.36
(1,2962)	2:48:B:ARG:HG3	2:48:B:ARG:H	1	0.36
(1,2829)	2:6:C:GLU:HG2	2:9:C:ALA:HB3	3	0.36
(1,2535)	2:36:C:ALA:HB1	2:40:B:ILE:HG13	4	0.36
(1,2502)	2:12:B:ILE:HB	2:12:B:ILE:HD11	5	0.36
(1,2493)	2:54:C:ILE:HB	2:54:C:ILE:HG23	2	0.36
(1,2493)	2:54:C:ILE:HB	2:54:C:ILE:HG23	7	0.36
(1,2482)	2:25:B:ILE:HB	2:19:B:ILE:HG22	2	0.36
(1,2475)	2:12:C:ILE:HG21	2:40:C:ILE:HD13	2	0.36
(1,2090)	2:8:B:ILE:HD12	2:3:B:ALA:HB1	6	0.36
(1,2077)	2:55:C:LEU:HD12	2:55:C:LEU:HG	10	0.36
(1,2076)	2:55:B:LEU:HD12	2:55:B:LEU:HG	1	0.36
(1,1810)	1:99:A:LEU:HG	1:103:A:GLN:HE21	10	0.36
(1,1793)	1:141:A:ASN:HB2	1:138:A:THR:H	6	0.36
(1,1683)	1:77:A:THR:H	1:76:A:LEU:HD12	4	0.36
(1,1683)	1:77:A:THR:H	1:76:A:LEU:HD13	6	0.36
(1,1460)	1:132:A:LEU:HD13	1:132:A:LEU:HA	4	0.36
(1,1419)	1:107:A:SER:HB3	1:108:A:GLU:H	4	0.36
(1,1198)	1:113:A:HIS:H	1:116:A:GLU:HB3	1	0.36
(1,1081)	1:140:A:ALA:HB1	1:141:A:ASN:H	8	0.36
(1,1071)	1:138:A:THR:H	1:138:A:THR:HG23	9	0.36
(1,1033)	1:106:A:ILE:HG13	1:106:A:ILE:H	8	0.36
(1,955)	1:131:A:PHE:HB3	1:131:A:PHE:H	1	0.36
(1,868)	1:144:A:ILE:HG22	1:145:A:THR:H	2	0.36
(1,783)	1:106:A:ILE:HG22	1:106:A:ILE:HB	5	0.36
(1,780)	1:148:A:ILE:HG23	1:148:A:ILE:HB	4	0.36
(1,669)	1:103:A:GLN:HG3	1:99:A:LEU:HD11	8	0.36
(1,494)	1:98:A:ILE:HA	1:101:A:ILE:HG12	5	0.36
(1,265)	1:114:A:ILE:HG12	1:103:A:GLN:HE22	8	0.36
(1,184)	1:130:A:LEU:HD21	1:130:A:LEU:H	3	0.36
(1,147)	1:132:A:LEU:HD23	1:98:A:ILE:H	7	0.36
(1,134)	1:125:A:VAL:HG21	1:125:A:VAL:HB	6	0.36
(1,132)	1:138:A:THR:HG22	1:141:A:ASN:HB3	1	0.36
(1,131)	1:111:A:ALA:HB3	1:105:A:LEU:HB2	3	0.36
(1,118)	1:97:A:THR:HG22	1:97:A:THR:H	4	0.36
(1,46)	1:88:A:ILE:HD13	1:88:A:ILE:HG12	1	0.36
(1,19)	1:98:A:ILE:HD13	1:132:A:LEU:HA	3	0.36
(3,139)	2:38:C:ASP:H	2:34:C:ASN:O	2	0.35
(3,33)	1:149:A:LYS:H	1:116:A:GLU:O	8	0.35
(1,4186)	1:120:A:LEU:HG	2:35:B:VAL:H	5	0.35
(1,4185)	1:120:A:LEU:HG	2:35:B:VAL:H	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4126)	2:19:B:ILE:HA	2:25:B:ILE:H	3	0.35
(1,4056)	2:17:B:SER:HA	2:18:B:SER:H	5	0.35
(1,4014)	2:60:B:PHE:HD1	2:8:B:ILE:HD13	2	0.35
(1,3939)	2:33:C:LEU:HD11	2:5:B:LYS:HE3	5	0.35
(1,3936)	2:13:B:VAL:HG21	2:48:B:ARG:HG3	6	0.35
(1,3830)	2:40:B:ILE:HD13	2:13:B:VAL:HB	9	0.35
(1,3761)	2:51:C:VAL:HG12	2:51:C:VAL:HB	5	0.35
(1,3761)	2:20:C:VAL:HG11	2:20:C:VAL:HB	6	0.35
(1,3751)	2:51:C:VAL:HG12	2:51:C:VAL:HB	5	0.35
(1,3751)	2:20:C:VAL:HG23	2:20:C:VAL:HB	7	0.35
(1,3659)	2:51:C:VAL:HG22	2:46:C:PHE:HE2	6	0.35
(1,3567)	2:19:C:ILE:HD11	2:5:B:LYS:HG2	8	0.35
(1,3477)	2:55:C:LEU:HD23	2:14:C:ASN:HD21	6	0.35
(1,3420)	2:51:B:VAL:H	2:54:B:ILE:HG12	2	0.35
(1,3316)	2:26:B:SER:H	2:33:B:LEU:HD11	10	0.35
(1,3290)	2:19:B:ILE:HG22	2:25:B:ILE:H	6	0.35
(1,3233)	2:72:C:ALA:H	2:72:C:ALA:HB1	5	0.35
(1,3231)	2:20:C:VAL:H	2:25:C:ILE:HG22	10	0.35
(1,3230)	2:20:B:VAL:H	2:25:B:ILE:HG23	9	0.35
(1,3092)	2:13:B:VAL:HG11	2:41:B:SER:H	6	0.35
(1,2829)	2:6:C:GLU:HG2	2:9:C:ALA:HB3	7	0.35
(1,2692)	2:50:B:ALA:HB3	2:47:B:GLU:HB2	6	0.35
(1,2545)	2:51:C:VAL:HG12	2:55:C:LEU:HG	2	0.35
(1,2493)	2:54:C:ILE:HB	2:54:C:ILE:HG22	10	0.35
(1,2492)	2:54:B:ILE:HB	2:54:B:ILE:HG23	9	0.35
(1,2356)	2:49:B:GLU:HG2	2:49:B:GLU:H	10	0.35
(1,2244)	2:55:B:LEU:HD22	2:11:B:LEU:HA	4	0.35
(1,2226)	2:5:B:LYS:HA	2:8:B:ILE:HG13	8	0.35
(1,2146)	2:23:B:LYS:HE3	2:23:B:LYS:HG3	3	0.35
(1,2114)	2:13:B:VAL:HG21	2:48:B:ARG:HG2	2	0.35
(1,2112)	2:13:B:VAL:HG23	2:51:B:VAL:HB	1	0.35
(1,2077)	2:55:C:LEU:HD12	2:55:C:LEU:HG	1	0.35
(1,2039)	2:5:C:LYS:HB3	2:44:C:PHE:HZ	2	0.35
(1,1995)	2:36:C:ALA:HB1	2:33:C:LEU:HD23	1	0.35
(1,1793)	1:141:A:ASN:HB2	1:138:A:THR:H	1	0.35
(1,1739)	1:118:A:LYS:H	1:118:A:LYS:HB3	2	0.35
(1,1739)	1:118:A:LYS:H	1:118:A:LYS:HB3	5	0.35
(1,1670)	1:135:A:LEU:HA	1:124:A:LYS:HE3	10	0.35
(1,1661)	1:149:A:LYS:HB3	1:149:A:LYS:HE3	10	0.35
(1,1532)	1:151:A:ASN:HA	1:152:A:LEU:HG	7	0.35
(1,1428)	1:106:A:ILE:HD13	1:102:A:LYS:HB3	5	0.35
(1,1266)	1:107:A:SER:H	1:106:A:ILE:HG21	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1236)	1:99:A:LEU:HD13	1:99:A:LEU:H	10	0.35
(1,1140)	1:82:A:GLN:HG2	1:82:A:GLN:H	2	0.35
(1,1132)	1:126:A:LEU:H	1:126:A:LEU:HB3	3	0.35
(1,1132)	1:126:A:LEU:H	1:126:A:LEU:HB3	9	0.35
(1,1068)	1:119:A:LEU:HD22	1:119:A:LEU:H	7	0.35
(1,955)	1:131:A:PHE:HB3	1:131:A:PHE:H	10	0.35
(1,898)	1:85:A:LYS:HB3	1:86:A:PHE:H	4	0.35
(1,783)	1:106:A:ILE:HG23	1:106:A:ILE:HB	2	0.35
(1,358)	1:95:A:SER:HB2	1:131:A:PHE:HD1	6	0.35
(1,158)	1:99:A:LEU:HD22	1:103:A:GLN:H	4	0.35
(1,134)	1:125:A:VAL:HG23	1:125:A:VAL:HB	2	0.35
(1,134)	1:125:A:VAL:HG21	1:125:A:VAL:HB	7	0.35
(1,112)	1:77:A:THR:HG23	1:78:A:LEU:H	9	0.35
(1,111)	1:126:A:LEU:HD12	1:124:A:LYS:HE2	2	0.35
(1,111)	1:126:A:LEU:HD13	1:124:A:LYS:HE2	5	0.35
(1,110)	1:126:A:LEU:HD13	1:125:A:VAL:HA	8	0.35
(1,13)	1:119:A:LEU:HD21	1:98:A:ILE:HA	10	0.35
(1,2)	1:120:A:LEU:HD13	1:120:A:LEU:H	7	0.35
(3,140)	2:38:C:ASP:N	2:34:C:ASN:O	1	0.34
(1,4171)	1:120:A:LEU:HB3	2:35:C:VAL:HG22	1	0.34
(1,4084)	2:14:B:ASN:H	2:12:B:ILE:HG21	3	0.34
(1,4056)	2:17:B:SER:HA	2:18:B:SER:H	9	0.34
(1,3971)	2:8:C:ILE:HD12	2:60:B:PHE:HE1	5	0.34
(1,3934)	2:55:B:LEU:HD12	2:7:B:GLU:HG2	1	0.34
(1,3851)	2:40:C:ILE:HG22	2:13:C:VAL:HB	6	0.34
(1,3831)	2:40:C:ILE:HD12	2:13:C:VAL:HB	1	0.34
(1,3803)	2:3:C:ALA:HB1	2:7:C:GLU:H	10	0.34
(1,3761)	2:20:C:VAL:HG22	2:20:C:VAL:HB	1	0.34
(1,3761)	2:20:C:VAL:HG22	2:20:C:VAL:HB	10	0.34
(1,3751)	2:20:C:VAL:HG22	2:20:C:VAL:HB	1	0.34
(1,3751)	2:20:C:VAL:HG22	2:20:C:VAL:HB	10	0.34
(1,3738)	2:68:B:ILE:HD13	2:11:C:LEU:HD21	2	0.34
(1,3727)	2:25:C:ILE:HG23	2:25:C:ILE:HG12	3	0.34
(1,3727)	2:25:C:ILE:HG21	2:25:C:ILE:HG12	5	0.34
(1,3684)	2:12:B:ILE:HD13	2:15:C:TYR:HD2	10	0.34
(1,3658)	2:51:B:VAL:HG21	2:46:B:PHE:HE2	6	0.34
(1,3592)	2:9:B:ALA:HA	2:12:B:ILE:HG23	9	0.34
(1,3564)	2:19:B:ILE:HB	2:19:B:ILE:HD11	10	0.34
(1,3320)	2:19:B:ILE:HG22	2:26:B:SER:H	6	0.34
(1,3320)	2:19:B:ILE:HG23	2:26:B:SER:H	9	0.34
(1,3258)	2:22:B:LYS:HG3	2:22:B:LYS:H	4	0.34
(1,3197)	2:14:C:ASN:H	2:48:C:ARG:HA	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2941)	2:44:C:PHE:HZ	2:33:B:LEU:HD22	3	0.34
(1,2880)	2:33:B:LEU:HD11	2:19:B:ILE:HD12	6	0.34
(1,2787)	2:20:C:VAL:HG11	2:34:C:ASN:HD22	10	0.34
(1,2652)	2:8:B:ILE:HG22	2:3:B:ALA:HB1	5	0.34
(1,2598)	2:13:B:VAL:HG13	2:41:B:SER:HA	2	0.34
(1,2551)	2:20:C:VAL:HG12	2:19:C:ILE:HB	8	0.34
(1,2492)	2:54:B:ILE:HB	2:54:B:ILE:HG21	6	0.34
(1,2347)	2:44:C:PHE:HB2	2:46:C:PHE:HD1	9	0.34
(1,2112)	2:13:B:VAL:HG21	2:51:B:VAL:HB	3	0.34
(1,2076)	2:55:B:LEU:HD13	2:55:B:LEU:HG	2	0.34
(1,2076)	2:55:B:LEU:HD11	2:55:B:LEU:HG	4	0.34
(1,2076)	2:55:B:LEU:HD11	2:55:B:LEU:HG	7	0.34
(1,2076)	2:55:B:LEU:HD13	2:55:B:LEU:HG	8	0.34
(1,2065)	2:55:C:LEU:HD23	2:51:C:VAL:HB	8	0.34
(1,2044)	2:5:B:LYS:HD2	2:44:B:PHE:HZ	6	0.34
(1,2038)	2:5:B:LYS:HB3	2:44:B:PHE:HZ	2	0.34
(1,1831)	1:148:A:ILE:HD13	1:148:A:ILE:H	6	0.34
(1,1784)	1:105:A:LEU:H	1:117:A:ILE:HD13	10	0.34
(1,1733)	1:129:A:ASN:H	1:97:A:THR:HG23	4	0.34
(1,1723)	1:102:A:LYS:H	1:117:A:ILE:HD11	3	0.34
(1,1661)	1:149:A:LYS:HB3	1:149:A:LYS:HE3	1	0.34
(1,1632)	1:147:A:MET:HG3	1:120:A:LEU:HB2	9	0.34
(1,1466)	1:117:A:ILE:HG23	1:117:A:ILE:HB	2	0.34
(1,955)	1:131:A:PHE:HB3	1:131:A:PHE:H	6	0.34
(1,945)	1:100:A:GLN:H	1:100:A:GLN:HG2	2	0.34
(1,720)	1:148:A:ILE:HD13	1:86:A:PHE:HZ	5	0.34
(1,533)	1:114:A:ILE:HA	1:114:A:ILE:HG12	3	0.34
(1,460)	1:126:A:LEU:HD13	1:120:A:LEU:HA	3	0.34
(1,418)	1:136:A:LYS:HG2	1:136:A:LYS:H	5	0.34
(1,235)	1:118:A:LYS:HB3	1:118:A:LYS:HE3	9	0.34
(1,184)	1:130:A:LEU:HD21	1:130:A:LEU:H	2	0.34
(1,177)	1:132:A:LEU:HD23	1:97:A:THR:HA	7	0.34
(1,172)	1:78:A:LEU:HD21	1:78:A:LEU:HG	9	0.34
(1,162)	1:78:A:LEU:HD23	1:92:A:PHE:HZ	4	0.34
(1,158)	1:99:A:LEU:HD21	1:103:A:GLN:H	10	0.34
(1,58)	1:114:A:ILE:HD13	1:99:A:LEU:HA	4	0.34
(1,46)	1:88:A:ILE:HD13	1:88:A:ILE:HG12	4	0.34
(1,4169)	1:81:A:ILE:HD12	2:31:C:ASP:OD1	3	0.33
(1,4050)	2:54:B:ILE:HB	2:50:B:ALA:H	7	0.33
(1,3911)	2:12:C:ILE:HG13	2:11:C:LEU:H	6	0.33
(1,3874)	2:15:B:TYR:HA	2:12:C:ILE:HD13	4	0.33
(1,3761)	2:51:C:VAL:HG12	2:51:C:VAL:HB	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3761)	2:51:C:VAL:HG12	2:51:C:VAL:HB	4	0.33
(1,3761)	2:51:C:VAL:HG12	2:51:C:VAL:HB	9	0.33
(1,3760)	2:20:B:VAL:HG23	2:20:B:VAL:HB	7	0.33
(1,3751)	2:51:C:VAL:HG12	2:51:C:VAL:HB	4	0.33
(1,3751)	2:51:C:VAL:HG12	2:51:C:VAL:HB	9	0.33
(1,3750)	2:20:B:VAL:HG23	2:20:B:VAL:HB	7	0.33
(1,3739)	2:68:C:ILE:HD11	2:11:B:LEU:HD23	10	0.33
(1,3725)	2:25:C:ILE:HG23	2:19:C:ILE:HB	4	0.33
(1,3705)	2:6:C:GLU:HA	2:46:C:PHE:HE1	4	0.33
(1,3659)	2:51:C:VAL:HG23	2:46:C:PHE:HE2	3	0.33
(1,3616)	2:12:B:ILE:HA	2:12:C:ILE:HD13	9	0.33
(1,3575)	2:33:C:LEU:HD23	2:43:B:ALA:HB2	4	0.33
(1,2962)	2:48:B:ARG:HG3	2:48:B:ARG:H	7	0.33
(1,2881)	2:33:C:LEU:HD11	2:19:C:ILE:HD11	6	0.33
(1,2852)	2:3:B:ALA:HB3	2:8:B:ILE:HA	5	0.33
(1,2694)	2:54:B:ILE:HG22	2:46:B:PHE:HB2	8	0.33
(1,2631)	2:51:C:VAL:HB	2:55:C:LEU:HG	3	0.33
(1,2630)	2:51:B:VAL:HB	2:55:B:LEU:HG	7	0.33
(1,2614)	2:13:B:VAL:HG13	2:48:B:ARG:HG2	7	0.33
(1,2565)	2:33:C:LEU:HD11	2:19:C:ILE:HG23	2	0.33
(1,2551)	2:20:C:VAL:HG13	2:19:C:ILE:HB	2	0.33
(1,2493)	2:54:C:ILE:HB	2:54:C:ILE:HG23	1	0.33
(1,2493)	2:54:C:ILE:HB	2:54:C:ILE:HG22	5	0.33
(1,2483)	2:25:C:ILE:HB	2:19:C:ILE:HG22	3	0.33
(1,2349)	2:54:C:ILE:HB	2:55:C:LEU:H	9	0.33
(1,2091)	2:8:C:ILE:HD12	2:3:C:ALA:HB1	5	0.33
(1,2090)	2:8:B:ILE:HD12	2:3:B:ALA:HB1	3	0.33
(1,2077)	2:55:C:LEU:HD13	2:55:C:LEU:HG	6	0.33
(1,2076)	2:55:B:LEU:HD13	2:55:B:LEU:HG	6	0.33
(1,2038)	2:5:B:LYS:HB3	2:44:B:PHE:HZ	8	0.33
(1,1802)	1:82:A:GLN:HE21	1:82:A:GLN:HB3	7	0.33
(1,1787)	1:111:A:ALA:H	1:106:A:ILE:HG23	10	0.33
(1,1736)	1:110:A:LYS:H	1:105:A:LEU:HB3	7	0.33
(1,1736)	1:110:A:LYS:H	1:105:A:LEU:HB3	9	0.33
(1,1545)	1:135:A:LEU:HA	1:124:A:LYS:HE3	10	0.33
(1,1467)	1:145:A:THR:HG23	1:82:A:GLN:HE22	1	0.33
(1,1466)	1:117:A:ILE:HG21	1:117:A:ILE:HB	4	0.33
(1,1466)	1:117:A:ILE:HG22	1:117:A:ILE:HB	8	0.33
(1,1403)	1:150:A:PRO:HD2	1:149:A:LYS:H	7	0.33
(1,1236)	1:99:A:LEU:HD13	1:99:A:LEU:H	1	0.33
(1,1236)	1:99:A:LEU:HD12	1:99:A:LEU:H	2	0.33
(1,1179)	1:82:A:GLN:H	1:80:A:LYS:HD2	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1011)	1:98:A:ILE:H	1:98:A:ILE:HG12	9	0.33
(1,889)	1:130:A:LEU:HB3	1:130:A:LEU:H	6	0.33
(1,889)	1:130:A:LEU:HB3	1:130:A:LEU:H	7	0.33
(1,783)	1:106:A:ILE:HG21	1:106:A:ILE:HB	3	0.33
(1,783)	1:106:A:ILE:HG22	1:106:A:ILE:HB	6	0.33
(1,783)	1:106:A:ILE:HG22	1:106:A:ILE:HB	9	0.33
(1,683)	1:106:A:ILE:HG12	1:106:A:ILE:H	8	0.33
(1,460)	1:126:A:LEU:HD13	1:120:A:LEU:HA	10	0.33
(1,281)	1:120:A:LEU:HB2	1:145:A:THR:HB	2	0.33
(1,261)	1:129:A:ASN:HB2	1:129:A:ASN:HD21	4	0.33
(1,183)	1:99:A:LEU:HD11	1:100:A:GLN:HE22	3	0.33
(1,172)	1:78:A:LEU:HD23	1:78:A:LEU:HG	3	0.33
(1,172)	1:78:A:LEU:HD23	1:78:A:LEU:HG	7	0.33
(1,112)	1:77:A:THR:HG21	1:78:A:LEU:H	2	0.33
(1,66)	1:83:A:ALA:HB3	1:83:A:ALA:H	7	0.33
(1,46)	1:88:A:ILE:HD13	1:88:A:ILE:HG12	8	0.33
(1,31)	1:106:A:ILE:HD12	1:112:A:SER:H	6	0.33
(3,140)	2:38:C:ASP:N	2:34:C:ASN:O	9	0.32
(1,4189)	1:124:A:LYS:H	2:38:C:ASP:H	10	0.32
(1,4015)	2:60:C:PHE:HD1	2:8:C:ILE:HD11	3	0.32
(1,3970)	2:8:B:ILE:HD13	2:60:B:PHE:HE1	8	0.32
(1,3968)	2:25:B:ILE:HG21	2:32:B:SER:H	4	0.32
(1,3962)	2:36:B:ALA:HB1	2:40:C:ILE:HA	8	0.32
(1,3929)	2:39:C:CYS:HB2	2:35:C:VAL:HB	1	0.32
(1,3801)	2:8:C:ILE:HG23	2:16:B:PHE:HD1	9	0.32
(1,3760)	2:51:B:VAL:HG12	2:51:B:VAL:HB	9	0.32
(1,3751)	2:51:C:VAL:HG12	2:51:C:VAL:HB	2	0.32
(1,3750)	2:51:B:VAL:HG12	2:51:B:VAL:HB	9	0.32
(1,3726)	2:25:B:ILE:HG22	2:30:B:ALA:HB2	1	0.32
(1,3726)	2:25:B:ILE:HG22	2:25:B:ILE:HG12	10	0.32
(1,3722)	2:25:B:ILE:HG21	2:5:C:LYS:HE3	2	0.32
(1,3705)	2:6:C:GLU:HA	2:46:C:PHE:HE1	1	0.32
(1,3664)	2:33:B:LEU:HD22	2:16:B:PHE:HD1	1	0.32
(1,3567)	2:19:C:ILE:HD11	2:5:B:LYS:HG2	7	0.32
(1,3566)	2:19:B:ILE:HD11	2:5:C:LYS:HG2	4	0.32
(1,3552)	2:25:B:ILE:HD13	2:24:B:GLU:HB3	2	0.32
(1,3551)	2:25:C:ILE:HD12	2:5:B:LYS:HE3	7	0.32
(1,3420)	2:51:B:VAL:H	2:54:B:ILE:HG12	8	0.32
(1,3320)	2:19:B:ILE:HG22	2:26:B:SER:H	2	0.32
(1,3316)	2:26:B:SER:H	2:33:B:LEU:HD12	3	0.32
(1,3253)	2:21:C:GLU:HB3	2:21:C:GLU:H	6	0.32
(1,2880)	2:33:B:LEU:HD11	2:19:B:ILE:HD12	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2829)	2:6:C:GLU:HG2	2:9:C:ALA:HB3	9	0.32
(1,2721)	2:54:C:ILE:HD12	2:6:C:GLU:HG3	9	0.32
(1,2702)	2:13:B:VAL:HA	2:40:B:ILE:HD11	6	0.32
(1,2563)	2:11:C:LEU:HD23	2:55:C:LEU:HD22	6	0.32
(1,2493)	2:54:C:ILE:HB	2:54:C:ILE:HG21	8	0.32
(1,2475)	2:12:C:ILE:HG21	2:40:C:ILE:HD12	7	0.32
(1,2474)	2:12:B:ILE:HG21	2:40:B:ILE:HD13	7	0.32
(1,2405)	2:8:C:ILE:HG23	2:15:B:TYR:H	3	0.32
(1,2366)	2:33:B:LEU:HD13	2:44:C:PHE:HZ	7	0.32
(1,2346)	2:44:B:PHE:HB2	2:46:B:PHE:HD1	5	0.32
(1,2077)	2:55:C:LEU:HD12	2:55:C:LEU:HG	3	0.32
(1,2076)	2:55:B:LEU:HD12	2:55:B:LEU:HG	9	0.32
(1,1803)	1:82:A:GLN:HE21	1:81:A:ILE:HG22	8	0.32
(1,1723)	1:102:A:LYS:H	1:117:A:ILE:HD11	8	0.32
(1,1419)	1:107:A:SER:HB3	1:108:A:GLU:H	5	0.32
(1,955)	1:131:A:PHE:HB3	1:131:A:PHE:H	5	0.32
(1,955)	1:131:A:PHE:HB3	1:131:A:PHE:H	8	0.32
(1,780)	1:148:A:ILE:HG21	1:148:A:ILE:HB	5	0.32
(1,734)	1:87:A:SER:HA	1:79:A:LYS:HD3	9	0.32
(1,732)	1:81:A:ILE:HA	1:79:A:LYS:HD3	9	0.32
(1,724)	1:148:A:ILE:HD13	1:80:A:LYS:HE3	5	0.32
(1,717)	1:120:A:LEU:HG	1:125:A:VAL:HA	2	0.32
(1,456)	1:149:A:LYS:HA	1:149:A:LYS:HE3	9	0.32
(1,265)	1:114:A:ILE:HG12	1:103:A:GLN:HE22	9	0.32
(1,229)	1:118:A:LYS:HB2	1:118:A:LYS:HE3	2	0.32
(1,138)	1:97:A:THR:HG21	1:97:A:THR:HB	4	0.32
(1,134)	1:125:A:VAL:HG22	1:125:A:VAL:HB	1	0.32
(1,134)	1:125:A:VAL:HG22	1:125:A:VAL:HB	3	0.32
(1,134)	1:125:A:VAL:HG23	1:125:A:VAL:HB	5	0.32
(1,134)	1:125:A:VAL:HG21	1:125:A:VAL:HB	9	0.32
(1,134)	1:125:A:VAL:HG21	1:125:A:VAL:HB	10	0.32
(1,110)	1:126:A:LEU:HD13	1:125:A:VAL:HA	6	0.32
(1,101)	1:77:A:THR:HG23	1:87:A:SER:HB3	1	0.32
(1,66)	1:83:A:ALA:HB3	1:83:A:ALA:H	2	0.32
(1,66)	1:83:A:ALA:HB3	1:83:A:ALA:H	9	0.32
(1,46)	1:88:A:ILE:HD11	1:88:A:ILE:HG12	10	0.32
(1,4189)	1:124:A:LYS:H	2:38:C:ASP:H	5	0.31
(1,4176)	1:145:A:THR:OG1	2:35:C:VAL:HG21	10	0.31
(1,4056)	2:17:B:SER:HA	2:18:B:SER:H	10	0.31
(1,4004)	2:44:B:PHE:HZ	2:25:C:ILE:HG21	4	0.31
(1,3962)	2:36:B:ALA:HB1	2:40:C:ILE:HA	5	0.31
(1,3935)	2:55:C:LEU:HD12	2:7:C:GLU:HG2	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3817)	2:6:C:GLU:HB2	2:46:C:PHE:HD1	10	0.31
(1,3760)	2:51:B:VAL:HG11	2:51:B:VAL:HB	2	0.31
(1,3760)	2:20:B:VAL:HG22	2:20:B:VAL:HB	5	0.31
(1,3750)	2:20:B:VAL:HG22	2:20:B:VAL:HB	5	0.31
(1,3744)	2:40:B:ILE:HD12	2:36:C:ALA:HB3	7	0.31
(1,3731)	2:12:C:ILE:HD12	2:13:C:VAL:HG13	4	0.31
(1,3722)	2:25:B:ILE:HG23	2:5:C:LYS:HE3	4	0.31
(1,3567)	2:19:C:ILE:HD11	2:5:B:LYS:HG2	2	0.31
(1,3068)	2:39:B:CYS:H	2:35:B:VAL:HB	5	0.31
(1,2946)	2:44:B:PHE:HB2	2:46:B:PHE:HE1	4	0.31
(1,2936)	2:6:B:GLU:HG2	2:44:B:PHE:HD1	2	0.31
(1,2631)	2:51:C:VAL:HB	2:55:C:LEU:HG	4	0.31
(1,2409)	2:19:C:ILE:HG23	2:44:B:PHE:HZ	6	0.31
(1,2346)	2:44:B:PHE:HB2	2:46:B:PHE:HD1	6	0.31
(1,2211)	2:22:C:LYS:HA	2:24:C:GLU:HB2	8	0.31
(1,2186)	2:30:B:ALA:HA	2:20:B:VAL:HG12	9	0.31
(1,2153)	2:48:C:ARG:HD3	2:48:C:ARG:HB3	2	0.31
(1,2090)	2:8:B:ILE:HD12	2:3:B:ALA:HB3	1	0.31
(1,2077)	2:55:C:LEU:HD12	2:55:C:LEU:HG	2	0.31
(1,2077)	2:55:C:LEU:HD11	2:55:C:LEU:HG	9	0.31
(1,2076)	2:55:B:LEU:HD12	2:55:B:LEU:HG	5	0.31
(1,2043)	2:5:C:LYS:HD3	2:44:C:PHE:HZ	9	0.31
(1,2038)	2:5:B:LYS:HB3	2:44:B:PHE:HZ	1	0.31
(1,1758)	1:83:A:ALA:H	1:85:A:LYS:HG2	2	0.31
(1,1716)	1:101:A:ILE:HG22	1:101:A:ILE:H	2	0.31
(1,1655)	1:81:A:ILE:HG12	1:81:A:ILE:HD13	10	0.31
(1,1611)	1:81:A:ILE:HB	1:81:A:ILE:HG23	3	0.31
(1,1611)	1:81:A:ILE:HB	1:81:A:ILE:HG22	4	0.31
(1,1611)	1:144:A:ILE:HB	1:144:A:ILE:HG21	8	0.31
(1,1466)	1:117:A:ILE:HG22	1:117:A:ILE:HB	3	0.31
(1,1159)	1:152:A:LEU:HG	1:152:A:LEU:H	2	0.31
(1,955)	1:131:A:PHE:HB3	1:131:A:PHE:H	9	0.31
(1,783)	1:106:A:ILE:HG22	1:106:A:ILE:HB	7	0.31
(1,780)	1:148:A:ILE:HG21	1:148:A:ILE:HB	7	0.31
(1,722)	1:148:A:ILE:HA	1:148:A:ILE:HD12	3	0.31
(1,638)	1:132:A:LEU:HB3	1:135:A:LEU:HD13	2	0.31
(1,533)	1:114:A:ILE:HA	1:114:A:ILE:HG12	5	0.31
(1,531)	1:137:A:VAL:HA	1:138:A:THR:HG23	2	0.31
(1,414)	1:118:A:LYS:HG2	1:118:A:LYS:H	1	0.31
(1,209)	1:151:A:ASN:HB3	1:151:A:ASN:HD21	9	0.31
(1,182)	1:132:A:LEU:HD12	1:92:A:PHE:HA	2	0.31
(1,172)	1:78:A:LEU:HD21	1:78:A:LEU:HG	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,172)	1:78:A:LEU:HD23	1:78:A:LEU:HG	8	0.31
(1,147)	1:132:A:LEU:HD23	1:98:A:ILE:H	4	0.31
(1,138)	1:97:A:THR:HG23	1:97:A:THR:HB	1	0.31
(1,138)	1:97:A:THR:HG21	1:97:A:THR:HB	8	0.31
(1,138)	1:97:A:THR:HG23	1:97:A:THR:HB	10	0.31
(1,134)	1:125:A:VAL:HG21	1:125:A:VAL:HB	4	0.31
(1,132)	1:138:A:THR:HG23	1:141:A:ASN:HB3	3	0.31
(1,110)	1:126:A:LEU:HD12	1:125:A:VAL:HA	5	0.31
(1,73)	1:88:A:ILE:HG23	1:90:A:HIS:HE1	2	0.31
(1,55)	1:114:A:ILE:HD13	1:103:A:GLN:HE22	1	0.31
(1,2)	1:120:A:LEU:HD13	1:120:A:LEU:H	10	0.31
(3,140)	2:38:C:ASP:N	2:34:C:ASN:O	3	0.3
(3,139)	2:38:C:ASP:H	2:34:C:ASN:O	4	0.3
(3,139)	2:38:C:ASP:H	2:34:C:ASN:O	10	0.3
(1,4169)	1:81:A:ILE:HD13	2:35:C:VAL:HG13	10	0.3
(1,4005)	2:44:C:PHE:HZ	2:25:B:ILE:HG21	1	0.3
(1,3968)	2:25:B:ILE:HG22	2:44:C:PHE:HD1	8	0.3
(1,3962)	2:36:B:ALA:HB1	2:40:C:ILE:HA	1	0.3
(1,3911)	2:12:C:ILE:HG13	2:11:C:LEU:H	8	0.3
(1,3816)	2:6:B:GLU:HB2	2:46:B:PHE:HD1	8	0.3
(1,3750)	2:51:B:VAL:HG11	2:51:B:VAL:HB	2	0.3
(1,3724)	2:25:B:ILE:HG21	2:19:B:ILE:HB	7	0.3
(1,3658)	2:51:B:VAL:HG23	2:46:B:PHE:HE2	1	0.3
(1,3629)	2:18:C:SER:HB3	2:19:C:ILE:HD13	6	0.3
(1,3575)	2:33:C:LEU:HD22	2:43:B:ALA:HB1	10	0.3
(1,3567)	2:19:C:ILE:HD12	2:5:B:LYS:HG2	5	0.3
(1,3527)	2:6:C:GLU:HG2	2:46:C:PHE:HD2	7	0.3
(1,3477)	2:55:C:LEU:HD23	2:14:C:ASN:HD21	2	0.3
(1,3453)	2:54:C:ILE:HG21	2:55:C:LEU:H	9	0.3
(1,3252)	2:21:B:GLU:HB3	2:21:B:GLU:H	2	0.3
(1,3139)	2:2:C:SER:H	2:3:C:ALA:H	6	0.3
(1,3092)	2:13:B:VAL:HG12	2:41:B:SER:H	3	0.3
(1,2791)	2:33:C:LEU:HD13	2:19:C:ILE:HB	6	0.3
(1,2715)	2:54:C:ILE:HD12	2:47:C:GLU:H	7	0.3
(1,2702)	2:13:B:VAL:HA	2:40:B:ILE:HD11	3	0.3
(1,2692)	2:50:B:ALA:HB3	2:47:B:GLU:HB2	3	0.3
(1,2614)	2:13:B:VAL:HG12	2:48:B:ARG:HG2	6	0.3
(1,2541)	2:36:C:ALA:HB1	2:33:C:LEU:HD12	6	0.3
(1,2540)	2:36:B:ALA:HB3	2:33:B:LEU:HD13	5	0.3
(1,2380)	2:55:B:LEU:HD12	2:60:B:PHE:HD2	2	0.3
(1,2126)	2:54:B:ILE:HB	2:13:B:VAL:HG23	2	0.3
(1,2113)	2:13:C:VAL:HG21	2:51:C:VAL:HB	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2077)	2:55:C:LEU:HD12	2:55:C:LEU:HG	5	0.3
(1,2064)	2:55:B:LEU:HD21	2:51:B:VAL:HB	8	0.3
(1,1811)	1:103:A:GLN:HE21	1:102:A:LYS:HB2	8	0.3
(1,1662)	1:149:A:LYS:HG3	1:149:A:LYS:HE3	10	0.3
(1,1659)	1:124:A:LYS:HE2	1:124:A:LYS:HD3	6	0.3
(1,1655)	1:81:A:ILE:HG12	1:81:A:ILE:HD12	4	0.3
(1,1655)	1:81:A:ILE:HG12	1:81:A:ILE:HD13	6	0.3
(1,1650)	1:137:A:VAL:HG22	1:137:A:VAL:HB	4	0.3
(1,1650)	1:137:A:VAL:HG22	1:137:A:VAL:HB	6	0.3
(1,1650)	1:74:A:VAL:HG23	1:74:A:VAL:HB	7	0.3
(1,1650)	1:137:A:VAL:HG22	1:137:A:VAL:HB	10	0.3
(1,1611)	1:81:A:ILE:HB	1:81:A:ILE:HG23	1	0.3
(1,1532)	1:151:A:ASN:HA	1:152:A:LEU:HG	1	0.3
(1,1479)	1:82:A:GLN:HG3	1:82:A:GLN:H	10	0.3
(1,1466)	1:117:A:ILE:HG21	1:117:A:ILE:HB	9	0.3
(1,1461)	1:126:A:LEU:HD21	1:145:A:THR:H	2	0.3
(1,1427)	1:106:A:ILE:HD12	1:104:A:HIS:H	1	0.3
(1,1033)	1:106:A:ILE:HG13	1:106:A:ILE:H	9	0.3
(1,809)	1:126:A:LEU:HB2	1:126:A:LEU:H	5	0.3
(1,779)	1:74:A:VAL:HG13	1:74:A:VAL:HB	9	0.3
(1,768)	1:76:A:LEU:HD13	1:132:A:LEU:HA	8	0.3
(1,252)	1:85:A:LYS:HB3	1:85:A:LYS:H	8	0.3
(1,184)	1:130:A:LEU:HD21	1:130:A:LEU:H	7	0.3
(1,182)	1:132:A:LEU:HD12	1:92:A:PHE:HA	5	0.3
(1,180)	1:132:A:LEU:HD11	1:96:A:ASP:HB2	1	0.3
(1,180)	1:132:A:LEU:HD11	1:96:A:ASP:HB2	5	0.3
(1,179)	1:120:A:LEU:HD21	1:147:A:MET:HG3	10	0.3
(1,172)	1:78:A:LEU:HD21	1:78:A:LEU:HG	5	0.3
(1,162)	1:78:A:LEU:HD23	1:92:A:PHE:HZ	10	0.3
(1,147)	1:132:A:LEU:HD23	1:98:A:ILE:H	8	0.3
(1,138)	1:97:A:THR:HG23	1:97:A:THR:HB	2	0.3
(1,138)	1:97:A:THR:HG21	1:97:A:THR:HB	3	0.3
(1,138)	1:97:A:THR:HG23	1:97:A:THR:HB	9	0.3
(1,114)	1:77:A:THR:HG23	1:79:A:LYS:H	7	0.3
(1,112)	1:77:A:THR:HG22	1:78:A:LEU:H	1	0.3
(1,112)	1:77:A:THR:HG23	1:78:A:LEU:H	4	0.3
(1,101)	1:77:A:THR:HG23	1:87:A:SER:HB3	10	0.3
(1,89)	1:101:A:ILE:HG23	1:119:A:LEU:HA	7	0.3
(1,67)	1:83:A:ALA:HB2	1:85:A:LYS:H	9	0.3
(1,66)	1:83:A:ALA:HB1	1:83:A:ALA:H	5	0.3
(1,55)	1:114:A:ILE:HD12	1:103:A:GLN:HE22	5	0.3
(1,34)	1:106:A:ILE:HD12	1:106:A:ILE:HB	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:106:A:ILE:HD11	1:113:A:HIS:HB3	7	0.3
(3,140)	2:38:C:ASP:N	2:34:C:ASN:O	2	0.29
(3,139)	2:38:C:ASP:H	2:34:C:ASN:O	7	0.29
(1,3962)	2:36:B:ALA:HB1	2:40:C:ILE:HA	6	0.29
(1,3939)	2:33:C:LEU:HD11	2:40:B:ILE:HA	2	0.29
(1,3911)	2:12:C:ILE:HG13	2:11:C:LEU:H	9	0.29
(1,3723)	2:25:C:ILE:HG21	2:5:B:LYS:HE3	7	0.29
(1,3692)	2:9:B:ALA:HA	2:46:B:PHE:HE1	8	0.29
(1,3683)	2:12:C:ILE:HD12	2:16:B:PHE:HD1	3	0.29
(1,3628)	2:18:B:SER:HB3	2:19:B:ILE:HD13	1	0.29
(1,3616)	2:12:B:ILE:HA	2:12:C:ILE:HD12	6	0.29
(1,3570)	2:13:B:VAL:HG21	2:50:B:ALA:HB2	6	0.29
(1,3543)	2:51:C:VAL:HG23	2:49:C:GLU:HG3	10	0.29
(1,3321)	2:19:C:ILE:HG23	2:26:C:SER:H	1	0.29
(1,3164)	2:7:B:GLU:H	2:7:B:GLU:HG3	2	0.29
(1,3153)	2:6:C:GLU:HG3	2:6:C:GLU:H	2	0.29
(1,3083)	2:41:C:SER:H	2:41:C:SER:HB3	3	0.29
(1,3082)	2:41:B:SER:H	2:41:B:SER:HB3	5	0.29
(1,3023)	2:48:C:ARG:HG2	2:48:C:ARG:H	8	0.29
(1,3015)	2:5:C:LYS:HG2	2:5:C:LYS:H	1	0.29
(1,2962)	2:48:B:ARG:HG3	2:48:B:ARG:H	6	0.29
(1,2630)	2:51:B:VAL:HB	2:55:B:LEU:HG	10	0.29
(1,2555)	2:20:C:VAL:HG11	2:30:C:ALA:HB3	6	0.29
(1,2501)	2:25:C:ILE:HG21	2:20:C:VAL:HB	3	0.29
(1,2408)	2:19:B:ILE:HG23	2:44:C:PHE:HZ	8	0.29
(1,2357)	2:49:C:GLU:HG2	2:49:C:GLU:H	8	0.29
(1,2347)	2:44:C:PHE:HB2	2:46:C:PHE:HD1	3	0.29
(1,2346)	2:44:B:PHE:HB2	2:46:B:PHE:HD1	3	0.29
(1,2227)	2:5:C:LYS:HA	2:8:C:ILE:HG13	6	0.29
(1,2211)	2:22:C:LYS:HA	2:24:C:GLU:HB2	2	0.29
(1,2193)	2:25:C:ILE:HD11	2:30:C:ALA:HA	2	0.29
(1,2077)	2:55:C:LEU:HD11	2:55:C:LEU:HG	7	0.29
(1,1994)	2:36:B:ALA:HB3	2:33:B:LEU:HD23	7	0.29
(1,1794)	1:138:A:THR:H	1:121:A:LEU:HD21	4	0.29
(1,1787)	1:111:A:ALA:H	1:106:A:ILE:HG23	8	0.29
(1,1723)	1:102:A:LYS:H	1:117:A:ILE:HD11	1	0.29
(1,1707)	1:120:A:LEU:H	1:119:A:LEU:HD12	2	0.29
(1,1655)	1:81:A:ILE:HG12	1:81:A:ILE:HD12	8	0.29
(1,1650)	1:137:A:VAL:HG22	1:137:A:VAL:HB	5	0.29
(1,1624)	1:132:A:LEU:HD11	1:93:A:SER:HA	5	0.29
(1,1611)	1:144:A:ILE:HB	1:144:A:ILE:HG21	10	0.29
(1,1466)	1:117:A:ILE:HG23	1:117:A:ILE:HB	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1466)	1:117:A:ILE:HG21	1:117:A:ILE:HB	7	0.29
(1,1461)	1:126:A:LEU:HD21	1:145:A:THR:H	4	0.29
(1,1450)	1:99:A:LEU:HD21	1:102:A:LYS:H	9	0.29
(1,1432)	1:117:A:ILE:HD11	1:117:A:ILE:HG13	10	0.29
(1,1338)	1:99:A:LEU:HD11	1:103:A:GLN:HE21	6	0.29
(1,1266)	1:107:A:SER:H	1:106:A:ILE:HG21	10	0.29
(1,1200)	1:113:A:HIS:H	1:106:A:ILE:HD13	5	0.29
(1,1133)	1:126:A:LEU:HD13	1:126:A:LEU:H	3	0.29
(1,1132)	1:126:A:LEU:H	1:126:A:LEU:HB3	7	0.29
(1,867)	1:145:A:THR:HG22	1:145:A:THR:H	2	0.29
(1,795)	1:80:A:LYS:HE3	1:86:A:PHE:HZ	3	0.29
(1,722)	1:148:A:ILE:HA	1:148:A:ILE:HD12	5	0.29
(1,703)	1:122:A:LYS:HE3	1:141:A:ASN:HD22	3	0.29
(1,686)	1:122:A:LYS:HA	1:122:A:LYS:HD3	1	0.29
(1,418)	1:136:A:LYS:HG2	1:136:A:LYS:H	10	0.29
(1,261)	1:129:A:ASN:HB2	1:129:A:ASN:HD21	2	0.29
(1,235)	1:118:A:LYS:HB3	1:118:A:LYS:HE3	4	0.29
(1,182)	1:132:A:LEU:HD12	1:92:A:PHE:HA	8	0.29
(1,138)	1:97:A:THR:HG21	1:97:A:THR:HB	5	0.29
(1,66)	1:83:A:ALA:HB3	1:83:A:ALA:H	6	0.29
(1,58)	1:114:A:ILE:HD12	1:99:A:LEU:HA	6	0.29
(1,28)	1:144:A:ILE:HD11	1:121:A:LEU:HA	3	0.29
(1,4189)	1:124:A:LYS:H	2:38:C:ASP:H	3	0.28
(1,4189)	1:124:A:LYS:H	2:38:C:ASP:H	7	0.28
(1,4181)	1:120:A:LEU:HD12	2:38:C:ASP:H	1	0.28
(1,4176)	1:145:A:THR:HG21	2:35:C:VAL:HG13	1	0.28
(1,3970)	2:8:B:ILE:HD13	2:60:B:PHE:HE1	2	0.28
(1,3723)	2:25:C:ILE:HG21	2:5:B:LYS:HE3	6	0.28
(1,3622)	2:40:B:ILE:HA	2:33:C:LEU:HG	8	0.28
(1,3563)	2:8:C:ILE:HD12	2:9:C:ALA:HA	3	0.28
(1,3562)	2:8:B:ILE:HD11	2:11:C:LEU:HA	1	0.28
(1,3421)	2:51:C:VAL:H	2:54:C:ILE:HG12	7	0.28
(1,3420)	2:51:B:VAL:H	2:54:B:ILE:HG12	5	0.28
(1,3320)	2:19:B:ILE:HG22	2:26:B:SER:H	8	0.28
(1,3317)	2:26:C:SER:H	2:33:C:LEU:HD13	1	0.28
(1,3316)	2:26:B:SER:H	2:33:B:LEU:HD12	6	0.28
(1,3175)	2:7:C:GLU:H	2:4:C:SER:HB3	2	0.28
(1,3152)	2:6:B:GLU:HG3	2:6:B:GLU:H	10	0.28
(1,3138)	2:2:B:SER:H	2:3:B:ALA:H	3	0.28
(1,3083)	2:41:C:SER:H	2:41:C:SER:HB3	1	0.28
(1,3082)	2:41:B:SER:H	2:41:B:SER:HB3	1	0.28
(1,3082)	2:41:B:SER:H	2:41:B:SER:HB3	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3082)	2:41:B:SER:H	2:41:B:SER:HB3	6	0.28
(1,3082)	2:41:B:SER:H	2:41:B:SER:HB3	9	0.28
(1,2963)	2:48:C:ARG:HG3	2:48:C:ARG:H	6	0.28
(1,2791)	2:33:C:LEU:HD12	2:19:C:ILE:HB	1	0.28
(1,2791)	2:33:C:LEU:HD13	2:19:C:ILE:HB	4	0.28
(1,2599)	2:13:C:VAL:HG11	2:41:C:SER:HA	2	0.28
(1,2564)	2:33:B:LEU:HD11	2:19:B:ILE:HG21	10	0.28
(1,2473)	2:12:C:ILE:HG23	2:13:C:VAL:HG12	1	0.28
(1,2186)	2:30:B:ALA:HA	2:20:B:VAL:HG12	10	0.28
(1,2183)	2:9:C:ALA:HA	2:40:C:ILE:HG22	3	0.28
(1,2114)	2:13:B:VAL:HG22	2:48:B:ARG:HG2	1	0.28
(1,2077)	2:55:C:LEU:HD11	2:55:C:LEU:HG	8	0.28
(1,1784)	1:105:A:LEU:H	1:117:A:ILE:HD13	6	0.28
(1,1766)	1:135:A:LEU:H	1:126:A:LEU:HD12	7	0.28
(1,1735)	1:109:A:GLU:H	1:108:A:GLU:HB2	6	0.28
(1,1716)	1:101:A:ILE:HG21	1:101:A:ILE:H	4	0.28
(1,1716)	1:101:A:ILE:HG21	1:101:A:ILE:H	5	0.28
(1,1716)	1:101:A:ILE:HG21	1:101:A:ILE:H	7	0.28
(1,1655)	1:81:A:ILE:HG12	1:81:A:ILE:HD13	7	0.28
(1,1650)	1:74:A:VAL:HG23	1:74:A:VAL:HB	2	0.28
(1,1650)	1:74:A:VAL:HG23	1:74:A:VAL:HB	8	0.28
(1,1611)	1:144:A:ILE:HB	1:144:A:ILE:HG23	7	0.28
(1,1466)	1:117:A:ILE:HG23	1:117:A:ILE:HB	1	0.28
(1,1060)	1:116:A:GLU:HG2	1:116:A:GLU:H	7	0.28
(1,1033)	1:106:A:ILE:HG13	1:106:A:ILE:H	7	0.28
(1,1011)	1:98:A:ILE:H	1:98:A:ILE:HG12	2	0.28
(1,783)	1:106:A:ILE:HG21	1:106:A:ILE:HB	1	0.28
(1,722)	1:148:A:ILE:HA	1:148:A:ILE:HD12	7	0.28
(1,511)	1:139:A:PRO:HD2	1:138:A:THR:HB	1	0.28
(1,511)	1:139:A:PRO:HD2	1:138:A:THR:HB	4	0.28
(1,460)	1:126:A:LEU:HD12	1:120:A:LEU:HA	5	0.28
(1,184)	1:130:A:LEU:HD21	1:130:A:LEU:H	6	0.28
(1,89)	1:101:A:ILE:HG23	1:119:A:LEU:HA	9	0.28
(1,66)	1:83:A:ALA:HB3	1:83:A:ALA:H	8	0.28
(1,4189)	1:124:A:LYS:H	2:38:C:ASP:H	9	0.27
(1,4186)	1:120:A:LEU:HG	2:35:B:VAL:H	6	0.27
(1,4185)	1:120:A:LEU:HG	2:35:B:VAL:H	6	0.27
(1,3911)	2:12:C:ILE:HG13	2:11:C:LEU:H	3	0.27
(1,3850)	2:40:B:ILE:HG23	2:13:B:VAL:HB	1	0.27
(1,3796)	2:8:B:ILE:HG21	2:9:B:ALA:HB2	9	0.27
(1,3623)	2:40:C:ILE:HA	2:33:B:LEU:HG	1	0.27
(1,3567)	2:19:C:ILE:HD12	2:5:B:LYS:HG2	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3476)	2:55:B:LEU:HD21	2:14:B:ASN:HD21	6	0.27
(1,3316)	2:26:B:SER:H	2:33:B:LEU:HD12	9	0.27
(1,3232)	2:72:B:ALA:H	2:72:B:ALA:HB2	3	0.27
(1,3162)	2:6:B:GLU:HB2	2:7:B:GLU:H	8	0.27
(1,3083)	2:41:C:SER:H	2:41:C:SER:HB3	2	0.27
(1,3083)	2:41:C:SER:H	2:41:C:SER:HB3	5	0.27
(1,3083)	2:41:C:SER:H	2:41:C:SER:HB3	6	0.27
(1,3083)	2:41:C:SER:H	2:41:C:SER:HB3	9	0.27
(1,3082)	2:41:B:SER:H	2:41:B:SER:HB3	3	0.27
(1,3082)	2:41:B:SER:H	2:41:B:SER:HB3	8	0.27
(1,3014)	2:5:B:LYS:HG2	2:5:B:LYS:H	1	0.27
(1,2962)	2:48:B:ARG:HG3	2:48:B:ARG:H	10	0.27
(1,2954)	2:16:B:PHE:HZ	2:12:C:ILE:HD13	7	0.27
(1,2614)	2:13:B:VAL:HG12	2:48:B:ARG:HG2	3	0.27
(1,2599)	2:13:C:VAL:HG12	2:41:C:SER:HA	4	0.27
(1,2599)	2:13:C:VAL:HG11	2:41:C:SER:HA	6	0.27
(1,2540)	2:36:B:ALA:HB3	2:33:B:LEU:HD13	10	0.27
(1,2521)	2:51:C:VAL:HA	2:54:C:ILE:HD11	2	0.27
(1,2499)	2:25:C:ILE:HG22	2:20:C:VAL:HG13	3	0.27
(1,2493)	2:54:C:ILE:HB	2:54:C:ILE:HG22	9	0.27
(1,2426)	2:68:B:ILE:HD13	2:60:C:PHE:HD2	5	0.27
(1,2409)	2:19:C:ILE:HG22	2:44:B:PHE:HZ	10	0.27
(1,2347)	2:44:C:PHE:HB2	2:46:C:PHE:HD1	6	0.27
(1,2346)	2:44:B:PHE:HB2	2:46:B:PHE:HD1	9	0.27
(1,2192)	2:25:B:ILE:HD12	2:30:B:ALA:HA	4	0.27
(1,2186)	2:30:B:ALA:HA	2:20:B:VAL:HG12	1	0.27
(1,2152)	2:48:B:ARG:HD3	2:48:B:ARG:HB3	3	0.27
(1,2077)	2:55:C:LEU:HD11	2:55:C:LEU:HG	4	0.27
(1,2076)	2:55:B:LEU:HD12	2:55:B:LEU:HG	10	0.27
(1,2039)	2:5:C:LYS:HB3	2:44:C:PHE:HZ	6	0.27
(1,1855)	2:16:C:PHE:HB2	2:16:C:PHE:H	6	0.27
(1,1792)	1:141:A:ASN:HB3	1:138:A:THR:H	7	0.27
(1,1716)	1:101:A:ILE:HG21	1:101:A:ILE:H	1	0.27
(1,1716)	1:101:A:ILE:HG21	1:101:A:ILE:H	9	0.27
(1,1716)	1:101:A:ILE:HG22	1:101:A:ILE:H	10	0.27
(1,1699)	1:98:A:ILE:HG22	1:128:A:ASP:H	9	0.27
(1,1673)	1:85:A:LYS:H	1:85:A:LYS:HG3	8	0.27
(1,1655)	1:81:A:ILE:HG12	1:81:A:ILE:HD12	3	0.27
(1,1655)	1:81:A:ILE:HG12	1:81:A:ILE:HD13	5	0.27
(1,1650)	1:74:A:VAL:HG22	1:74:A:VAL:HB	3	0.27
(1,1650)	1:137:A:VAL:HG23	1:137:A:VAL:HB	9	0.27
(1,1611)	1:81:A:ILE:HB	1:81:A:ILE:HG22	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1528)	1:121:A:LEU:HA	1:122:A:LYS:HB3	7	0.27
(1,1392)	1:144:A:ILE:HG12	1:144:A:ILE:H	2	0.27
(1,1350)	1:141:A:ASN:HB3	1:141:A:ASN:HD21	6	0.27
(1,1132)	1:126:A:LEU:H	1:126:A:LEU:HB3	5	0.27
(1,1060)	1:116:A:GLU:HG2	1:116:A:GLU:H	4	0.27
(1,1041)	1:108:A:GLU:HG3	1:108:A:GLU:H	9	0.27
(1,980)	1:101:A:ILE:HG13	1:101:A:ILE:H	3	0.27
(1,955)	1:131:A:PHE:HB3	1:131:A:PHE:H	4	0.27
(1,955)	1:131:A:PHE:HB3	1:131:A:PHE:H	7	0.27
(1,898)	1:85:A:LYS:HB3	1:86:A:PHE:H	9	0.27
(1,780)	1:148:A:ILE:HG22	1:148:A:ILE:HB	6	0.27
(1,779)	1:74:A:VAL:HG11	1:74:A:VAL:HB	2	0.27
(1,779)	1:74:A:VAL:HG13	1:74:A:VAL:HB	4	0.27
(1,779)	1:74:A:VAL:HG11	1:74:A:VAL:HB	5	0.27
(1,700)	1:79:A:LYS:HE3	1:81:A:ILE:HA	1	0.27
(1,683)	1:106:A:ILE:HG12	1:106:A:ILE:H	5	0.27
(1,625)	1:101:A:ILE:HB	1:98:A:ILE:HG21	2	0.27
(1,547)	1:150:A:PRO:HD3	1:149:A:LYS:HA	8	0.27
(1,535)	1:150:A:PRO:HA	1:116:A:GLU:HG3	3	0.27
(1,513)	1:145:A:THR:HB	1:120:A:LEU:HD23	3	0.27
(1,437)	1:94:A:PRO:HD2	1:74:A:VAL:HG11	4	0.27
(1,158)	1:99:A:LEU:HD21	1:103:A:GLN:H	7	0.27
(1,138)	1:97:A:THR:HG23	1:97:A:THR:HB	7	0.27
(1,37)	1:106:A:ILE:HD13	1:114:A:ILE:HA	1	0.27
(1,31)	1:106:A:ILE:HD13	1:112:A:SER:H	8	0.27
(1,4175)	1:125:A:VAL:HG22	2:39:C:CYS:HG	5	0.26
(1,4008)	2:44:B:PHE:HZ	2:19:C:ILE:HG21	1	0.26
(1,3936)	2:13:B:VAL:HG22	2:48:B:ARG:HG3	10	0.26
(1,3932)	2:18:B:SER:HB3	2:22:B:LYS:HE3	6	0.26
(1,3888)	2:18:B:SER:HB3	2:22:B:LYS:HD3	6	0.26
(1,3828)	2:40:B:ILE:HD13	2:37:B:MET:HG3	10	0.26
(1,3724)	2:25:B:ILE:HG22	2:19:B:ILE:HB	6	0.26
(1,3692)	2:9:B:ALA:HA	2:46:B:PHE:HE1	9	0.26
(1,3561)	2:25:C:ILE:HD13	2:25:C:ILE:HG13	5	0.26
(1,3557)	2:25:C:ILE:HD12	2:5:B:LYS:HD2	5	0.26
(1,3541)	2:51:C:VAL:HG23	2:52:C:SER:HB3	6	0.26
(1,3292)	2:25:B:ILE:HG23	2:25:B:ILE:H	1	0.26
(1,3253)	2:21:C:GLU:HB3	2:21:C:GLU:H	3	0.26
(1,3138)	2:2:B:SER:H	2:3:B:ALA:H	2	0.26
(1,3118)	2:48:B:ARG:HB3	2:49:B:GLU:H	5	0.26
(1,3093)	2:13:C:VAL:HG11	2:41:C:SER:H	3	0.26
(1,3083)	2:41:C:SER:H	2:41:C:SER:HB3	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3083)	2:41:C:SER:H	2:41:C:SER:HB3	7	0.26
(1,3083)	2:41:C:SER:H	2:41:C:SER:HB3	10	0.26
(1,3082)	2:41:B:SER:H	2:41:B:SER:HB3	4	0.26
(1,3082)	2:41:B:SER:H	2:41:B:SER:HB3	10	0.26
(1,3044)	2:47:B:GLU:HB2	2:50:B:ALA:H	6	0.26
(1,2947)	2:44:C:PHE:HB2	2:46:C:PHE:HE2	5	0.26
(1,2790)	2:33:B:LEU:HD13	2:19:B:ILE:HB	10	0.26
(1,2702)	2:13:B:VAL:HA	2:40:B:ILE:HD13	1	0.26
(1,2685)	2:50:C:ALA:HB1	2:46:C:PHE:HB3	4	0.26
(1,2650)	2:8:B:ILE:HG22	2:19:C:ILE:HG12	10	0.26
(1,2630)	2:51:B:VAL:HB	2:55:B:LEU:HG	6	0.26
(1,2599)	2:13:C:VAL:HG13	2:41:C:SER:HA	1	0.26
(1,2599)	2:13:C:VAL:HG11	2:41:C:SER:HA	3	0.26
(1,2585)	2:49:C:GLU:HG3	2:49:C:GLU:HA	10	0.26
(1,2565)	2:33:C:LEU:HD11	2:19:C:ILE:HG23	8	0.26
(1,2501)	2:25:C:ILE:HG21	2:20:C:VAL:HB	6	0.26
(1,2472)	2:12:B:ILE:HG21	2:13:B:VAL:HG11	6	0.26
(1,2409)	2:19:C:ILE:HG23	2:44:B:PHE:HZ	3	0.26
(1,2226)	2:5:B:LYS:HA	2:8:B:ILE:HG13	10	0.26
(1,2183)	2:9:C:ALA:HA	2:40:C:ILE:HG23	9	0.26
(1,2183)	2:9:C:ALA:HA	2:40:C:ILE:HG23	10	0.26
(1,2091)	2:8:C:ILE:HD13	2:3:C:ALA:HB1	3	0.26
(1,2061)	2:55:C:LEU:HD23	2:14:C:ASN:H	8	0.26
(1,1766)	1:135:A:LEU:H	1:126:A:LEU:HD12	3	0.26
(1,1760)	1:152:A:LEU:HB3	1:153:A:GLU:H	9	0.26
(1,1680)	1:145:A:THR:H	1:79:A:LYS:HB2	4	0.26
(1,1662)	1:149:A:LYS:HG3	1:149:A:LYS:HE3	4	0.26
(1,1623)	1:126:A:LEU:HG	1:124:A:LYS:HE3	9	0.26
(1,1611)	1:81:A:ILE:HB	1:81:A:ILE:HG23	5	0.26
(1,1611)	1:81:A:ILE:HB	1:81:A:ILE:HG22	9	0.26
(1,1609)	1:114:A:ILE:HB	1:114:A:ILE:HG23	3	0.26
(1,1609)	1:114:A:ILE:HB	1:114:A:ILE:HG22	9	0.26
(1,1466)	1:117:A:ILE:HG22	1:117:A:ILE:HB	6	0.26
(1,1465)	1:117:A:ILE:HG23	1:102:A:LYS:HB3	1	0.26
(1,1432)	1:117:A:ILE:HD12	1:117:A:ILE:HG13	7	0.26
(1,1159)	1:152:A:LEU:HG	1:152:A:LEU:H	7	0.26
(1,1133)	1:126:A:LEU:HD13	1:126:A:LEU:H	6	0.26
(1,1070)	1:111:A:ALA:HB3	1:111:A:ALA:H	6	0.26
(1,1060)	1:116:A:GLU:HG2	1:116:A:GLU:H	9	0.26
(1,949)	1:100:A:GLN:H	1:99:A:LEU:HD13	4	0.26
(1,761)	1:106:A:ILE:HA	1:106:A:ILE:HG23	7	0.26
(1,722)	1:148:A:ILE:HA	1:148:A:ILE:HD11	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,655)	1:81:A:ILE:HG12	1:145:A:THR:HA	1	0.26
(1,494)	1:98:A:ILE:HA	1:101:A:ILE:HG12	1	0.26
(1,494)	1:98:A:ILE:HA	1:101:A:ILE:HG12	10	0.26
(1,460)	1:126:A:LEU:HD13	1:120:A:LEU:HA	7	0.26
(1,437)	1:94:A:PRO:HD2	1:74:A:VAL:HG11	9	0.26
(1,261)	1:129:A:ASN:HB2	1:129:A:ASN:HD21	9	0.26
(1,172)	1:78:A:LEU:HD21	1:78:A:LEU:HG	6	0.26
(1,158)	1:99:A:LEU:HD21	1:103:A:GLN:H	6	0.26
(1,156)	1:99:A:LEU:HD21	1:103:A:GLN:HE21	1	0.26
(1,138)	1:97:A:THR:HG21	1:97:A:THR:HB	6	0.26
(1,112)	1:77:A:THR:HG23	1:78:A:LEU:H	7	0.26
(1,106)	1:126:A:LEU:HD11	1:121:A:LEU:H	2	0.26
(1,75)	1:98:A:ILE:HG22	1:128:A:ASP:HA	1	0.26
(1,75)	1:98:A:ILE:HG22	1:128:A:ASP:HA	3	0.26
(1,66)	1:83:A:ALA:HB3	1:83:A:ALA:H	1	0.26
(3,140)	2:38:C:ASP:N	2:34:C:ASN:O	4	0.25
(1,4189)	1:124:A:LYS:H	2:38:C:ASP:H	8	0.25
(1,4177)	1:147:A:MET:HE1	2:35:C:VAL:HG11	8	0.25
(1,4175)	1:125:A:VAL:HG12	2:39:C:CYS:HG	1	0.25
(1,4161)	2:38:C:ASP:H	2:40:C:ILE:HD12	9	0.25
(1,4126)	2:19:B:ILE:HA	2:25:B:ILE:H	1	0.25
(1,3968)	2:25:B:ILE:HG23	2:32:B:SER:H	2	0.25
(1,3938)	2:33:B:LEU:HD12	2:40:C:ILE:HA	5	0.25
(1,3911)	2:12:C:ILE:HG13	2:11:C:LEU:H	7	0.25
(1,3692)	2:9:B:ALA:HA	2:46:B:PHE:HE1	6	0.25
(1,3683)	2:12:C:ILE:HD13	2:16:B:PHE:HD1	2	0.25
(1,3561)	2:25:C:ILE:HD13	2:25:C:ILE:HG13	3	0.25
(1,3560)	2:25:B:ILE:HD12	2:25:B:ILE:HG13	2	0.25
(1,3560)	2:25:B:ILE:HD11	2:25:B:ILE:HG13	7	0.25
(1,3421)	2:51:C:VAL:H	2:54:C:ILE:HG12	10	0.25
(1,3321)	2:19:C:ILE:HG22	2:26:C:SER:H	2	0.25
(1,3232)	2:72:B:ALA:H	2:72:B:ALA:HB2	6	0.25
(1,3230)	2:20:B:VAL:H	2:25:B:ILE:HG23	10	0.25
(1,3174)	2:7:B:GLU:H	2:4:B:SER:HB3	8	0.25
(1,3158)	2:42:B:GLU:HB3	2:42:B:GLU:H	7	0.25
(1,3158)	2:42:B:GLU:HB3	2:42:B:GLU:H	10	0.25
(1,3100)	2:23:B:LYS:HG3	2:23:B:LYS:H	9	0.25
(1,3083)	2:41:C:SER:H	2:41:C:SER:HB3	8	0.25
(1,3008)	2:4:B:SER:HB2	2:5:B:LYS:H	2	0.25
(1,2946)	2:44:B:PHE:HB2	2:46:B:PHE:HE1	10	0.25
(1,2845)	2:64:C:HIS:HB2	2:64:C:HIS:H	4	0.25
(1,2693)	2:50:C:ALA:HB3	2:47:C:GLU:HB2	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2692)	2:50:B:ALA:HB3	2:47:B:GLU:HB2	1	0.25
(1,2594)	2:57:B:LYS:HB3	2:68:C:ILE:HG13	4	0.25
(1,2535)	2:36:C:ALA:HB2	2:40:B:ILE:HG13	2	0.25
(1,2520)	2:51:B:VAL:HA	2:54:B:ILE:HD13	6	0.25
(1,2483)	2:25:C:ILE:HB	2:19:C:ILE:HG21	9	0.25
(1,2427)	2:68:C:ILE:HD11	2:60:B:PHE:HD2	1	0.25
(1,2426)	2:68:B:ILE:HD13	2:60:C:PHE:HD1	6	0.25
(1,2423)	2:25:C:ILE:HD12	2:44:B:PHE:HZ	7	0.25
(1,2389)	2:20:C:VAL:HG22	2:34:C:ASN:HD22	2	0.25
(1,2298)	2:19:B:ILE:HA	2:22:B:LYS:HD3	7	0.25
(1,2254)	2:36:B:ALA:HA	2:35:B:VAL:HG21	3	0.25
(1,2183)	2:9:C:ALA:HA	2:40:C:ILE:HG22	6	0.25
(1,2183)	2:9:C:ALA:HA	2:40:C:ILE:HG23	8	0.25
(1,2076)	2:55:B:LEU:HD13	2:55:B:LEU:HG	3	0.25
(1,1845)	2:13:C:VAL:HA	2:13:C:VAL:HG23	2	0.25
(1,1845)	2:13:C:VAL:HA	2:13:C:VAL:HG23	7	0.25
(1,1716)	1:101:A:ILE:HG21	1:101:A:ILE:H	6	0.25
(1,1716)	1:101:A:ILE:HG21	1:101:A:ILE:H	8	0.25
(1,1647)	1:136:A:LYS:HG3	1:136:A:LYS:HE3	10	0.25
(1,1614)	1:150:A:PRO:HB2	1:152:A:LEU:HD12	4	0.25
(1,1611)	1:81:A:ILE:HB	1:81:A:ILE:HG21	2	0.25
(1,1609)	1:114:A:ILE:HB	1:114:A:ILE:HG23	4	0.25
(1,1411)	1:116:A:GLU:HG3	1:151:A:ASN:H	7	0.25
(1,1160)	1:152:A:LEU:H	1:150:A:PRO:HB2	2	0.25
(1,1159)	1:152:A:LEU:HG	1:152:A:LEU:H	9	0.25
(1,1157)	1:152:A:LEU:HA	1:152:A:LEU:H	6	0.25
(1,1139)	1:82:A:GLN:HG3	1:82:A:GLN:H	10	0.25
(1,809)	1:126:A:LEU:HB2	1:126:A:LEU:H	7	0.25
(1,791)	1:136:A:LYS:HG3	1:136:A:LYS:HE3	9	0.25
(1,787)	1:120:A:LEU:HG	1:120:A:LEU:HD21	5	0.25
(1,779)	1:74:A:VAL:HG11	1:74:A:VAL:HB	10	0.25
(1,756)	1:146:A:VAL:HG22	1:119:A:LEU:HA	8	0.25
(1,749)	1:124:A:LYS:HG2	1:125:A:VAL:HA	2	0.25
(1,697)	1:79:A:LYS:HE3	1:79:A:LYS:HG3	2	0.25
(1,642)	1:97:A:THR:HG21	1:100:A:GLN:HG3	9	0.25
(1,624)	1:141:A:ASN:HB3	1:121:A:LEU:HD13	7	0.25
(1,440)	1:83:A:ALA:HA	1:85:A:LYS:HE3	1	0.25
(1,418)	1:136:A:LYS:HG2	1:136:A:LYS:H	7	0.25
(1,180)	1:132:A:LEU:HD11	1:96:A:ASP:HB2	3	0.25
(1,139)	1:125:A:VAL:HG22	1:125:A:VAL:HA	5	0.25
(1,112)	1:77:A:THR:HG23	1:78:A:LEU:H	10	0.25
(1,58)	1:114:A:ILE:HD12	1:99:A:LEU:HA	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:144:A:ILE:HD11	1:143:A:THR:H	4	0.25
(1,2)	1:120:A:LEU:HD13	1:120:A:LEU:H	8	0.25
(3,140)	2:38:C:ASP:N	2:34:C:ASN:O	10	0.24
(1,4186)	1:120:A:LEU:HG	2:35:B:VAL:H	3	0.24
(1,4185)	1:120:A:LEU:HG	2:35:B:VAL:H	3	0.24
(1,3796)	2:8:B:ILE:HG21	2:9:B:ALA:HB3	6	0.24
(1,3725)	2:25:C:ILE:HG23	2:19:C:ILE:HB	5	0.24
(1,3693)	2:9:C:ALA:HA	2:46:C:PHE:HE1	2	0.24
(1,3665)	2:33:C:LEU:HD23	2:44:B:PHE:HZ	6	0.24
(1,3665)	2:33:C:LEU:HD23	2:44:B:PHE:HZ	7	0.24
(1,3589)	2:5:C:LYS:HE2	2:19:B:ILE:HG21	2	0.24
(1,3563)	2:8:C:ILE:HD11	2:9:C:ALA:HA	4	0.24
(1,3560)	2:25:B:ILE:HD11	2:25:B:ILE:HG13	1	0.24
(1,3355)	2:37:C:MET:H	2:40:C:ILE:HD13	2	0.24
(1,3232)	2:72:B:ALA:H	2:72:B:ALA:HB2	2	0.24
(1,3153)	2:6:C:GLU:HG3	2:6:C:GLU:H	4	0.24
(1,2881)	2:33:C:LEU:HD12	2:19:C:ILE:HD11	7	0.24
(1,2790)	2:33:B:LEU:HD13	2:19:B:ILE:HB	1	0.24
(1,2712)	2:54:B:ILE:HD12	2:51:B:VAL:H	2	0.24
(1,2698)	2:54:B:ILE:HG23	2:6:B:GLU:HG3	5	0.24
(1,2647)	2:55:C:LEU:HD13	2:11:C:LEU:HD22	1	0.24
(1,2646)	2:55:B:LEU:HD13	2:11:B:LEU:HD23	9	0.24
(1,2555)	2:20:C:VAL:HG13	2:30:C:ALA:HB3	7	0.24
(1,2540)	2:36:B:ALA:HB3	2:33:B:LEU:HD13	9	0.24
(1,2404)	2:8:B:ILE:HG22	2:15:C:TYR:H	9	0.24
(1,2357)	2:49:C:GLU:HG2	2:49:C:GLU:H	9	0.24
(1,2347)	2:44:C:PHE:HB2	2:46:C:PHE:HD1	10	0.24
(1,2234)	2:27:B:GLU:HA	2:30:B:ALA:HB1	1	0.24
(1,2192)	2:25:B:ILE:HD12	2:30:B:ALA:HA	5	0.24
(1,2114)	2:13:B:VAL:HG21	2:48:B:ARG:HG2	7	0.24
(1,2091)	2:8:C:ILE:HD12	2:3:C:ALA:HB1	10	0.24
(1,2067)	2:55:C:LEU:HD21	2:55:C:LEU:HG	2	0.24
(1,2067)	2:55:C:LEU:HD22	2:55:C:LEU:HG	10	0.24
(1,2066)	2:55:B:LEU:HD22	2:55:B:LEU:HG	9	0.24
(1,1854)	2:16:B:PHE:HB2	2:16:B:PHE:H	7	0.24
(1,1845)	2:13:C:VAL:HA	2:13:C:VAL:HG22	4	0.24
(1,1845)	2:13:C:VAL:HA	2:13:C:VAL:HG22	5	0.24
(1,1845)	2:13:C:VAL:HA	2:13:C:VAL:HG22	6	0.24
(1,1845)	2:13:C:VAL:HA	2:13:C:VAL:HG23	8	0.24
(1,1844)	2:13:B:VAL:HA	2:13:B:VAL:HG23	6	0.24
(1,1745)	1:82:A:GLN:H	1:81:A:ILE:HG22	5	0.24
(1,1716)	1:101:A:ILE:HG22	1:101:A:ILE:H	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1683)	1:77:A:THR:H	1:76:A:LEU:HD12	7	0.24
(1,1661)	1:149:A:LYS:HB3	1:149:A:LYS:HE3	7	0.24
(1,1655)	1:81:A:ILE:HG12	1:81:A:ILE:HD13	9	0.24
(1,1623)	1:126:A:LEU:HG	1:124:A:LYS:HE3	1	0.24
(1,1319)	1:82:A:GLN:HG3	1:82:A:GLN:HE21	8	0.24
(1,1157)	1:152:A:LEU:HA	1:152:A:LEU:H	5	0.24
(1,1132)	1:126:A:LEU:H	1:126:A:LEU:HB3	4	0.24
(1,1132)	1:126:A:LEU:H	1:126:A:LEU:HB3	8	0.24
(1,1071)	1:138:A:THR:H	1:138:A:THR:HG23	2	0.24
(1,1033)	1:106:A:ILE:HG13	1:106:A:ILE:H	6	0.24
(1,809)	1:126:A:LEU:HB2	1:126:A:LEU:H	6	0.24
(1,779)	1:74:A:VAL:HG11	1:74:A:VAL:HB	3	0.24
(1,779)	1:74:A:VAL:HG11	1:74:A:VAL:HB	6	0.24
(1,769)	1:132:A:LEU:HA	1:135:A:LEU:HD13	1	0.24
(1,760)	1:106:A:ILE:HG21	1:107:A:SER:HA	3	0.24
(1,725)	1:148:A:ILE:HD13	1:80:A:LYS:HD3	3	0.24
(1,722)	1:148:A:ILE:HA	1:148:A:ILE:HD12	8	0.24
(1,697)	1:79:A:LYS:HE3	1:79:A:LYS:HG3	9	0.24
(1,585)	1:91:A:ASP:HB3	1:92:A:PHE:HA	1	0.24
(1,266)	1:114:A:ILE:HG12	1:114:A:ILE:H	1	0.24
(1,235)	1:118:A:LYS:HB3	1:118:A:LYS:HE3	7	0.24
(1,134)	1:125:A:VAL:HG22	1:125:A:VAL:HB	8	0.24
(1,112)	1:77:A:THR:HG21	1:78:A:LEU:H	5	0.24
(1,111)	1:126:A:LEU:HD11	1:124:A:LYS:HE2	10	0.24
(3,140)	2:38:C:ASP:N	2:34:C:ASN:O	7	0.23
(1,4177)	1:147:A:MET:HG2	2:35:B:VAL:HG22	9	0.23
(1,4160)	2:38:B:ASP:H	2:40:B:ILE:HD13	10	0.23
(1,4126)	2:19:B:ILE:HA	2:25:B:ILE:H	6	0.23
(1,4005)	2:46:C:PHE:HE2	2:54:C:ILE:HG21	7	0.23
(1,4004)	2:44:B:PHE:HZ	2:25:C:ILE:HG23	9	0.23
(1,3968)	2:25:B:ILE:HG21	2:32:B:SER:H	10	0.23
(1,3963)	2:36:C:ALA:HB2	2:40:B:ILE:HA	1	0.23
(1,3954)	2:5:B:LYS:HD3	2:19:C:ILE:HG21	6	0.23
(1,3890)	2:18:B:SER:HB3	2:19:B:ILE:HG12	1	0.23
(1,3770)	2:30:B:ALA:HA	2:20:B:VAL:HG22	7	0.23
(1,3722)	2:25:B:ILE:HG23	2:5:C:LYS:HE3	9	0.23
(1,3693)	2:9:C:ALA:HA	2:46:C:PHE:HE1	1	0.23
(1,3658)	2:51:B:VAL:HG23	2:46:B:PHE:HE2	10	0.23
(1,3566)	2:19:B:ILE:HD11	2:5:C:LYS:HG2	1	0.23
(1,3563)	2:8:C:ILE:HD13	2:11:C:LEU:HA	5	0.23
(1,3561)	2:25:C:ILE:HD13	2:25:C:ILE:HG13	1	0.23
(1,3561)	2:25:C:ILE:HD13	2:25:C:ILE:HG13	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3253)	2:21:C:GLU:HB3	2:21:C:GLU:H	5	0.23
(1,3164)	2:7:B:GLU:H	2:7:B:GLU:HG3	6	0.23
(1,3163)	2:6:C:GLU:HB2	2:7:C:GLU:H	10	0.23
(1,3153)	2:6:C:GLU:HG3	2:6:C:GLU:H	9	0.23
(1,2963)	2:48:C:ARG:HG3	2:48:C:ARG:H	1	0.23
(1,2936)	2:6:B:GLU:HG2	2:44:B:PHE:HD1	8	0.23
(1,2810)	2:25:B:ILE:HA	2:33:B:LEU:HD13	7	0.23
(1,2775)	2:71:C:SER:HB3	2:68:C:ILE:H	9	0.23
(1,2713)	2:54:C:ILE:HD11	2:51:C:VAL:H	2	0.23
(1,2641)	2:33:C:LEU:HD13	2:20:C:VAL:HG11	2	0.23
(1,2629)	2:37:C:MET:HB3	2:17:C:SER:HB3	3	0.23
(1,2500)	2:25:B:ILE:HG21	2:20:B:VAL:HB	8	0.23
(1,2405)	2:8:C:ILE:HG21	2:15:B:TYR:H	4	0.23
(1,2346)	2:44:B:PHE:HB2	2:46:B:PHE:HD1	4	0.23
(1,2153)	2:48:C:ARG:HD3	2:48:C:ARG:HB3	5	0.23
(1,2153)	2:48:C:ARG:HD3	2:48:C:ARG:HB3	7	0.23
(1,2113)	2:13:C:VAL:HG22	2:51:C:VAL:HB	3	0.23
(1,2112)	2:13:B:VAL:HG21	2:51:B:VAL:HB	4	0.23
(1,2067)	2:55:C:LEU:HD21	2:55:C:LEU:HG	3	0.23
(1,2067)	2:55:C:LEU:HD22	2:55:C:LEU:HG	4	0.23
(1,2066)	2:55:B:LEU:HD22	2:55:B:LEU:HG	5	0.23
(1,1995)	2:36:C:ALA:HB2	2:33:C:LEU:HD21	4	0.23
(1,1855)	2:16:C:PHE:HB2	2:16:C:PHE:H	7	0.23
(1,1844)	2:13:B:VAL:HA	2:13:B:VAL:HG21	5	0.23
(1,1844)	2:13:B:VAL:HA	2:13:B:VAL:HG23	8	0.23
(1,1810)	1:99:A:LEU:HG	1:103:A:GLN:HE21	7	0.23
(1,1801)	1:82:A:GLN:HE22	1:81:A:ILE:HG21	2	0.23
(1,1697)	1:78:A:LEU:HD11	1:90:A:HIS:H	10	0.23
(1,1609)	1:114:A:ILE:HB	1:114:A:ILE:HG22	6	0.23
(1,1466)	1:117:A:ILE:HG22	1:117:A:ILE:HB	10	0.23
(1,1319)	1:82:A:GLN:HG3	1:82:A:GLN:HE21	10	0.23
(1,1236)	1:99:A:LEU:HD11	1:99:A:LEU:H	5	0.23
(1,1157)	1:152:A:LEU:HA	1:152:A:LEU:H	2	0.23
(1,1141)	1:82:A:GLN:H	1:80:A:LYS:HG2	9	0.23
(1,1081)	1:140:A:ALA:HB3	1:141:A:ASN:H	5	0.23
(1,1011)	1:98:A:ILE:H	1:98:A:ILE:HG12	5	0.23
(1,958)	1:121:A:LEU:H	1:126:A:LEU:HB3	10	0.23
(1,955)	1:131:A:PHE:HB3	1:131:A:PHE:H	3	0.23
(1,809)	1:126:A:LEU:HB2	1:126:A:LEU:H	8	0.23
(1,809)	1:126:A:LEU:HB2	1:126:A:LEU:H	9	0.23
(1,779)	1:74:A:VAL:HG13	1:74:A:VAL:HB	7	0.23
(1,722)	1:148:A:ILE:HA	1:148:A:ILE:HD12	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,722)	1:148:A:ILE:HA	1:148:A:ILE:HD13	10	0.23
(1,719)	1:148:A:ILE:HD12	1:112:A:SER:H	6	0.23
(1,655)	1:81:A:ILE:HG12	1:145:A:THR:HA	4	0.23
(1,642)	1:97:A:THR:HG22	1:100:A:GLN:HG3	4	0.23
(1,494)	1:98:A:ILE:HA	1:101:A:ILE:HG12	7	0.23
(1,144)	1:140:A:ALA:HB2	1:140:A:ALA:HA	2	0.23
(1,116)	1:125:A:VAL:HG22	1:120:A:LEU:H	8	0.23
(1,113)	1:77:A:THR:HG23	1:88:A:ILE:H	3	0.23
(1,89)	1:101:A:ILE:HG23	1:119:A:LEU:HA	6	0.23
(1,66)	1:83:A:ALA:HB3	1:83:A:ALA:H	4	0.23
(1,31)	1:106:A:ILE:HD11	1:112:A:SER:H	7	0.23
(1,28)	1:144:A:ILE:HD11	1:121:A:LEU:HA	10	0.23
(1,10)	1:120:A:LEU:HD12	1:120:A:LEU:HG	1	0.23
(3,34)	1:149:A:LYS:N	1:116:A:GLU:O	2	0.22
(3,33)	1:149:A:LYS:H	1:116:A:GLU:O	6	0.22
(1,4169)	1:81:A:ILE:HG22	2:42:B:GLU:HG3	5	0.22
(1,4098)	2:17:B:SER:H	2:12:B:ILE:HG21	8	0.22
(1,3891)	2:18:C:SER:HB3	2:19:C:ILE:HG12	5	0.22
(1,3725)	2:25:C:ILE:HG21	2:19:C:ILE:HB	2	0.22
(1,3725)	2:25:C:ILE:HG22	2:19:C:ILE:HB	10	0.22
(1,3714)	2:19:B:ILE:HG22	2:24:B:GLU:HB3	9	0.22
(1,3704)	2:6:B:GLU:HA	2:46:B:PHE:HE1	2	0.22
(1,3664)	2:33:B:LEU:HD23	2:44:C:PHE:HZ	10	0.22
(1,3643)	2:68:C:ILE:HB	2:71:C:SER:H	5	0.22
(1,3570)	2:13:B:VAL:HG22	2:48:B:ARG:HG3	10	0.22
(1,3561)	2:25:C:ILE:HD13	2:25:C:ILE:HG13	7	0.22
(1,3561)	2:25:C:ILE:HD12	2:25:C:ILE:HG13	8	0.22
(1,3561)	2:25:C:ILE:HD13	2:25:C:ILE:HG13	9	0.22
(1,3561)	2:25:C:ILE:HD13	2:25:C:ILE:HG13	10	0.22
(1,3560)	2:25:B:ILE:HD11	2:25:B:ILE:HG13	5	0.22
(1,3233)	2:72:C:ALA:H	2:72:C:ALA:HB2	6	0.22
(1,3230)	2:20:B:VAL:H	2:25:B:ILE:HG23	4	0.22
(1,2963)	2:48:C:ARG:HG3	2:48:C:ARG:H	4	0.22
(1,2962)	2:48:B:ARG:HG3	2:48:B:ARG:H	9	0.22
(1,2955)	2:16:C:PHE:HZ	2:12:B:ILE:HD12	5	0.22
(1,2940)	2:44:B:PHE:HZ	2:33:C:LEU:HD22	10	0.22
(1,2811)	2:25:C:ILE:HA	2:33:C:LEU:HD11	8	0.22
(1,2712)	2:54:B:ILE:HD11	2:51:B:VAL:H	4	0.22
(1,2691)	2:50:C:ALA:HB1	2:47:C:GLU:HB3	9	0.22
(1,2512)	2:54:B:ILE:HD12	2:54:B:ILE:HG22	3	0.22
(1,2489)	2:68:C:ILE:HG23	2:68:C:ILE:HG13	4	0.22
(1,2489)	2:68:C:ILE:HG22	2:68:C:ILE:HG13	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2489)	2:68:C:ILE:HG22	2:68:C:ILE:HG13	6	0.22
(1,2488)	2:68:B:ILE:HG21	2:68:B:ILE:HG13	1	0.22
(1,2488)	2:68:B:ILE:HG22	2:68:B:ILE:HG13	7	0.22
(1,2488)	2:68:B:ILE:HG21	2:68:B:ILE:HG13	10	0.22
(1,2483)	2:25:C:ILE:HB	2:19:C:ILE:HG22	4	0.22
(1,2423)	2:25:C:ILE:HD12	2:44:B:PHE:HZ	10	0.22
(1,2346)	2:44:B:PHE:HB2	2:46:B:PHE:HD1	10	0.22
(1,2296)	2:19:B:ILE:HA	2:22:B:LYS:HB2	9	0.22
(1,2258)	2:51:B:VAL:HA	2:54:B:ILE:HB	3	0.22
(1,2148)	2:5:B:LYS:HE3	2:25:C:ILE:HG22	1	0.22
(1,2067)	2:55:C:LEU:HD21	2:55:C:LEU:HG	6	0.22
(1,2066)	2:55:B:LEU:HD23	2:55:B:LEU:HG	1	0.22
(1,2066)	2:55:B:LEU:HD22	2:55:B:LEU:HG	8	0.22
(1,1995)	2:36:C:ALA:HB1	2:33:C:LEU:HD21	2	0.22
(1,1893)	2:23:C:LYS:HA	2:23:C:LYS:HG3	8	0.22
(1,1845)	2:13:C:VAL:HA	2:13:C:VAL:HG21	1	0.22
(1,1845)	2:13:C:VAL:HA	2:13:C:VAL:HG23	3	0.22
(1,1844)	2:13:B:VAL:HA	2:13:B:VAL:HG22	7	0.22
(1,1808)	1:99:A:LEU:HG	1:103:A:GLN:HE22	6	0.22
(1,1736)	1:110:A:LYS:H	1:105:A:LEU:HB3	4	0.22
(1,1707)	1:144:A:ILE:HG23	1:120:A:LEU:H	1	0.22
(1,1609)	1:114:A:ILE:HB	1:114:A:ILE:HG21	1	0.22
(1,1573)	1:137:A:VAL:HA	1:137:A:VAL:HG21	8	0.22
(1,1528)	1:121:A:LEU:HA	1:122:A:LYS:HB3	8	0.22
(1,1432)	1:117:A:ILE:HD12	1:117:A:ILE:HG13	9	0.22
(1,1167)	1:124:A:LYS:HG2	1:125:A:VAL:H	8	0.22
(1,1157)	1:152:A:LEU:HA	1:152:A:LEU:H	1	0.22
(1,1157)	1:152:A:LEU:HA	1:152:A:LEU:H	3	0.22
(1,1060)	1:116:A:GLU:HG2	1:116:A:GLU:H	3	0.22
(1,1060)	1:116:A:GLU:HG2	1:116:A:GLU:H	10	0.22
(1,955)	1:131:A:PHE:HB3	1:131:A:PHE:H	2	0.22
(1,867)	1:145:A:THR:HG22	1:145:A:THR:H	8	0.22
(1,809)	1:126:A:LEU:HB2	1:126:A:LEU:H	4	0.22
(1,779)	1:74:A:VAL:HG13	1:74:A:VAL:HB	1	0.22
(1,758)	1:113:A:HIS:HA	1:114:A:ILE:HG22	7	0.22
(1,756)	1:146:A:VAL:HG21	1:119:A:LEU:HA	3	0.22
(1,634)	1:114:A:ILE:HB	1:113:A:HIS:HA	1	0.22
(1,585)	1:91:A:ASP:HB3	1:92:A:PHE:HA	6	0.22
(1,533)	1:114:A:ILE:HA	1:114:A:ILE:HG12	6	0.22
(1,513)	1:145:A:THR:HB	1:120:A:LEU:HD23	9	0.22
(1,506)	1:112:A:SER:HA	1:106:A:ILE:HD13	6	0.22
(1,494)	1:98:A:ILE:HA	1:101:A:ILE:HG12	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,418)	1:136:A:LYS:HG2	1:136:A:LYS:H	8	0.22
(1,261)	1:129:A:ASN:HB2	1:129:A:ASN:HD21	1	0.22
(1,261)	1:129:A:ASN:HB2	1:129:A:ASN:HD21	6	0.22
(1,235)	1:118:A:LYS:HB3	1:118:A:LYS:HE3	10	0.22
(1,201)	1:144:A:ILE:HG23	1:120:A:LEU:H	1	0.22
(1,184)	1:130:A:LEU:HD21	1:130:A:LEU:H	4	0.22
(1,156)	1:99:A:LEU:HD21	1:103:A:GLN:HE21	9	0.22
(1,119)	1:97:A:THR:HG22	1:131:A:PHE:HD1	1	0.22
(1,66)	1:83:A:ALA:HB1	1:83:A:ALA:H	3	0.22
(1,66)	1:83:A:ALA:HB3	1:83:A:ALA:H	10	0.22
(1,31)	1:106:A:ILE:HD13	1:112:A:SER:H	5	0.22
(3,34)	1:149:A:LYS:N	1:116:A:GLU:O	8	0.21
(1,4023)	2:44:C:PHE:HZ	2:9:C:ALA:H	9	0.21
(1,4009)	2:16:C:PHE:HZ	2:12:B:ILE:HG21	7	0.21
(1,3911)	2:12:C:ILE:HG13	2:11:C:LEU:H	2	0.21
(1,3823)	2:40:C:ILE:HD11	2:36:C:ALA:HA	6	0.21
(1,3817)	2:6:C:GLU:HB2	2:46:C:PHE:HD1	9	0.21
(1,3800)	2:8:B:ILE:HG22	2:16:C:PHE:HD1	5	0.21
(1,3727)	2:25:C:ILE:HG22	2:30:C:ALA:HB3	4	0.21
(1,3575)	2:33:C:LEU:HD23	2:43:B:ALA:HB2	6	0.21
(1,3574)	2:33:B:LEU:HD22	2:43:C:ALA:HB1	2	0.21
(1,3574)	2:33:B:LEU:HD23	2:43:C:ALA:HB1	5	0.21
(1,3560)	2:25:B:ILE:HD11	2:25:B:ILE:HG13	3	0.21
(1,3559)	2:25:C:ILE:HD11	2:25:C:ILE:HG12	2	0.21
(1,3559)	2:25:C:ILE:HD11	2:25:C:ILE:HG12	3	0.21
(1,3558)	2:25:B:ILE:HD12	2:25:B:ILE:HG12	2	0.21
(1,3558)	2:25:B:ILE:HD12	2:25:B:ILE:HG12	4	0.21
(1,3320)	2:19:B:ILE:HG23	2:26:B:SER:H	10	0.21
(1,3261)	2:22:C:LYS:HG2	2:22:C:LYS:H	7	0.21
(1,3253)	2:21:C:GLU:HB3	2:21:C:GLU:H	8	0.21
(1,3252)	2:21:B:GLU:HB3	2:21:B:GLU:H	4	0.21
(1,3230)	2:20:B:VAL:H	2:25:B:ILE:HG23	5	0.21
(1,3197)	2:14:C:ASN:H	2:48:C:ARG:HA	6	0.21
(1,3158)	2:42:B:GLU:HB3	2:42:B:GLU:H	4	0.21
(1,3154)	2:4:B:SER:HB3	2:6:B:GLU:H	2	0.21
(1,2965)	2:48:C:ARG:HB3	2:48:C:ARG:H	8	0.21
(1,2960)	2:3:B:ALA:HB1	2:3:B:ALA:H	5	0.21
(1,2947)	2:44:C:PHE:HB2	2:46:C:PHE:HE2	10	0.21
(1,2904)	2:48:B:ARG:HG3	2:48:B:ARG:HE	9	0.21
(1,2798)	2:48:B:ARG:HA	2:51:B:VAL:HG11	5	0.21
(1,2791)	2:33:C:LEU:HD12	2:19:C:ILE:HB	7	0.21
(1,2564)	2:33:B:LEU:HD12	2:19:B:ILE:HG21	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2500)	2:25:B:ILE:HG21	2:20:B:VAL:HB	3	0.21
(1,2499)	2:25:C:ILE:HG22	2:20:C:VAL:HG13	6	0.21
(1,2404)	2:8:B:ILE:HG22	2:15:C:TYR:H	6	0.21
(1,2347)	2:44:C:PHE:HB2	2:46:C:PHE:HD1	8	0.21
(1,2309)	2:52:C:SER:HA	2:55:C:LEU:HD13	7	0.21
(1,2186)	2:30:B:ALA:HA	2:20:B:VAL:HG13	4	0.21
(1,2153)	2:48:C:ARG:HD3	2:48:C:ARG:HB3	9	0.21
(1,2112)	2:13:B:VAL:HG23	2:51:B:VAL:HB	9	0.21
(1,2066)	2:55:B:LEU:HD23	2:55:B:LEU:HG	4	0.21
(1,2038)	2:5:B:LYS:HB3	2:44:B:PHE:HZ	5	0.21
(1,1855)	2:16:C:PHE:HB2	2:16:C:PHE:H	1	0.21
(1,1855)	2:16:C:PHE:HB2	2:16:C:PHE:H	4	0.21
(1,1844)	2:13:B:VAL:HA	2:13:B:VAL:HG22	2	0.21
(1,1844)	2:13:B:VAL:HA	2:13:B:VAL:HG22	4	0.21
(1,1789)	1:127:A:HIS:H	1:98:A:ILE:HG23	1	0.21
(1,1719)	1:95:A:SER:HB3	1:95:A:SER:H	2	0.21
(1,1699)	1:98:A:ILE:HG23	1:128:A:ASP:H	8	0.21
(1,1655)	1:81:A:ILE:HG12	1:81:A:ILE:HD13	1	0.21
(1,1650)	1:74:A:VAL:HG22	1:74:A:VAL:HB	1	0.21
(1,1606)	1:130:A:LEU:HB2	1:130:A:LEU:HD21	3	0.21
(1,1573)	1:137:A:VAL:HA	1:137:A:VAL:HG21	10	0.21
(1,1432)	1:117:A:ILE:HD13	1:117:A:ILE:HG13	2	0.21
(1,1432)	1:117:A:ILE:HD12	1:117:A:ILE:HG13	5	0.21
(1,1428)	1:106:A:ILE:HD13	1:102:A:LYS:HB3	2	0.21
(1,1411)	1:116:A:GLU:HG3	1:151:A:ASN:H	10	0.21
(1,1392)	1:144:A:ILE:HG12	1:144:A:ILE:H	6	0.21
(1,1266)	1:107:A:SER:H	1:106:A:ILE:HG21	4	0.21
(1,1266)	1:107:A:SER:H	1:106:A:ILE:HG21	7	0.21
(1,1265)	1:107:A:SER:H	1:108:A:GLU:HG3	7	0.21
(1,1236)	1:99:A:LEU:HD13	1:99:A:LEU:H	6	0.21
(1,1236)	1:99:A:LEU:HD13	1:99:A:LEU:H	7	0.21
(1,1236)	1:99:A:LEU:HD13	1:99:A:LEU:H	9	0.21
(1,1140)	1:82:A:GLN:HG2	1:82:A:GLN:H	10	0.21
(1,1060)	1:116:A:GLU:HG2	1:116:A:GLU:H	6	0.21
(1,958)	1:121:A:LEU:H	1:126:A:LEU:HB3	8	0.21
(1,949)	1:100:A:GLN:H	1:99:A:LEU:HD13	8	0.21
(1,787)	1:120:A:LEU:HG	1:120:A:LEU:HD23	4	0.21
(1,787)	1:120:A:LEU:HG	1:120:A:LEU:HD23	9	0.21
(1,785)	1:122:A:LYS:HD3	1:121:A:LEU:HD12	7	0.21
(1,761)	1:106:A:ILE:HA	1:106:A:ILE:HG23	6	0.21
(1,756)	1:146:A:VAL:HG21	1:119:A:LEU:HA	4	0.21
(1,624)	1:141:A:ASN:HB3	1:121:A:LEU:HD13	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,585)	1:91:A:ASP:HB3	1:92:A:PHE:HA	4	0.21
(1,531)	1:137:A:VAL:HA	1:138:A:THR:HG23	8	0.21
(1,281)	1:120:A:LEU:HB2	1:145:A:THR:HB	1	0.21
(1,184)	1:130:A:LEU:HD21	1:130:A:LEU:H	5	0.21
(1,144)	1:140:A:ALA:HB2	1:140:A:ALA:HA	3	0.21
(1,144)	1:140:A:ALA:HB3	1:140:A:ALA:HA	9	0.21
(1,119)	1:97:A:THR:HG22	1:131:A:PHE:HD1	9	0.21
(1,111)	1:126:A:LEU:HD11	1:124:A:LYS:HE2	8	0.21
(1,26)	1:144:A:ILE:HD11	1:121:A:LEU:H	8	0.21
(1,10)	1:120:A:LEU:HD12	1:120:A:LEU:HG	5	0.21
(1,5)	1:119:A:LEU:HD23	1:102:A:LYS:H	7	0.21
(1,4186)	1:120:A:LEU:HG	2:35:C:VAL:H	1	0.2
(1,4185)	1:120:A:LEU:HG	2:35:C:VAL:H	1	0.2
(1,4014)	2:60:B:PHE:HD1	2:8:B:ILE:HD13	8	0.2
(1,3955)	2:5:C:LYS:HD3	2:19:B:ILE:HD11	10	0.2
(1,3815)	2:5:C:LYS:HG2	2:5:C:LYS:H	10	0.2
(1,3797)	2:8:C:ILE:HG23	2:9:C:ALA:HB1	7	0.2
(1,3725)	2:25:C:ILE:HG23	2:19:C:ILE:HB	1	0.2
(1,3623)	2:40:C:ILE:HA	2:33:B:LEU:HG	4	0.2
(1,3567)	2:19:C:ILE:HD12	2:5:B:LYS:HG2	1	0.2
(1,3563)	2:8:C:ILE:HD13	2:11:C:LEU:HA	1	0.2
(1,3562)	2:8:B:ILE:HD11	2:9:B:ALA:HA	2	0.2
(1,3559)	2:25:C:ILE:HD13	2:25:C:ILE:HG12	5	0.2
(1,3558)	2:25:B:ILE:HD13	2:25:B:ILE:HG12	6	0.2
(1,3558)	2:25:B:ILE:HD12	2:25:B:ILE:HG12	9	0.2
(1,3252)	2:21:B:GLU:HB3	2:21:B:GLU:H	7	0.2
(1,3231)	2:20:C:VAL:H	2:25:C:ILE:HG22	5	0.2
(1,3230)	2:20:B:VAL:H	2:25:B:ILE:HG21	3	0.2
(1,3139)	2:2:C:SER:H	2:3:C:ALA:H	5	0.2
(1,2962)	2:48:B:ARG:HG3	2:48:B:ARG:H	2	0.2
(1,2946)	2:44:B:PHE:HB2	2:46:B:PHE:HE2	2	0.2
(1,2910)	2:19:B:ILE:HD13	2:16:B:PHE:H	2	0.2
(1,2880)	2:33:B:LEU:HD11	2:19:B:ILE:HD12	8	0.2
(1,2836)	2:40:B:ILE:HB	2:13:B:VAL:HG12	7	0.2
(1,2784)	2:51:B:VAL:HG22	2:14:B:ASN:H	8	0.2
(1,2640)	2:33:B:LEU:HD11	2:20:B:VAL:HG11	5	0.2
(1,2598)	2:13:B:VAL:HG12	2:41:B:SER:HA	6	0.2
(1,2489)	2:68:C:ILE:HG22	2:68:C:ILE:HG13	9	0.2
(1,2488)	2:68:B:ILE:HG22	2:68:B:ILE:HG13	2	0.2
(1,2475)	2:12:C:ILE:HG23	2:40:C:ILE:HD11	9	0.2
(1,2423)	2:25:C:ILE:HD12	2:44:B:PHE:HZ	1	0.2
(1,2309)	2:52:C:SER:HA	2:55:C:LEU:HD13	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2309)	2:52:C:SER:HA	2:55:C:LEU:HD12	6	0.2
(1,2308)	2:52:B:SER:HA	2:55:B:LEU:HD11	5	0.2
(1,2299)	2:19:C:ILE:HA	2:22:C:LYS:HD3	3	0.2
(1,2297)	2:19:C:ILE:HA	2:22:C:LYS:HB2	1	0.2
(1,2152)	2:48:B:ARG:HD3	2:48:B:ARG:HB3	7	0.2
(1,2067)	2:55:C:LEU:HD22	2:55:C:LEU:HG	1	0.2
(1,2067)	2:55:C:LEU:HD22	2:55:C:LEU:HG	5	0.2
(1,2066)	2:55:B:LEU:HD22	2:55:B:LEU:HG	6	0.2
(1,2066)	2:55:B:LEU:HD22	2:55:B:LEU:HG	7	0.2
(1,2066)	2:55:B:LEU:HD23	2:55:B:LEU:HG	10	0.2
(1,1854)	2:16:B:PHE:HB2	2:16:B:PHE:H	6	0.2
(1,1803)	1:82:A:GLN:HE21	1:81:A:ILE:HG22	9	0.2
(1,1761)	1:82:A:GLN:H	1:80:A:LYS:HD2	5	0.2
(1,1699)	1:98:A:ILE:HG22	1:128:A:ASP:H	5	0.2
(1,1683)	1:77:A:THR:H	1:76:A:LEU:HD11	1	0.2
(1,1609)	1:114:A:ILE:HB	1:114:A:ILE:HG23	2	0.2
(1,1550)	1:85:A:LYS:HA	1:85:A:LYS:HG3	6	0.2
(1,1460)	1:120:A:LEU:HD22	1:125:A:VAL:HA	3	0.2
(1,1432)	1:117:A:ILE:HD12	1:117:A:ILE:HG13	1	0.2
(1,1193)	1:112:A:SER:HB3	1:113:A:HIS:H	5	0.2
(1,1179)	1:82:A:GLN:H	1:80:A:LYS:HD2	2	0.2
(1,1157)	1:152:A:LEU:HA	1:152:A:LEU:H	4	0.2
(1,1157)	1:152:A:LEU:HA	1:152:A:LEU:H	9	0.2
(1,1033)	1:106:A:ILE:HG13	1:106:A:ILE:H	4	0.2
(1,833)	1:105:A:LEU:HD11	1:105:A:LEU:HG	10	0.2
(1,787)	1:120:A:LEU:HG	1:120:A:LEU:HD22	10	0.2
(1,769)	1:132:A:LEU:HA	1:135:A:LEU:HD13	2	0.2
(1,761)	1:106:A:ILE:HA	1:106:A:ILE:HG23	9	0.2
(1,756)	1:146:A:VAL:HG21	1:119:A:LEU:HA	10	0.2
(1,723)	1:111:A:ALA:HA	1:148:A:ILE:HD13	3	0.2
(1,722)	1:148:A:ILE:HA	1:148:A:ILE:HD11	9	0.2
(1,513)	1:145:A:THR:HB	1:120:A:LEU:HD22	5	0.2
(1,209)	1:151:A:ASN:HB3	1:151:A:ASN:HD21	6	0.2
(1,114)	1:77:A:THR:HG23	1:79:A:LYS:H	3	0.2
(1,112)	1:77:A:THR:HG23	1:78:A:LEU:H	8	0.2
(1,16)	1:98:A:ILE:HD11	1:98:A:ILE:HG12	8	0.2
(1,10)	1:120:A:LEU:HD12	1:120:A:LEU:HG	4	0.2
(3,33)	1:149:A:LYS:H	1:116:A:GLU:O	5	0.19
(1,4186)	1:120:A:LEU:HG	2:35:C:VAL:H	10	0.19
(1,4185)	1:120:A:LEU:HG	2:35:C:VAL:H	10	0.19
(1,4161)	2:38:C:ASP:H	2:40:C:ILE:HD12	10	0.19
(1,3910)	2:12:B:ILE:HG13	2:11:B:LEU:H	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3891)	2:18:C:SER:HB3	2:19:C:ILE:HG12	7	0.19
(1,3797)	2:8:C:ILE:HG23	2:9:C:ALA:HB1	2	0.19
(1,3727)	2:25:C:ILE:HG21	2:25:C:ILE:HG12	1	0.19
(1,3629)	2:18:C:SER:HB3	2:19:C:ILE:HD13	8	0.19
(1,3559)	2:25:C:ILE:HD11	2:25:C:ILE:HG12	1	0.19
(1,3559)	2:25:C:ILE:HD11	2:25:C:ILE:HG12	6	0.19
(1,3558)	2:25:B:ILE:HD12	2:25:B:ILE:HG12	1	0.19
(1,3558)	2:25:B:ILE:HD12	2:25:B:ILE:HG12	7	0.19
(1,3550)	2:25:B:ILE:HD11	2:5:C:LYS:HE3	6	0.19
(1,3232)	2:72:B:ALA:H	2:72:B:ALA:HB2	1	0.19
(1,3182)	2:12:B:ILE:HD12	2:9:B:ALA:H	6	0.19
(1,3154)	2:4:B:SER:HB3	2:6:B:GLU:H	3	0.19
(1,3068)	2:39:B:CYS:H	2:35:B:VAL:HB	10	0.19
(1,3050)	2:16:B:PHE:HB3	2:16:B:PHE:H	2	0.19
(1,3019)	2:9:C:ALA:H	2:9:C:ALA:HB3	6	0.19
(1,2978)	2:25:B:ILE:HD12	2:30:B:ALA:H	8	0.19
(1,2947)	2:44:C:PHE:HB2	2:46:C:PHE:HE1	4	0.19
(1,2947)	2:44:C:PHE:HB2	2:46:C:PHE:HE1	9	0.19
(1,2941)	2:44:C:PHE:HZ	2:33:B:LEU:HD23	5	0.19
(1,2940)	2:44:B:PHE:HZ	2:33:C:LEU:HD22	5	0.19
(1,2784)	2:51:B:VAL:HG22	2:14:B:ASN:H	7	0.19
(1,2702)	2:13:B:VAL:HA	2:40:B:ILE:HD11	8	0.19
(1,2631)	2:51:C:VAL:HB	2:55:C:LEU:HG	10	0.19
(1,2585)	2:49:C:GLU:HG3	2:49:C:GLU:HA	5	0.19
(1,2565)	2:33:C:LEU:HD12	2:19:C:ILE:HG21	4	0.19
(1,2489)	2:68:C:ILE:HG22	2:68:C:ILE:HG13	7	0.19
(1,2489)	2:68:C:ILE:HG23	2:68:C:ILE:HG13	8	0.19
(1,2483)	2:25:C:ILE:HB	2:19:C:ILE:HG23	5	0.19
(1,2356)	2:49:B:GLU:HG2	2:49:B:GLU:H	5	0.19
(1,2347)	2:44:C:PHE:HB2	2:46:C:PHE:HD1	5	0.19
(1,2258)	2:51:B:VAL:HA	2:54:B:ILE:HB	4	0.19
(1,2067)	2:55:C:LEU:HD21	2:55:C:LEU:HG	7	0.19
(1,2067)	2:55:C:LEU:HD21	2:55:C:LEU:HG	9	0.19
(1,2060)	2:55:B:LEU:HD21	2:14:B:ASN:H	2	0.19
(1,2013)	2:47:C:GLU:HG3	2:47:C:GLU:H	3	0.19
(1,1845)	2:13:C:VAL:HA	2:13:C:VAL:HG22	10	0.19
(1,1810)	1:99:A:LEU:HG	1:103:A:GLN:HE21	3	0.19
(1,1793)	1:141:A:ASN:HB2	1:138:A:THR:H	3	0.19
(1,1766)	1:135:A:LEU:H	1:126:A:LEU:HD12	10	0.19
(1,1609)	1:114:A:ILE:HB	1:114:A:ILE:HG22	8	0.19
(1,1532)	1:151:A:ASN:HA	1:152:A:LEU:HG	9	0.19
(1,1295)	1:129:A:ASN:H	1:97:A:THR:HB	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1266)	1:107:A:SER:H	1:106:A:ILE:HG21	9	0.19
(1,1157)	1:152:A:LEU:HA	1:152:A:LEU:H	8	0.19
(1,1070)	1:111:A:ALA:HB2	1:111:A:ALA:H	10	0.19
(1,958)	1:121:A:LEU:H	1:126:A:LEU:HB3	5	0.19
(1,889)	1:130:A:LEU:HB3	1:130:A:LEU:H	3	0.19
(1,868)	1:144:A:ILE:HG23	1:145:A:THR:H	7	0.19
(1,833)	1:105:A:LEU:HD12	1:105:A:LEU:HG	2	0.19
(1,809)	1:126:A:LEU:HB2	1:126:A:LEU:H	10	0.19
(1,779)	1:74:A:VAL:HG11	1:74:A:VAL:HB	8	0.19
(1,673)	1:81:A:ILE:HG13	1:145:A:THR:HA	6	0.19
(1,652)	1:146:A:VAL:HB	1:146:A:VAL:HG23	2	0.19
(1,652)	1:146:A:VAL:HB	1:146:A:VAL:HG22	7	0.19
(1,585)	1:91:A:ASP:HB3	1:92:A:PHE:HA	9	0.19
(1,547)	1:150:A:PRO:HD3	1:149:A:LYS:HA	4	0.19
(1,506)	1:112:A:SER:HA	1:106:A:ILE:HD11	5	0.19
(1,281)	1:120:A:LEU:HB2	1:145:A:THR:HB	6	0.19
(1,209)	1:151:A:ASN:HB3	1:151:A:ASN:HD21	10	0.19
(1,186)	1:120:A:LEU:HD21	1:120:A:LEU:H	3	0.19
(1,184)	1:130:A:LEU:HD21	1:130:A:LEU:H	10	0.19
(1,182)	1:132:A:LEU:HD12	1:92:A:PHE:HA	4	0.19
(1,144)	1:140:A:ALA:HB3	1:140:A:ALA:HA	1	0.19
(1,144)	1:140:A:ALA:HB3	1:140:A:ALA:HA	4	0.19
(1,144)	1:140:A:ALA:HB3	1:140:A:ALA:HA	6	0.19
(1,121)	1:111:A:ALA:HB1	1:112:A:SER:H	6	0.19
(1,112)	1:77:A:THR:HG23	1:78:A:LEU:H	3	0.19
(1,27)	1:144:A:ILE:HD12	1:143:A:THR:H	9	0.19
(1,16)	1:98:A:ILE:HD11	1:98:A:ILE:HG12	9	0.19
(1,16)	1:98:A:ILE:HD13	1:98:A:ILE:HG12	10	0.19
(1,10)	1:120:A:LEU:HD11	1:120:A:LEU:HG	2	0.19
(1,10)	1:120:A:LEU:HD12	1:120:A:LEU:HG	6	0.19
(1,10)	1:120:A:LEU:HD11	1:120:A:LEU:HG	10	0.19
(3,89)	2:38:B:ASP:H	2:34:B:ASN:O	2	0.18
(1,4177)	1:147:A:MET:HG3	2:35:B:VAL:HG22	5	0.18
(1,4177)	1:147:A:MET:HE2	2:35:C:VAL:HG11	6	0.18
(1,4176)	1:145:A:THR:HG21	2:35:C:VAL:HG11	8	0.18
(1,4176)	1:145:A:THR:OG1	2:35:C:VAL:HG22	9	0.18
(1,4008)	2:44:B:PHE:HZ	2:19:C:ILE:HG23	6	0.18
(1,4003)	2:44:C:PHE:HZ	2:25:B:ILE:HG21	1	0.18
(1,3970)	2:8:B:ILE:HD13	2:60:B:PHE:HE1	6	0.18
(1,3968)	2:25:B:ILE:HG21	2:32:B:SER:H	5	0.18
(1,3963)	2:36:C:ALA:HB2	2:40:B:ILE:HA	7	0.18
(1,3891)	2:18:C:SER:HB3	2:22:C:LYS:HG3	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3850)	2:40:B:ILE:HG23	2:13:B:VAL:HB	10	0.18
(1,3803)	2:3:C:ALA:HB1	2:7:C:GLU:H	5	0.18
(1,3730)	2:12:B:ILE:HD11	2:13:B:VAL:HG11	8	0.18
(1,3728)	2:12:B:ILE:HD12	2:12:C:ILE:HA	9	0.18
(1,3726)	2:25:B:ILE:HG23	2:30:B:ALA:HB1	3	0.18
(1,3717)	2:19:C:ILE:HG21	2:19:C:ILE:HG12	8	0.18
(1,3605)	2:34:C:ASN:HA	2:20:C:VAL:HG11	5	0.18
(1,3563)	2:8:C:ILE:HD12	2:9:C:ALA:HA	2	0.18
(1,3560)	2:25:B:ILE:HD12	2:25:B:ILE:HG13	10	0.18
(1,3559)	2:25:C:ILE:HD11	2:25:C:ILE:HG12	7	0.18
(1,3559)	2:25:C:ILE:HD11	2:25:C:ILE:HG12	9	0.18
(1,3559)	2:25:C:ILE:HD11	2:25:C:ILE:HG12	10	0.18
(1,3527)	2:6:C:GLU:HG2	2:46:C:PHE:HD2	3	0.18
(1,3526)	2:6:B:GLU:HG2	2:46:B:PHE:HD2	2	0.18
(1,3196)	2:14:B:ASN:H	2:48:B:ARG:HA	2	0.18
(1,3051)	2:16:C:PHE:HB3	2:16:C:PHE:H	3	0.18
(1,3051)	2:16:C:PHE:HB3	2:16:C:PHE:H	8	0.18
(1,3048)	2:50:B:ALA:H	2:13:B:VAL:HG13	7	0.18
(1,3045)	2:47:C:GLU:HB2	2:50:C:ALA:H	5	0.18
(1,3014)	2:5:B:LYS:HG2	2:5:B:LYS:H	10	0.18
(1,2937)	2:6:C:GLU:HG2	2:44:C:PHE:HD1	1	0.18
(1,2821)	2:5:C:LYS:HE2	2:24:B:GLU:HB3	9	0.18
(1,2810)	2:25:B:ILE:HA	2:33:B:LEU:HD12	3	0.18
(1,2615)	2:13:C:VAL:HG11	2:48:C:ARG:HG2	6	0.18
(1,2556)	2:35:B:VAL:HG11	2:36:B:ALA:HB1	3	0.18
(1,2520)	2:51:B:VAL:HA	2:54:B:ILE:HD13	7	0.18
(1,2512)	2:54:B:ILE:HD12	2:54:B:ILE:HG22	8	0.18
(1,2498)	2:25:B:ILE:HG22	2:20:B:VAL:HG11	3	0.18
(1,2497)	2:25:C:ILE:HG22	2:24:C:GLU:HB2	5	0.18
(1,2488)	2:68:B:ILE:HG23	2:68:B:ILE:HG13	4	0.18
(1,2381)	2:55:C:LEU:HD13	2:60:C:PHE:HD2	8	0.18
(1,2356)	2:49:B:GLU:HG2	2:49:B:GLU:H	9	0.18
(1,2346)	2:44:B:PHE:HB2	2:46:B:PHE:HD1	2	0.18
(1,2270)	2:20:B:VAL:HA	2:25:B:ILE:HG23	4	0.18
(1,2066)	2:55:B:LEU:HD22	2:55:B:LEU:HG	3	0.18
(1,1854)	2:16:B:PHE:HB2	2:16:B:PHE:H	3	0.18
(1,1854)	2:16:B:PHE:HB2	2:16:B:PHE:H	4	0.18
(1,1723)	1:102:A:LYS:H	1:117:A:ILE:HD11	6	0.18
(1,1639)	1:148:A:ILE:HD12	1:148:A:ILE:H	9	0.18
(1,1532)	1:151:A:ASN:HA	1:152:A:LEU:HG	6	0.18
(1,1458)	1:126:A:LEU:HD23	1:126:A:LEU:HA	1	0.18
(1,1432)	1:117:A:ILE:HD12	1:117:A:ILE:HG13	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1428)	1:106:A:ILE:HD12	1:102:A:LYS:HB3	3	0.18
(1,1351)	1:141:A:ASN:HD21	1:121:A:LEU:HG	1	0.18
(1,1339)	1:103:A:GLN:HG2	1:103:A:GLN:HE21	8	0.18
(1,1157)	1:152:A:LEU:HA	1:152:A:LEU:H	10	0.18
(1,1081)	1:140:A:ALA:HB1	1:141:A:ASN:H	3	0.18
(1,1081)	1:140:A:ALA:HB1	1:141:A:ASN:H	7	0.18
(1,787)	1:120:A:LEU:HG	1:120:A:LEU:HD23	6	0.18
(1,727)	1:88:A:ILE:HG12	1:86:A:PHE:HD2	6	0.18
(1,652)	1:146:A:VAL:HB	1:146:A:VAL:HG22	3	0.18
(1,652)	1:146:A:VAL:HB	1:146:A:VAL:HG23	8	0.18
(1,652)	1:146:A:VAL:HB	1:146:A:VAL:HG22	9	0.18
(1,610)	1:108:A:GLU:HG3	1:107:A:SER:HB3	7	0.18
(1,209)	1:151:A:ASN:HB3	1:151:A:ASN:HD21	3	0.18
(1,196)	1:117:A:ILE:HG21	1:119:A:LEU:HA	4	0.18
(1,193)	1:117:A:ILE:HG23	1:118:A:LYS:H	4	0.18
(1,177)	1:132:A:LEU:HD23	1:97:A:THR:HA	4	0.18
(1,155)	1:135:A:LEU:HD12	1:137:A:VAL:H	10	0.18
(1,144)	1:140:A:ALA:HB3	1:140:A:ALA:HA	8	0.18
(1,144)	1:140:A:ALA:HB2	1:140:A:ALA:HA	10	0.18
(1,116)	1:125:A:VAL:HG22	1:120:A:LEU:H	9	0.18
(1,113)	1:77:A:THR:HG21	1:88:A:ILE:H	2	0.18
(1,111)	1:126:A:LEU:HD11	1:124:A:LYS:HE2	4	0.18
(1,75)	1:98:A:ILE:HG22	1:128:A:ASP:HA	8	0.18
(1,51)	1:88:A:ILE:HD12	1:92:A:PHE:HZ	8	0.18
(1,29)	1:144:A:ILE:HD11	1:144:A:ILE:HA	10	0.18
(1,10)	1:120:A:LEU:HD12	1:120:A:LEU:HG	7	0.18
(3,89)	2:38:B:ASP:H	2:34:B:ASN:O	3	0.17
(1,4009)	2:16:C:PHE:HZ	2:12:B:ILE:HG22	5	0.17
(1,3954)	2:5:B:LYS:HD3	2:19:C:ILE:HG23	7	0.17
(1,3822)	2:40:B:ILE:HD11	2:36:B:ALA:HA	4	0.17
(1,3727)	2:25:C:ILE:HG23	2:25:C:ILE:HG12	6	0.17
(1,3717)	2:19:C:ILE:HG21	2:19:C:ILE:HG12	2	0.17
(1,3716)	2:19:B:ILE:HG21	2:19:B:ILE:HG12	10	0.17
(1,3692)	2:9:B:ALA:HA	2:46:B:PHE:HE1	1	0.17
(1,3589)	2:5:C:LYS:HE2	2:19:B:ILE:HD11	10	0.17
(1,3574)	2:33:B:LEU:HD23	2:43:C:ALA:HB1	10	0.17
(1,3560)	2:25:B:ILE:HD11	2:43:C:ALA:HB1	4	0.17
(1,3558)	2:25:B:ILE:HD12	2:25:B:ILE:HG12	5	0.17
(1,3421)	2:51:C:VAL:H	2:54:C:ILE:HG12	9	0.17
(1,3321)	2:19:C:ILE:HG22	2:26:C:SER:H	4	0.17
(1,3155)	2:4:C:SER:HB3	2:6:C:GLU:H	6	0.17
(1,3139)	2:2:C:SER:H	2:3:C:ALA:H	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3051)	2:16:C:PHE:HB3	2:16:C:PHE:H	2	0.17
(1,3050)	2:16:B:PHE:HB3	2:16:B:PHE:H	9	0.17
(1,3019)	2:9:C:ALA:H	2:9:C:ALA:HB3	1	0.17
(1,3019)	2:9:C:ALA:H	2:9:C:ALA:HB1	4	0.17
(1,3018)	2:9:B:ALA:H	2:9:B:ALA:HB3	3	0.17
(1,3018)	2:9:B:ALA:H	2:9:B:ALA:HB3	7	0.17
(1,3018)	2:9:B:ALA:H	2:9:B:ALA:HB2	10	0.17
(1,2881)	2:33:C:LEU:HD12	2:19:C:ILE:HD11	10	0.17
(1,2862)	2:37:B:MET:HA	2:37:B:MET:HG2	4	0.17
(1,2786)	2:20:B:VAL:HG13	2:34:B:ASN:HD22	1	0.17
(1,2784)	2:51:B:VAL:HG22	2:14:B:ASN:H	6	0.17
(1,2558)	2:55:B:LEU:HD22	2:13:B:VAL:HG21	9	0.17
(1,2489)	2:68:C:ILE:HG21	2:68:C:ILE:HG13	1	0.17
(1,2465)	2:71:C:SER:HB3	2:71:C:SER:H	7	0.17
(1,2422)	2:25:B:ILE:HD12	2:44:C:PHE:HZ	10	0.17
(1,2405)	2:8:C:ILE:HG21	2:15:B:TYR:H	1	0.17
(1,2404)	2:8:B:ILE:HG22	2:15:C:TYR:H	3	0.17
(1,2389)	2:20:C:VAL:HG22	2:34:C:ASN:HD22	6	0.17
(1,2346)	2:44:B:PHE:HB2	2:46:B:PHE:HD1	8	0.17
(1,2149)	2:5:C:LYS:HE3	2:25:B:ILE:HG23	1	0.17
(1,2070)	2:51:B:VAL:HG22	2:14:B:ASN:HA	7	0.17
(1,2067)	2:55:C:LEU:HD21	2:55:C:LEU:HG	8	0.17
(1,2066)	2:55:B:LEU:HD22	2:55:B:LEU:HG	2	0.17
(1,1892)	2:23:B:LYS:HA	2:23:B:LYS:HG3	6	0.17
(1,1845)	2:13:C:VAL:HA	2:13:C:VAL:HG21	9	0.17
(1,1844)	2:13:B:VAL:HA	2:13:B:VAL:HG21	3	0.17
(1,1844)	2:13:B:VAL:HA	2:13:B:VAL:HG21	10	0.17
(1,1789)	1:126:A:LEU:HD11	1:127:A:HIS:H	10	0.17
(1,1771)	1:81:A:ILE:HG12	1:81:A:ILE:H	7	0.17
(1,1707)	1:144:A:ILE:HG23	1:120:A:LEU:H	9	0.17
(1,1616)	1:83:A:ALA:HB2	1:84:A:PRO:HB2	5	0.17
(1,1609)	1:114:A:ILE:HB	1:114:A:ILE:HG23	5	0.17
(1,1609)	1:114:A:ILE:HB	1:114:A:ILE:HG22	10	0.17
(1,1528)	1:121:A:LEU:HA	1:122:A:LYS:HB3	6	0.17
(1,1465)	1:117:A:ILE:HG22	1:102:A:LYS:HB3	4	0.17
(1,1438)	1:101:A:ILE:HG23	1:78:A:LEU:HB3	6	0.17
(1,1432)	1:117:A:ILE:HD12	1:117:A:ILE:HG13	3	0.17
(1,1392)	1:144:A:ILE:HG12	1:144:A:ILE:H	3	0.17
(1,1157)	1:152:A:LEU:HA	1:152:A:LEU:H	7	0.17
(1,1141)	1:82:A:GLN:H	1:80:A:LYS:HG2	5	0.17
(1,1132)	1:126:A:LEU:H	1:126:A:LEU:HB3	6	0.17
(1,1081)	1:140:A:ALA:HB3	1:141:A:ASN:H	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,869)	1:144:A:ILE:HD11	1:145:A:THR:H	7	0.17
(1,833)	1:105:A:LEU:HD11	1:105:A:LEU:HG	6	0.17
(1,833)	1:105:A:LEU:HD13	1:105:A:LEU:HG	9	0.17
(1,760)	1:106:A:ILE:HG21	1:107:A:SER:HA	5	0.17
(1,738)	1:115:A:SER:HA	1:114:A:ILE:HG13	4	0.17
(1,738)	1:115:A:SER:HA	1:114:A:ILE:HG13	9	0.17
(1,724)	1:148:A:ILE:HD13	1:80:A:LYS:HE3	7	0.17
(1,683)	1:106:A:ILE:HG12	1:106:A:ILE:H	10	0.17
(1,669)	1:103:A:GLN:HG3	1:99:A:LEU:HD11	6	0.17
(1,652)	1:146:A:VAL:HB	1:146:A:VAL:HG22	1	0.17
(1,638)	1:132:A:LEU:HB3	1:135:A:LEU:HD12	5	0.17
(1,511)	1:139:A:PRO:HD2	1:138:A:THR:HB	6	0.17
(1,461)	1:96:A:ASP:HA	1:97:A:THR:HG22	2	0.17
(1,265)	1:114:A:ILE:HG12	1:103:A:GLN:HE22	3	0.17
(1,261)	1:129:A:ASN:HB2	1:129:A:ASN:HD21	7	0.17
(1,210)	1:151:A:ASN:HB2	1:151:A:ASN:HD21	2	0.17
(1,201)	1:144:A:ILE:HG23	1:120:A:LEU:H	9	0.17
(1,180)	1:132:A:LEU:HD11	1:96:A:ASP:HB2	8	0.17
(1,67)	1:83:A:ALA:HB2	1:85:A:LYS:H	10	0.17
(1,4183)	1:120:A:LEU:HD12	2:35:B:VAL:H	3	0.16
(1,4175)	1:125:A:VAL:HG13	2:31:B:ASP:HB3	2	0.16
(1,4009)	2:44:C:PHE:HZ	2:19:B:ILE:HG23	8	0.16
(1,3727)	2:25:C:ILE:HG21	2:30:C:ALA:HB2	10	0.16
(1,3726)	2:25:B:ILE:HG22	2:30:B:ALA:HB2	9	0.16
(1,3717)	2:19:C:ILE:HG23	2:19:C:ILE:HG12	6	0.16
(1,3717)	2:19:C:ILE:HG21	2:19:C:ILE:HG12	9	0.16
(1,3716)	2:19:B:ILE:HG21	2:19:B:ILE:HG12	9	0.16
(1,3477)	2:55:C:LEU:HD23	2:14:C:ASN:HD21	10	0.16
(1,3476)	2:55:B:LEU:HD21	2:14:B:ASN:HD21	4	0.16
(1,3420)	2:51:B:VAL:H	2:54:B:ILE:HG12	10	0.16
(1,3317)	2:26:C:SER:H	2:33:C:LEU:HD11	9	0.16
(1,3232)	2:72:B:ALA:H	2:72:B:ALA:HB2	10	0.16
(1,3205)	2:50:C:ALA:H	2:51:C:VAL:H	9	0.16
(1,3152)	2:6:B:GLU:HG3	2:6:B:GLU:H	1	0.16
(1,3051)	2:16:C:PHE:HB3	2:16:C:PHE:H	5	0.16
(1,3051)	2:16:C:PHE:HB3	2:16:C:PHE:H	10	0.16
(1,3050)	2:16:B:PHE:HB3	2:16:B:PHE:H	1	0.16
(1,3050)	2:16:B:PHE:HB3	2:16:B:PHE:H	5	0.16
(1,3050)	2:16:B:PHE:HB3	2:16:B:PHE:H	8	0.16
(1,3050)	2:16:B:PHE:HB3	2:16:B:PHE:H	10	0.16
(1,2876)	2:13:B:VAL:HB	2:14:B:ASN:HA	8	0.16
(1,2820)	2:5:B:LYS:HE2	2:24:C:GLU:HB3	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2653)	2:8:C:ILE:HG22	2:3:C:ALA:HB3	8	0.16
(1,2614)	2:13:B:VAL:HG12	2:48:B:ARG:HG2	10	0.16
(1,2598)	2:13:B:VAL:HG13	2:41:B:SER:HA	3	0.16
(1,2598)	2:13:B:VAL:HG12	2:41:B:SER:HA	10	0.16
(1,2563)	2:11:C:LEU:HD21	2:55:C:LEU:HD22	7	0.16
(1,2489)	2:68:C:ILE:HG23	2:68:C:ILE:HG13	2	0.16
(1,2488)	2:68:B:ILE:HG21	2:68:B:ILE:HG13	5	0.16
(1,2488)	2:68:B:ILE:HG21	2:68:B:ILE:HG13	8	0.16
(1,2475)	2:12:C:ILE:HG21	2:40:C:ILE:HD11	1	0.16
(1,2475)	2:12:C:ILE:HG23	2:40:C:ILE:HD11	10	0.16
(1,2472)	2:12:B:ILE:HG22	2:13:B:VAL:HG13	4	0.16
(1,2405)	2:8:C:ILE:HG21	2:15:B:TYR:H	6	0.16
(1,2315)	2:37:C:MET:HA	2:40:C:ILE:HD13	2	0.16
(1,2308)	2:52:B:SER:HA	2:55:B:LEU:HD13	2	0.16
(1,2188)	2:30:B:ALA:HA	2:25:B:ILE:HG22	3	0.16
(1,2187)	2:30:C:ALA:HA	2:20:C:VAL:HG13	10	0.16
(1,2152)	2:48:B:ARG:HD3	2:48:B:ARG:HB3	2	0.16
(1,2152)	2:48:B:ARG:HD3	2:48:B:ARG:HB3	8	0.16
(1,2113)	2:13:C:VAL:HG22	2:51:C:VAL:HB	10	0.16
(1,2085)	2:25:C:ILE:HD11	2:25:C:ILE:HG21	4	0.16
(1,1893)	2:23:C:LYS:HA	2:23:C:LYS:HG3	3	0.16
(1,1892)	2:23:B:LYS:HA	2:23:B:LYS:HG3	8	0.16
(1,1844)	2:13:B:VAL:HA	2:13:B:VAL:HG23	1	0.16
(1,1808)	1:103:A:GLN:HE22	1:114:A:ILE:HG13	10	0.16
(1,1792)	1:141:A:ASN:HB3	1:138:A:THR:H	6	0.16
(1,1789)	1:126:A:LEU:HD11	1:127:A:HIS:H	3	0.16
(1,1789)	1:127:A:HIS:H	1:98:A:ILE:HG23	9	0.16
(1,1719)	1:93:A:SER:HB3	1:95:A:SER:H	5	0.16
(1,1616)	1:83:A:ALA:HB1	1:84:A:PRO:HB2	2	0.16
(1,1432)	1:117:A:ILE:HD12	1:117:A:ILE:HG13	8	0.16
(1,1428)	1:106:A:ILE:HD11	1:102:A:LYS:HB3	9	0.16
(1,1350)	1:141:A:ASN:HB3	1:141:A:ASN:HD21	7	0.16
(1,1159)	1:152:A:LEU:HG	1:152:A:LEU:H	4	0.16
(1,1133)	1:126:A:LEU:HD12	1:126:A:LEU:H	5	0.16
(1,1081)	1:140:A:ALA:HB1	1:141:A:ASN:H	1	0.16
(1,1060)	1:116:A:GLU:HG2	1:116:A:GLU:H	1	0.16
(1,833)	1:105:A:LEU:HD12	1:105:A:LEU:HG	5	0.16
(1,795)	1:80:A:LYS:HE3	1:86:A:PHE:HZ	7	0.16
(1,787)	1:120:A:LEU:HG	1:120:A:LEU:HD21	1	0.16
(1,787)	1:120:A:LEU:HG	1:120:A:LEU:HD21	2	0.16
(1,760)	1:106:A:ILE:HG21	1:107:A:SER:HA	8	0.16
(1,756)	1:146:A:VAL:HG21	1:119:A:LEU:HA	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,749)	1:124:A:LYS:HG2	1:125:A:VAL:HA	10	0.16
(1,732)	1:81:A:ILE:HA	1:79:A:LYS:HD3	1	0.16
(1,725)	1:148:A:ILE:HD13	1:80:A:LYS:HD3	6	0.16
(1,686)	1:122:A:LYS:HA	1:122:A:LYS:HD3	6	0.16
(1,642)	1:97:A:THR:HG21	1:100:A:GLN:HG3	5	0.16
(1,638)	1:132:A:LEU:HB3	1:135:A:LEU:HD13	3	0.16
(1,625)	1:101:A:ILE:HB	1:98:A:ILE:HG21	6	0.16
(1,547)	1:150:A:PRO:HD3	1:149:A:LYS:HA	3	0.16
(1,533)	1:114:A:ILE:HA	1:114:A:ILE:HG12	8	0.16
(1,494)	1:98:A:ILE:HA	1:101:A:ILE:HG12	2	0.16
(1,231)	1:149:A:LYS:HB3	1:149:A:LYS:HE3	3	0.16
(1,182)	1:132:A:LEU:HD12	1:92:A:PHE:HA	3	0.16
(1,155)	1:135:A:LEU:HD12	1:137:A:VAL:H	9	0.16
(1,117)	1:125:A:VAL:HG22	1:126:A:LEU:H	9	0.16
(1,111)	1:126:A:LEU:HD11	1:124:A:LYS:HE2	6	0.16
(1,108)	1:126:A:LEU:HD11	1:125:A:VAL:H	2	0.16
(1,89)	1:101:A:ILE:HG23	1:119:A:LEU:HA	4	0.16
(1,26)	1:144:A:ILE:HD12	1:121:A:LEU:H	3	0.16
(1,16)	1:98:A:ILE:HD13	1:98:A:ILE:HG12	1	0.16
(1,16)	1:98:A:ILE:HD11	1:98:A:ILE:HG12	4	0.16
(1,4004)	2:44:B:PHE:HZ	2:25:C:ILE:HG22	3	0.15
(1,3983)	2:15:C:TYR:HD2	2:12:B:ILE:HD13	10	0.15
(1,3969)	2:25:C:ILE:HG22	2:32:C:SER:H	7	0.15
(1,3910)	2:12:B:ILE:HG13	2:11:B:LEU:H	1	0.15
(1,3716)	2:19:B:ILE:HG22	2:19:B:ILE:HG12	1	0.15
(1,3716)	2:19:B:ILE:HG23	2:19:B:ILE:HG12	2	0.15
(1,3575)	2:33:C:LEU:HD23	2:43:B:ALA:HB2	7	0.15
(1,3558)	2:25:B:ILE:HD12	2:25:B:ILE:HG12	3	0.15
(1,3540)	2:51:B:VAL:HG23	2:52:B:SER:HB3	8	0.15
(1,3476)	2:55:B:LEU:HD21	2:14:B:ASN:HD21	2	0.15
(1,3324)	2:27:B:GLU:HG3	2:27:B:GLU:H	7	0.15
(1,3318)	2:25:B:ILE:HG13	2:26:B:SER:H	8	0.15
(1,3233)	2:72:C:ALA:H	2:72:C:ALA:HB2	8	0.15
(1,3220)	2:34:B:ASN:HA	2:17:B:SER:H	1	0.15
(1,3175)	2:7:C:GLU:H	2:4:C:SER:HB3	3	0.15
(1,3174)	2:7:B:GLU:H	2:4:B:SER:HB3	6	0.15
(1,3158)	2:42:B:GLU:HB3	2:42:B:GLU:H	2	0.15
(1,3154)	2:4:B:SER:HB3	2:6:B:GLU:H	7	0.15
(1,3139)	2:2:C:SER:H	2:3:C:ALA:H	1	0.15
(1,3138)	2:2:B:SER:H	2:3:B:ALA:H	5	0.15
(1,3051)	2:16:C:PHE:HB3	2:16:C:PHE:H	9	0.15
(1,3050)	2:16:B:PHE:HB3	2:16:B:PHE:H	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3013)	2:5:C:LYS:HG3	2:5:C:LYS:H	9	0.15
(1,3011)	2:5:C:LYS:HB2	2:5:C:LYS:H	8	0.15
(1,2954)	2:16:B:PHE:HZ	2:12:C:ILE:HD12	8	0.15
(1,2810)	2:25:B:ILE:HA	2:33:B:LEU:HD12	6	0.15
(1,2488)	2:68:B:ILE:HG21	2:68:B:ILE:HG13	3	0.15
(1,2464)	2:71:B:SER:HB3	2:71:B:SER:H	7	0.15
(1,2405)	2:8:C:ILE:HG21	2:15:B:TYR:H	2	0.15
(1,2356)	2:49:B:GLU:HG2	2:49:B:GLU:H	1	0.15
(1,2346)	2:44:B:PHE:HB2	2:46:B:PHE:HD1	7	0.15
(1,2308)	2:52:B:SER:HA	2:55:B:LEU:HD11	9	0.15
(1,2281)	2:12:C:ILE:HA	2:12:C:ILE:HG13	5	0.15
(1,2183)	2:9:C:ALA:HA	2:40:C:ILE:HG22	7	0.15
(1,2178)	2:9:B:ALA:HA	2:12:B:ILE:HD11	2	0.15
(1,2158)	2:13:B:VAL:HG23	2:48:B:ARG:HD3	4	0.15
(1,2114)	2:13:B:VAL:HG23	2:48:B:ARG:HG2	3	0.15
(1,2062)	2:55:B:LEU:HD21	2:14:B:ASN:HB2	8	0.15
(1,1855)	2:16:C:PHE:HB2	2:16:C:PHE:H	9	0.15
(1,1844)	2:13:B:VAL:HA	2:13:B:VAL:HG21	9	0.15
(1,1829)	1:147:A:MET:H	1:119:A:LEU:HD11	7	0.15
(1,1810)	1:103:A:GLN:HE21	1:114:A:ILE:HG13	5	0.15
(1,1808)	1:103:A:GLN:HE22	1:114:A:ILE:HG13	7	0.15
(1,1801)	1:82:A:GLN:HE22	1:81:A:ILE:HG22	4	0.15
(1,1794)	1:138:A:THR:H	1:121:A:LEU:HD21	10	0.15
(1,1745)	1:82:A:GLN:H	1:81:A:ILE:HG22	9	0.15
(1,1606)	1:152:A:LEU:HB2	1:152:A:LEU:HD12	7	0.15
(1,1591)	1:87:A:SER:HB3	1:88:A:ILE:HG12	9	0.15
(1,1573)	1:137:A:VAL:HA	1:137:A:VAL:HG21	4	0.15
(1,1567)	1:143:A:THR:HB	1:144:A:ILE:HB	6	0.15
(1,1460)	1:120:A:LEU:HD22	1:125:A:VAL:HA	1	0.15
(1,1455)	1:132:A:LEU:HD23	1:94:A:PRO:HA	2	0.15
(1,1417)	1:73:A:MET:HB3	1:74:A:VAL:H	3	0.15
(1,1417)	1:73:A:MET:HB3	1:74:A:VAL:H	10	0.15
(1,1412)	1:151:A:ASN:HA	1:151:A:ASN:H	9	0.15
(1,1327)	1:100:A:GLN:HE21	1:99:A:LEU:HB2	6	0.15
(1,889)	1:130:A:LEU:HB3	1:130:A:LEU:H	4	0.15
(1,833)	1:105:A:LEU:HD11	1:105:A:LEU:HG	7	0.15
(1,769)	1:132:A:LEU:HA	1:135:A:LEU:HD13	3	0.15
(1,761)	1:106:A:ILE:HA	1:106:A:ILE:HG22	2	0.15
(1,720)	1:148:A:ILE:HD11	1:86:A:PHE:HZ	6	0.15
(1,652)	1:146:A:VAL:HB	1:146:A:VAL:HG23	10	0.15
(1,638)	1:132:A:LEU:HB3	1:135:A:LEU:HD13	9	0.15
(1,487)	1:139:A:PRO:HD2	1:138:A:THR:HA	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:132:A:LEU:HD12	1:92:A:PHE:HB2	8	0.15
(1,144)	1:140:A:ALA:HB2	1:140:A:ALA:HA	5	0.15
(1,144)	1:140:A:ALA:HB3	1:140:A:ALA:HA	7	0.15
(1,112)	1:77:A:THR:HG23	1:78:A:LEU:H	6	0.15
(1,110)	1:126:A:LEU:HD13	1:125:A:VAL:HA	3	0.15
(1,67)	1:83:A:ALA:HB2	1:85:A:LYS:H	3	0.15
(1,61)	1:117:A:ILE:HD12	1:112:A:SER:H	3	0.15
(1,61)	1:117:A:ILE:HD12	1:112:A:SER:H	6	0.15
(1,52)	1:81:A:ILE:HD13	1:81:A:ILE:H	2	0.15
(1,16)	1:98:A:ILE:HD12	1:98:A:ILE:HG12	2	0.15
(1,16)	1:98:A:ILE:HD11	1:98:A:ILE:HG12	3	0.15
(1,16)	1:98:A:ILE:HD11	1:98:A:ILE:HG12	6	0.15
(1,10)	1:120:A:LEU:HD12	1:120:A:LEU:HG	8	0.15
(3,18)	1:144:A:ILE:N	1:77:A:THR:O	9	0.14
(1,4177)	1:147:A:MET:HE1	2:35:C:VAL:HG13	4	0.14
(1,4163)	2:38:C:ASP:H	2:35:C:VAL:HG11	5	0.14
(1,4047)	2:15:C:TYR:H	2:8:B:ILE:HG22	3	0.14
(1,4008)	2:44:B:PHE:HZ	2:19:C:ILE:HG22	10	0.14
(1,3739)	2:68:C:ILE:HD13	2:11:B:LEU:HD23	8	0.14
(1,3726)	2:25:B:ILE:HG23	2:30:B:ALA:HB1	7	0.14
(1,3717)	2:19:C:ILE:HG22	2:19:C:ILE:HG12	4	0.14
(1,3658)	2:51:B:VAL:HG22	2:46:B:PHE:HE2	3	0.14
(1,3642)	2:68:B:ILE:HB	2:71:B:SER:H	9	0.14
(1,3605)	2:34:C:ASN:HA	2:20:C:VAL:HG11	1	0.14
(1,3593)	2:9:C:ALA:HA	2:12:C:ILE:HG21	4	0.14
(1,3563)	2:8:C:ILE:HD12	2:9:C:ALA:HA	8	0.14
(1,3562)	2:8:B:ILE:HD11	2:9:B:ALA:HA	3	0.14
(1,3560)	2:25:B:ILE:HD11	2:43:C:ALA:HB3	9	0.14
(1,3559)	2:25:C:ILE:HD13	2:25:C:ILE:HG12	8	0.14
(1,3558)	2:25:B:ILE:HD12	2:25:B:ILE:HG12	8	0.14
(1,3550)	2:25:B:ILE:HD11	2:5:C:LYS:HE3	8	0.14
(1,3420)	2:51:B:VAL:H	2:54:B:ILE:HG12	9	0.14
(1,3355)	2:37:C:MET:H	2:40:C:ILE:HD11	4	0.14
(1,3105)	2:51:C:VAL:HB	2:52:C:SER:H	10	0.14
(1,3050)	2:16:B:PHE:HB3	2:16:B:PHE:H	4	0.14
(1,3050)	2:16:B:PHE:HB3	2:16:B:PHE:H	6	0.14
(1,3018)	2:9:B:ALA:H	2:9:B:ALA:HB2	4	0.14
(1,2863)	2:37:C:MET:HA	2:37:C:MET:HG2	3	0.14
(1,2851)	2:26:C:SER:HB2	2:28:C:ASP:H	8	0.14
(1,2821)	2:5:C:LYS:HE2	2:24:B:GLU:HB3	8	0.14
(1,2811)	2:25:C:ILE:HA	2:33:C:LEU:HD13	2	0.14
(1,2701)	2:54:C:ILE:HG22	2:55:C:LEU:HA	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2693)	2:50:C:ALA:HB1	2:47:C:GLU:HB2	5	0.14
(1,2606)	2:35:B:VAL:HG12	2:34:B:ASN:HB2	3	0.14
(1,2556)	2:35:B:VAL:HG12	2:36:B:ALA:HB1	10	0.14
(1,2541)	2:36:C:ALA:HB1	2:33:C:LEU:HD12	2	0.14
(1,2500)	2:25:B:ILE:HG21	2:20:B:VAL:HB	6	0.14
(1,2475)	2:12:C:ILE:HG23	2:40:C:ILE:HD12	8	0.14
(1,2474)	2:12:B:ILE:HG22	2:40:B:ILE:HD13	3	0.14
(1,2473)	2:12:C:ILE:HG23	2:13:C:VAL:HG13	4	0.14
(1,2464)	2:71:B:SER:HB3	2:71:B:SER:H	3	0.14
(1,2464)	2:71:B:SER:HB3	2:71:B:SER:H	6	0.14
(1,2422)	2:25:B:ILE:HD13	2:44:C:PHE:HZ	9	0.14
(1,2405)	2:8:C:ILE:HG21	2:15:B:TYR:H	5	0.14
(1,2388)	2:20:B:VAL:HG21	2:34:B:ASN:HD22	5	0.14
(1,2380)	2:55:B:LEU:HD13	2:60:B:PHE:HD1	9	0.14
(1,2309)	2:52:C:SER:HA	2:55:C:LEU:HD11	3	0.14
(1,2271)	2:20:C:VAL:HA	2:25:C:ILE:HG21	8	0.14
(1,2270)	2:20:B:VAL:HA	2:25:B:ILE:HG23	5	0.14
(1,2152)	2:48:B:ARG:HD3	2:48:B:ARG:HB3	6	0.14
(1,1854)	2:16:B:PHE:HB2	2:16:B:PHE:H	8	0.14
(1,1854)	2:16:B:PHE:HB2	2:16:B:PHE:H	10	0.14
(1,1818)	1:99:A:LEU:HD23	1:129:A:ASN:HD22	9	0.14
(1,1625)	1:150:A:PRO:HG2	1:152:A:LEU:HD12	10	0.14
(1,1609)	1:114:A:ILE:HB	1:114:A:ILE:HG22	7	0.14
(1,1424)	1:98:A:ILE:HD11	1:131:A:PHE:H	2	0.14
(1,1200)	1:113:A:HIS:H	1:106:A:ILE:HD13	8	0.14
(1,1070)	1:111:A:ALA:HB2	1:111:A:ALA:H	3	0.14
(1,1033)	1:106:A:ILE:HG13	1:106:A:ILE:H	2	0.14
(1,1008)	1:97:A:THR:HB	1:98:A:ILE:H	5	0.14
(1,809)	1:126:A:LEU:HB2	1:126:A:LEU:H	2	0.14
(1,809)	1:126:A:LEU:HB2	1:126:A:LEU:H	3	0.14
(1,787)	1:120:A:LEU:HG	1:120:A:LEU:HD23	8	0.14
(1,762)	1:119:A:LEU:HA	1:144:A:ILE:HG23	10	0.14
(1,761)	1:106:A:ILE:HA	1:106:A:ILE:HG23	4	0.14
(1,756)	1:146:A:VAL:HG21	1:119:A:LEU:HA	7	0.14
(1,725)	1:148:A:ILE:HD13	1:80:A:LYS:HD3	7	0.14
(1,683)	1:106:A:ILE:HG12	1:106:A:ILE:H	4	0.14
(1,673)	1:81:A:ILE:HG13	1:145:A:THR:HA	7	0.14
(1,533)	1:114:A:ILE:HA	1:114:A:ILE:HG12	2	0.14
(1,514)	1:138:A:THR:HB	1:141:A:ASN:HB2	8	0.14
(1,414)	1:118:A:LYS:HG2	1:118:A:LYS:H	10	0.14
(1,262)	1:80:A:LYS:HD3	1:86:A:PHE:HZ	9	0.14
(1,184)	1:130:A:LEU:HD23	1:130:A:LEU:H	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,154)	1:135:A:LEU:HD12	1:136:A:LYS:H	9	0.14
(1,152)	1:78:A:LEU:HD12	1:144:A:ILE:H	2	0.14
(1,116)	1:125:A:VAL:HG22	1:120:A:LEU:H	10	0.14
(1,19)	1:98:A:ILE:HD13	1:132:A:LEU:HA	4	0.14
(1,19)	1:98:A:ILE:HD13	1:132:A:LEU:HA	9	0.14
(1,16)	1:98:A:ILE:HD11	1:98:A:ILE:HG12	5	0.14
(3,90)	2:38:B:ASP:N	2:34:B:ASN:O	2	0.13
(3,89)	2:38:B:ASP:H	2:34:B:ASN:O	5	0.13
(3,18)	1:144:A:ILE:N	1:77:A:THR:O	5	0.13
(3,9)	1:86:A:PHE:H	1:80:A:LYS:O	4	0.13
(1,4175)	1:125:A:VAL:H	2:42:C:GLU:OE2	8	0.13
(1,4168)	1:79:A:LYS:HZ2	2:31:C:ASP:HB3	5	0.13
(1,4153)	2:54:C:ILE:H	2:55:C:LEU:HD13	4	0.13
(1,4008)	2:44:B:PHE:HZ	2:19:C:ILE:HG23	3	0.13
(1,3800)	2:8:B:ILE:HG23	2:16:C:PHE:HD1	4	0.13
(1,3797)	2:8:C:ILE:HG23	2:9:C:ALA:HB1	1	0.13
(1,3796)	2:8:B:ILE:HG21	2:9:B:ALA:HB3	3	0.13
(1,3727)	2:25:C:ILE:HG23	2:30:C:ALA:HB2	2	0.13
(1,3717)	2:19:C:ILE:HG23	2:19:C:ILE:HG12	7	0.13
(1,3717)	2:19:C:ILE:HG22	2:19:C:ILE:HG12	10	0.13
(1,3716)	2:19:B:ILE:HG23	2:19:B:ILE:HG12	3	0.13
(1,3716)	2:19:B:ILE:HG21	2:19:B:ILE:HG12	7	0.13
(1,3714)	2:19:B:ILE:HG23	2:24:B:GLU:HB3	4	0.13
(1,3704)	2:6:B:GLU:HA	2:46:B:PHE:HE1	4	0.13
(1,3617)	2:12:C:ILE:HA	2:12:B:ILE:HD11	4	0.13
(1,3574)	2:33:B:LEU:HD23	2:43:C:ALA:HB1	1	0.13
(1,3574)	2:33:B:LEU:HD22	2:43:C:ALA:HB1	6	0.13
(1,3562)	2:8:B:ILE:HD12	2:11:B:LEU:HA	5	0.13
(1,3477)	2:55:C:LEU:HD23	2:14:C:ASN:HD21	8	0.13
(1,3288)	2:25:B:ILE:H	2:25:B:ILE:HD12	1	0.13
(1,3197)	2:14:C:ASN:H	2:48:C:ARG:HA	7	0.13
(1,3196)	2:14:B:ASN:H	2:48:B:ARG:HA	6	0.13
(1,3175)	2:7:C:GLU:H	2:4:C:SER:HB3	7	0.13
(1,3068)	2:39:B:CYS:H	2:35:B:VAL:HB	9	0.13
(1,3051)	2:16:C:PHE:HB3	2:16:C:PHE:H	1	0.13
(1,3051)	2:16:C:PHE:HB3	2:16:C:PHE:H	4	0.13
(1,3018)	2:9:B:ALA:H	2:9:B:ALA:HB2	1	0.13
(1,3018)	2:9:B:ALA:H	2:9:B:ALA:HB3	6	0.13
(1,3011)	2:5:C:LYS:HB2	2:5:C:LYS:H	2	0.13
(1,3011)	2:5:C:LYS:HB2	2:5:C:LYS:H	5	0.13
(1,3011)	2:5:C:LYS:HB2	2:5:C:LYS:H	7	0.13
(1,2877)	2:13:C:VAL:HB	2:14:C:ASN:HA	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2844)	2:64:B:HIS:HB2	2:64:B:HIS:H	4	0.13
(1,2821)	2:5:C:LYS:HE2	2:24:B:GLU:HB3	10	0.13
(1,2820)	2:5:B:LYS:HE2	2:24:C:GLU:HB3	1	0.13
(1,2660)	2:19:B:ILE:HG23	2:15:B:TYR:HD1	2	0.13
(1,2641)	2:33:C:LEU:HD13	2:20:C:VAL:HG13	9	0.13
(1,2629)	2:37:C:MET:HB3	2:17:C:SER:HB3	2	0.13
(1,2549)	2:20:C:VAL:HG13	2:20:C:VAL:HB	4	0.13
(1,2548)	2:20:B:VAL:HG12	2:20:B:VAL:HB	8	0.13
(1,2496)	2:25:B:ILE:HG23	2:24:B:GLU:HB2	5	0.13
(1,2489)	2:68:C:ILE:HG22	2:68:C:ILE:HG13	3	0.13
(1,2488)	2:68:B:ILE:HG22	2:68:B:ILE:HG13	9	0.13
(1,2474)	2:12:B:ILE:HG22	2:40:B:ILE:HD13	2	0.13
(1,2261)	2:51:C:VAL:HG23	2:51:C:VAL:HA	1	0.13
(1,2259)	2:51:C:VAL:HA	2:54:C:ILE:HB	8	0.13
(1,2245)	2:55:C:LEU:HD23	2:11:C:LEU:HA	9	0.13
(1,2152)	2:48:B:ARG:HD3	2:48:B:ARG:HB3	10	0.13
(1,2114)	2:13:B:VAL:HG22	2:48:B:ARG:HG2	10	0.13
(1,2113)	2:13:C:VAL:HG22	2:51:C:VAL:HB	8	0.13
(1,2072)	2:51:B:VAL:HG21	2:51:B:VAL:HB	9	0.13
(1,1854)	2:16:B:PHE:HB2	2:16:B:PHE:H	5	0.13
(1,1736)	1:110:A:LYS:H	1:105:A:LEU:HB3	8	0.13
(1,1733)	1:129:A:ASN:H	1:97:A:THR:HG23	5	0.13
(1,1573)	1:137:A:VAL:HA	1:137:A:VAL:HG23	2	0.13
(1,1573)	1:137:A:VAL:HA	1:137:A:VAL:HG21	6	0.13
(1,1479)	1:82:A:GLN:HG3	1:82:A:GLN:H	2	0.13
(1,1438)	1:101:A:ILE:HG23	1:78:A:LEU:HB3	7	0.13
(1,1412)	1:151:A:ASN:HA	1:151:A:ASN:H	1	0.13
(1,1412)	1:151:A:ASN:HA	1:151:A:ASN:H	4	0.13
(1,1412)	1:151:A:ASN:HA	1:151:A:ASN:H	6	0.13
(1,1211)	1:81:A:ILE:H	1:82:A:GLN:HG2	6	0.13
(1,1197)	1:92:A:PHE:HB3	1:93:A:SER:H	10	0.13
(1,1070)	1:111:A:ALA:HB2	1:111:A:ALA:H	7	0.13
(1,833)	1:105:A:LEU:HD11	1:105:A:LEU:HG	3	0.13
(1,833)	1:105:A:LEU:HD11	1:105:A:LEU:HG	4	0.13
(1,787)	1:120:A:LEU:HG	1:120:A:LEU:HD22	7	0.13
(1,764)	1:121:A:LEU:HA	1:121:A:LEU:HD12	4	0.13
(1,762)	1:119:A:LEU:HA	1:144:A:ILE:HG23	4	0.13
(1,761)	1:106:A:ILE:HA	1:106:A:ILE:HG23	5	0.13
(1,638)	1:132:A:LEU:HB3	1:135:A:LEU:HD13	1	0.13
(1,547)	1:150:A:PRO:HD3	1:149:A:LYS:HA	5	0.13
(1,536)	1:77:A:THR:HA	1:89:A:GLU:HG2	2	0.13
(1,533)	1:114:A:ILE:HA	1:114:A:ILE:HG12	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,418)	1:136:A:LYS:HG2	1:136:A:LYS:H	9	0.13
(1,209)	1:151:A:ASN:HB3	1:151:A:ASN:HD21	7	0.13
(1,188)	1:101:A:ILE:HG13	1:101:A:ILE:HG23	3	0.13
(1,154)	1:135:A:LEU:HD12	1:136:A:LYS:H	1	0.13
(1,148)	1:132:A:LEU:HD22	1:92:A:PHE:HD2	8	0.13
(1,133)	1:138:A:THR:HG22	1:141:A:ASN:HB2	6	0.13
(1,118)	1:97:A:THR:HG22	1:97:A:THR:H	3	0.13
(1,116)	1:125:A:VAL:HG22	1:120:A:LEU:H	7	0.13
(1,103)	1:143:A:THR:HG23	1:143:A:THR:HB	2	0.13
(1,103)	1:143:A:THR:HG23	1:143:A:THR:HB	3	0.13
(1,103)	1:143:A:THR:HG21	1:143:A:THR:HB	4	0.13
(1,78)	1:148:A:ILE:HG23	1:148:A:ILE:HA	6	0.13
(1,58)	1:114:A:ILE:HD13	1:99:A:LEU:HA	5	0.13
(1,44)	1:88:A:ILE:HD13	1:78:A:LEU:HB3	7	0.13
(1,5)	1:119:A:LEU:HD21	1:102:A:LYS:H	6	0.13
(1,2)	1:120:A:LEU:HD13	1:120:A:LEU:H	4	0.13
(3,17)	1:144:A:ILE:H	1:77:A:THR:O	9	0.12
(3,9)	1:86:A:PHE:H	1:80:A:LYS:O	5	0.12
(3,9)	1:86:A:PHE:H	1:80:A:LYS:O	10	0.12
(1,4124)	2:25:B:ILE:H	2:30:B:ALA:HB1	8	0.12
(1,4098)	2:17:B:SER:H	2:12:B:ILE:HG23	1	0.12
(1,4046)	2:15:B:TYR:H	2:8:C:ILE:HG21	2	0.12
(1,3982)	2:15:B:TYR:HD2	2:12:C:ILE:HD12	7	0.12
(1,3963)	2:36:C:ALA:HB2	2:40:B:ILE:HA	2	0.12
(1,3889)	2:18:C:SER:HB3	2:22:C:LYS:HD3	8	0.12
(1,3851)	2:40:C:ILE:HG22	2:13:C:VAL:HB	5	0.12
(1,3753)	2:33:C:LEU:HB2	2:33:C:LEU:HD13	1	0.12
(1,3724)	2:25:B:ILE:HG23	2:19:B:ILE:HB	9	0.12
(1,3716)	2:19:B:ILE:HG23	2:19:B:ILE:HG12	8	0.12
(1,3664)	2:33:B:LEU:HD23	2:44:C:PHE:HZ	9	0.12
(1,3592)	2:9:B:ALA:HA	2:12:B:ILE:HG21	7	0.12
(1,3544)	2:51:B:VAL:HG21	2:48:B:ARG:HB3	8	0.12
(1,3186)	2:40:B:ILE:H	2:13:B:VAL:HG11	4	0.12
(1,3165)	2:7:C:GLU:H	2:7:C:GLU:HG3	9	0.12
(1,3071)	2:40:C:ILE:HG13	2:40:C:ILE:H	4	0.12
(1,3071)	2:40:C:ILE:HG13	2:40:C:ILE:H	7	0.12
(1,3051)	2:16:C:PHE:HB3	2:16:C:PHE:H	7	0.12
(1,3026)	2:55:B:LEU:HB2	2:56:B:GLY:H	4	0.12
(1,3026)	2:55:B:LEU:HB2	2:56:B:GLY:H	5	0.12
(1,3026)	2:55:B:LEU:HB2	2:56:B:GLY:H	10	0.12
(1,3019)	2:9:C:ALA:H	2:9:C:ALA:HB1	7	0.12
(1,3011)	2:5:C:LYS:HB2	2:5:C:LYS:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3011)	2:5:C:LYS:HB2	2:5:C:LYS:H	4	0.12
(1,3010)	2:5:B:LYS:HB2	2:5:B:LYS:H	3	0.12
(1,3010)	2:5:B:LYS:HB2	2:5:B:LYS:H	5	0.12
(1,3010)	2:5:B:LYS:HB2	2:5:B:LYS:H	6	0.12
(1,3010)	2:5:B:LYS:HB2	2:5:B:LYS:H	7	0.12
(1,3010)	2:5:B:LYS:HB2	2:5:B:LYS:H	9	0.12
(1,2951)	2:60:C:PHE:HD2	2:54:C:ILE:HB	2	0.12
(1,2863)	2:37:C:MET:HA	2:37:C:MET:HG2	4	0.12
(1,2820)	2:5:B:LYS:HE2	2:24:C:GLU:HB3	4	0.12
(1,2811)	2:25:C:ILE:HA	2:33:C:LEU:HD11	7	0.12
(1,2659)	2:12:C:ILE:HG22	2:15:C:TYR:HD2	3	0.12
(1,2630)	2:51:B:VAL:HB	2:55:B:LEU:HG	5	0.12
(1,2614)	2:13:B:VAL:HG12	2:48:B:ARG:HG2	4	0.12
(1,2555)	2:20:C:VAL:HG13	2:30:C:ALA:HB3	3	0.12
(1,2549)	2:20:C:VAL:HG11	2:20:C:VAL:HB	7	0.12
(1,2544)	2:51:B:VAL:HG11	2:55:B:LEU:HG	8	0.12
(1,2497)	2:25:C:ILE:HG22	2:24:C:GLU:HB2	1	0.12
(1,2488)	2:68:B:ILE:HG21	2:68:B:ILE:HG13	6	0.12
(1,2465)	2:71:C:SER:HB3	2:71:C:SER:H	2	0.12
(1,2405)	2:8:C:ILE:HG21	2:15:B:TYR:H	10	0.12
(1,2347)	2:44:C:PHE:HB2	2:46:C:PHE:HD1	4	0.12
(1,2187)	2:30:C:ALA:HA	2:20:C:VAL:HG13	1	0.12
(1,2085)	2:25:C:ILE:HD11	2:25:C:ILE:HG22	6	0.12
(1,2072)	2:51:B:VAL:HG21	2:51:B:VAL:HB	3	0.12
(1,2072)	2:51:B:VAL:HG22	2:51:B:VAL:HB	8	0.12
(1,1893)	2:23:C:LYS:HA	2:23:C:LYS:HG3	6	0.12
(1,1855)	2:16:C:PHE:HB2	2:16:C:PHE:H	5	0.12
(1,1855)	2:16:C:PHE:HB2	2:16:C:PHE:H	10	0.12
(1,1813)	1:141:A:ASN:HD22	1:122:A:LYS:HG2	8	0.12
(1,1802)	1:82:A:GLN:HE21	1:82:A:GLN:HB3	6	0.12
(1,1760)	1:152:A:LEU:HB3	1:153:A:GLU:H	1	0.12
(1,1629)	1:105:A:LEU:HD13	1:90:A:HIS:HE1	2	0.12
(1,1624)	1:132:A:LEU:HD11	1:93:A:SER:HA	2	0.12
(1,1573)	1:137:A:VAL:HA	1:137:A:VAL:HG21	3	0.12
(1,1532)	1:151:A:ASN:HA	1:152:A:LEU:HG	3	0.12
(1,1476)	1:85:A:LYS:HB2	1:85:A:LYS:HE3	8	0.12
(1,1460)	1:132:A:LEU:HD13	1:132:A:LEU:HA	10	0.12
(1,1432)	1:117:A:ILE:HD12	1:117:A:ILE:HG13	4	0.12
(1,1417)	1:73:A:MET:HB3	1:74:A:VAL:H	7	0.12
(1,1399)	1:80:A:LYS:HE3	1:148:A:ILE:H	2	0.12
(1,1236)	1:99:A:LEU:HD13	1:99:A:LEU:H	4	0.12
(1,1186)	1:135:A:LEU:HB2	1:135:A:LEU:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1179)	1:82:A:GLN:H	1:80:A:LYS:HD2	5	0.12
(1,1071)	1:138:A:THR:H	1:138:A:THR:HG21	3	0.12
(1,1071)	1:138:A:THR:H	1:138:A:THR:HG23	8	0.12
(1,1041)	1:108:A:GLU:HG3	1:108:A:GLU:H	10	0.12
(1,787)	1:120:A:LEU:HG	1:120:A:LEU:HD23	3	0.12
(1,767)	1:99:A:LEU:HD21	1:128:A:ASP:HA	2	0.12
(1,749)	1:124:A:LYS:HG2	1:125:A:VAL:HA	4	0.12
(1,670)	1:130:A:LEU:HG	1:131:A:PHE:H	5	0.12
(1,661)	1:76:A:LEU:HD23	1:76:A:LEU:HA	2	0.12
(1,652)	1:146:A:VAL:HB	1:146:A:VAL:HG22	4	0.12
(1,652)	1:146:A:VAL:HB	1:146:A:VAL:HG23	6	0.12
(1,625)	1:101:A:ILE:HB	1:98:A:ILE:HG22	7	0.12
(1,559)	1:115:A:SER:HA	1:114:A:ILE:HG21	3	0.12
(1,545)	1:99:A:LEU:HA	1:99:A:LEU:HD12	2	0.12
(1,182)	1:132:A:LEU:HD12	1:92:A:PHE:HA	7	0.12
(1,117)	1:125:A:VAL:HG22	1:126:A:LEU:H	6	0.12
(1,103)	1:143:A:THR:HG22	1:143:A:THR:HB	5	0.12
(1,103)	1:143:A:THR:HG23	1:143:A:THR:HB	9	0.12
(1,101)	1:77:A:THR:HG21	1:87:A:SER:HB3	5	0.12
(1,67)	1:83:A:ALA:HB2	1:85:A:LYS:H	8	0.12
(1,19)	1:98:A:ILE:HD13	1:132:A:LEU:HA	8	0.12
(1,15)	1:98:A:ILE:HD13	1:98:A:ILE:HG13	10	0.12
(1,5)	1:119:A:LEU:HD23	1:102:A:LYS:H	8	0.12
(1,5)	1:119:A:LEU:HD23	1:102:A:LYS:H	9	0.12
(3,18)	1:144:A:ILE:N	1:77:A:THR:O	4	0.11
(3,18)	1:144:A:ILE:N	1:77:A:THR:O	7	0.11
(3,15)	1:77:A:THR:H	1:142:A:SER:O	2	0.11
(3,9)	1:86:A:PHE:H	1:80:A:LYS:O	9	0.11
(1,4160)	2:38:B:ASP:H	2:40:B:ILE:HD13	5	0.11
(1,4126)	2:19:B:ILE:HA	2:25:B:ILE:H	9	0.11
(1,4085)	2:14:C:ASN:H	2:12:C:ILE:HG22	3	0.11
(1,4012)	2:44:B:PHE:HZ	2:5:B:LYS:HE2	7	0.11
(1,3971)	2:8:C:ILE:HD11	2:60:C:PHE:HE1	3	0.11
(1,3963)	2:36:C:ALA:HB2	2:40:B:ILE:HA	6	0.11
(1,3918)	2:16:B:PHE:HB3	2:40:B:ILE:HD13	1	0.11
(1,3891)	2:18:C:SER:HB3	2:19:C:ILE:HG12	3	0.11
(1,3830)	2:40:B:ILE:HD13	2:13:B:VAL:HB	5	0.11
(1,3726)	2:25:B:ILE:HG22	2:30:B:ALA:HB2	4	0.11
(1,3725)	2:25:C:ILE:HG22	2:19:C:ILE:HB	6	0.11
(1,3723)	2:25:C:ILE:HG21	2:5:B:LYS:HE3	8	0.11
(1,3723)	2:25:C:ILE:HG22	2:5:B:LYS:HE3	9	0.11
(1,3717)	2:19:C:ILE:HG23	2:19:C:ILE:HG12	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3716)	2:19:B:ILE:HG22	2:19:B:ILE:HG12	4	0.11
(1,3658)	2:51:B:VAL:HG23	2:46:B:PHE:HE2	5	0.11
(1,3561)	2:25:C:ILE:HD13	2:25:C:ILE:HG13	4	0.11
(1,3558)	2:25:B:ILE:HD13	2:25:B:ILE:HG12	10	0.11
(1,3551)	2:25:C:ILE:HD12	2:5:B:LYS:HE3	1	0.11
(1,3197)	2:14:C:ASN:H	2:48:C:ARG:HA	9	0.11
(1,3174)	2:7:B:GLU:H	2:4:B:SER:HB3	3	0.11
(1,3154)	2:4:B:SER:HB3	2:6:B:GLU:H	6	0.11
(1,3059)	2:26:C:SER:HB2	2:26:C:SER:H	8	0.11
(1,3050)	2:16:B:PHE:HB3	2:16:B:PHE:H	7	0.11
(1,3045)	2:47:C:GLU:HB2	2:50:C:ALA:H	3	0.11
(1,3011)	2:5:C:LYS:HB2	2:5:C:LYS:H	6	0.11
(1,3010)	2:5:B:LYS:HB2	2:5:B:LYS:H	2	0.11
(1,3010)	2:5:B:LYS:HB2	2:5:B:LYS:H	4	0.11
(1,2963)	2:48:C:ARG:HG3	2:48:C:ARG:H	8	0.11
(1,2876)	2:13:B:VAL:HB	2:14:B:ASN:HA	1	0.11
(1,2829)	2:6:C:GLU:HG2	2:9:C:ALA:HB3	10	0.11
(1,2693)	2:50:C:ALA:HB3	2:47:C:GLU:HB2	8	0.11
(1,2691)	2:50:C:ALA:HB3	2:47:C:GLU:HB3	7	0.11
(1,2690)	2:50:B:ALA:HB3	2:47:B:GLU:HB3	1	0.11
(1,2652)	2:8:B:ILE:HG23	2:3:B:ALA:HB3	2	0.11
(1,2631)	2:51:C:VAL:HB	2:55:C:LEU:HG	8	0.11
(1,2556)	2:35:B:VAL:HG11	2:36:B:ALA:HB1	6	0.11
(1,2548)	2:20:B:VAL:HG11	2:20:B:VAL:HB	7	0.11
(1,2548)	2:20:B:VAL:HG12	2:20:B:VAL:HB	10	0.11
(1,2496)	2:25:B:ILE:HG21	2:24:B:GLU:HB2	6	0.11
(1,2482)	2:25:B:ILE:HB	2:19:B:ILE:HG23	5	0.11
(1,2479)	2:19:C:ILE:HB	2:19:C:ILE:HG21	9	0.11
(1,2479)	2:19:C:ILE:HB	2:19:C:ILE:HG22	10	0.11
(1,2426)	2:68:B:ILE:HD12	2:60:C:PHE:HD1	9	0.11
(1,2423)	2:25:C:ILE:HD12	2:44:B:PHE:HZ	4	0.11
(1,2404)	2:8:B:ILE:HG22	2:15:C:TYR:H	2	0.11
(1,2404)	2:8:B:ILE:HG21	2:15:C:TYR:H	4	0.11
(1,2261)	2:51:C:VAL:HG22	2:51:C:VAL:HA	5	0.11
(1,2227)	2:5:C:LYS:HA	2:8:C:ILE:HG13	10	0.11
(1,2153)	2:48:C:ARG:HD3	2:48:C:ARG:HB3	6	0.11
(1,2111)	2:13:C:VAL:HG23	2:13:C:VAL:HB	5	0.11
(1,2073)	2:51:C:VAL:HG21	2:51:C:VAL:HB	7	0.11
(1,2065)	2:55:C:LEU:HD23	2:51:C:VAL:HB	7	0.11
(1,2035)	2:5:C:LYS:HB2	2:44:C:PHE:HZ	7	0.11
(1,1968)	2:34:B:ASN:HB3	2:34:B:ASN:HD21	3	0.11
(1,1966)	2:34:B:ASN:HB2	2:34:B:ASN:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1892)	2:23:B:LYS:HA	2:23:B:LYS:HG3	2	0.11
(1,1743)	1:126:A:LEU:H	1:120:A:LEU:HB2	1	0.11
(1,1616)	1:83:A:ALA:HB2	1:84:A:PRO:HB2	9	0.11
(1,1603)	1:141:A:ASN:HB2	1:121:A:LEU:HD12	5	0.11
(1,1550)	1:85:A:LYS:HA	1:85:A:LYS:HG2	2	0.11
(1,1539)	1:117:A:ILE:HG21	1:118:A:LYS:HA	7	0.11
(1,1427)	1:106:A:ILE:HD11	1:104:A:HIS:H	3	0.11
(1,1412)	1:151:A:ASN:HA	1:151:A:ASN:H	2	0.11
(1,1412)	1:151:A:ASN:HA	1:151:A:ASN:H	7	0.11
(1,1412)	1:151:A:ASN:HA	1:151:A:ASN:H	10	0.11
(1,1391)	1:143:A:THR:H	1:141:A:ASN:HB3	1	0.11
(1,1272)	1:111:A:ALA:H	1:106:A:ILE:HD11	1	0.11
(1,1194)	1:92:A:PHE:HB2	1:93:A:SER:H	5	0.11
(1,1186)	1:135:A:LEU:HB2	1:135:A:LEU:H	8	0.11
(1,1053)	1:115:A:SER:H	1:114:A:ILE:HG13	1	0.11
(1,958)	1:121:A:LEU:H	1:126:A:LEU:HB3	3	0.11
(1,833)	1:105:A:LEU:HD11	1:105:A:LEU:HG	1	0.11
(1,768)	1:76:A:LEU:HD13	1:132:A:LEU:HA	9	0.11
(1,766)	1:76:A:LEU:HA	1:76:A:LEU:HD12	9	0.11
(1,762)	1:119:A:LEU:HA	1:144:A:ILE:HG23	8	0.11
(1,751)	1:149:A:LYS:HG2	1:149:A:LYS:HE3	4	0.11
(1,738)	1:115:A:SER:HA	1:114:A:ILE:HG13	10	0.11
(1,683)	1:106:A:ILE:HG12	1:106:A:ILE:H	3	0.11
(1,609)	1:108:A:GLU:HA	1:108:A:GLU:HG3	6	0.11
(1,487)	1:139:A:PRO:HD2	1:138:A:THR:HA	3	0.11
(1,437)	1:94:A:PRO:HD2	1:74:A:VAL:HG11	1	0.11
(1,437)	1:94:A:PRO:HD2	1:74:A:VAL:HG11	8	0.11
(1,281)	1:120:A:LEU:HB2	1:145:A:THR:HB	4	0.11
(1,261)	1:129:A:ASN:HB2	1:129:A:ASN:HD21	3	0.11
(1,247)	1:103:A:GLN:HG2	1:100:A:GLN:HE22	10	0.11
(1,209)	1:151:A:ASN:HB3	1:151:A:ASN:HD21	4	0.11
(1,188)	1:101:A:ILE:HG13	1:101:A:ILE:HG23	1	0.11
(1,181)	1:132:A:LEU:HD12	1:92:A:PHE:HB2	5	0.11
(1,119)	1:97:A:THR:HG22	1:131:A:PHE:HD2	7	0.11
(1,92)	1:101:A:ILE:HG23	1:101:A:ILE:HB	9	0.11
(1,89)	1:101:A:ILE:HG23	1:119:A:LEU:HA	8	0.11
(1,16)	1:98:A:ILE:HD11	1:98:A:ILE:HG12	7	0.11
(1,15)	1:98:A:ILE:HD12	1:98:A:ILE:HG13	1	0.11
(1,15)	1:98:A:ILE:HD13	1:98:A:ILE:HG13	8	0.11
(3,18)	1:144:A:ILE:N	1:77:A:THR:O	8	0.1
(3,9)	1:86:A:PHE:H	1:80:A:LYS:O	1	0.1
(1,4013)	2:44:C:PHE:HZ	2:5:C:LYS:HE2	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3968)	2:25:B:ILE:HG22	2:44:C:PHE:HD1	3	0.1
(1,3717)	2:19:C:ILE:HG21	2:19:C:ILE:HG12	1	0.1
(1,3704)	2:6:B:GLU:HA	2:44:B:PHE:HZ	5	0.1
(1,3421)	2:51:C:VAL:H	2:54:C:ILE:HG12	1	0.1
(1,3253)	2:21:C:GLU:HB3	2:21:C:GLU:H	2	0.1
(1,3233)	2:72:C:ALA:H	2:72:C:ALA:HB1	1	0.1
(1,3177)	2:7:C:GLU:H	2:4:C:SER:HB2	9	0.1
(1,3174)	2:7:B:GLU:H	2:4:B:SER:HB3	7	0.1
(1,3059)	2:26:C:SER:HB2	2:26:C:SER:H	5	0.1
(1,3058)	2:26:B:SER:HB2	2:26:B:SER:H	8	0.1
(1,3019)	2:9:C:ALA:H	2:9:C:ALA:HB1	3	0.1
(1,2946)	2:44:B:PHE:HB2	2:46:B:PHE:HE1	9	0.1
(1,2690)	2:50:B:ALA:HB3	2:47:B:GLU:HB3	7	0.1
(1,2658)	2:12:B:ILE:HG23	2:15:B:TYR:HD2	8	0.1
(1,2549)	2:20:C:VAL:HG11	2:20:C:VAL:HB	3	0.1
(1,2549)	2:20:C:VAL:HG11	2:20:C:VAL:HB	10	0.1
(1,2465)	2:71:C:SER:HB3	2:71:C:SER:H	6	0.1
(1,2261)	2:51:C:VAL:HG23	2:51:C:VAL:HA	7	0.1
(1,2175)	2:9:C:ALA:HA	2:12:C:ILE:HB	5	0.1
(1,2167)	2:44:C:PHE:HB3	2:44:C:PHE:HB2	7	0.1
(1,2166)	2:44:B:PHE:HB3	2:44:B:PHE:HB2	3	0.1
(1,2166)	2:44:B:PHE:HB3	2:44:B:PHE:HB2	10	0.1
(1,2111)	2:13:C:VAL:HG21	2:13:C:VAL:HB	2	0.1
(1,2072)	2:51:B:VAL:HG22	2:51:B:VAL:HB	4	0.1
(1,2072)	2:51:B:VAL:HG22	2:51:B:VAL:HB	5	0.1
(1,1968)	2:34:B:ASN:HB3	2:34:B:ASN:HD21	8	0.1
(1,1855)	2:16:C:PHE:HB2	2:16:C:PHE:H	3	0.1
(1,1723)	1:102:A:LYS:H	1:117:A:ILE:HD12	2	0.1
(1,1550)	1:85:A:LYS:HA	1:85:A:LYS:HG3	10	0.1
(1,1428)	1:106:A:ILE:HD12	1:102:A:LYS:HB3	10	0.1
(1,1323)	1:100:A:GLN:HE21	1:99:A:LEU:HB3	6	0.1
(1,1211)	1:81:A:ILE:H	1:82:A:GLN:HG2	10	0.1
(1,1186)	1:135:A:LEU:HB2	1:135:A:LEU:H	9	0.1
(1,597)	1:109:A:GLU:HA	1:109:A:GLU:HG3	9	0.1
(1,245)	1:103:A:GLN:HG2	1:103:A:GLN:H	10	0.1
(1,193)	1:117:A:ILE:HG22	1:118:A:LYS:H	2	0.1
(1,162)	1:78:A:LEU:HD23	1:92:A:PHE:HZ	1	0.1
(1,55)	1:114:A:ILE:HD12	1:103:A:GLN:HE22	4	0.1
(1,15)	1:98:A:ILE:HD13	1:98:A:ILE:HG13	9	0.1
(1,10)	1:120:A:LEU:HD12	1:120:A:LEU:HG	3	0.1
(1,3)	1:120:A:LEU:HD13	1:119:A:LEU:H	10	0.1

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

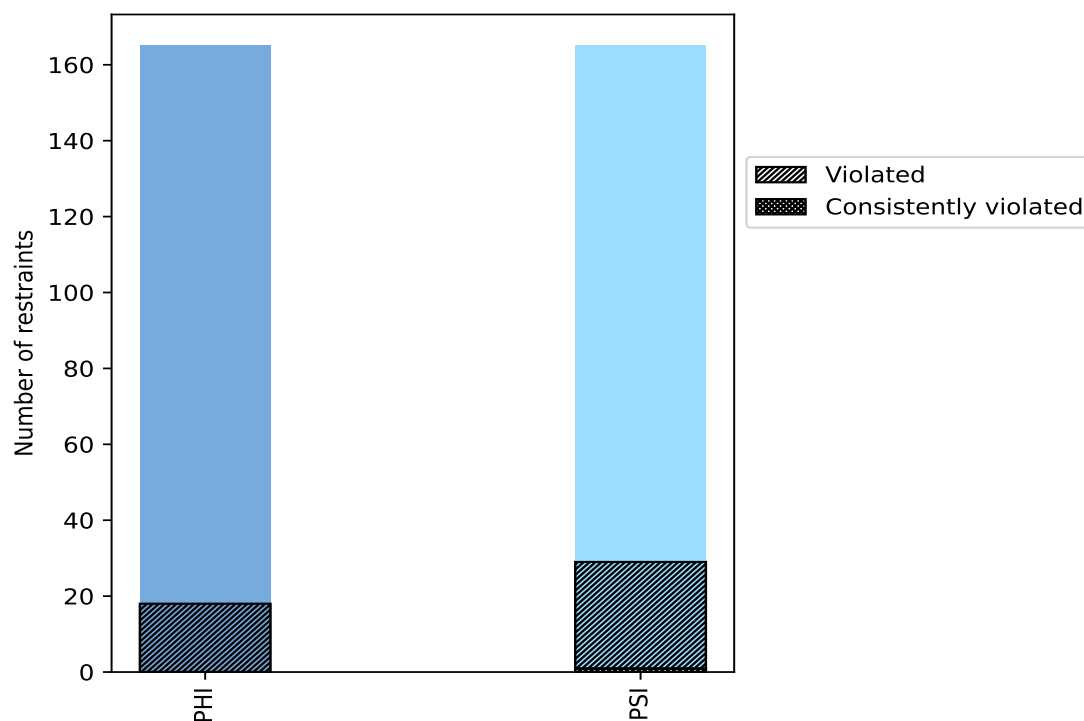
10.1 Summary of dihedral-angle violations [i](#)

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	165	50.0	18	10.9	5.5	0	0.0	0.0
PSI	165	50.0	29	17.6	8.8	1	0.6	0.3
Total	330	100.0	47	14.2	14.2	1	0.3	0.3

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](#)



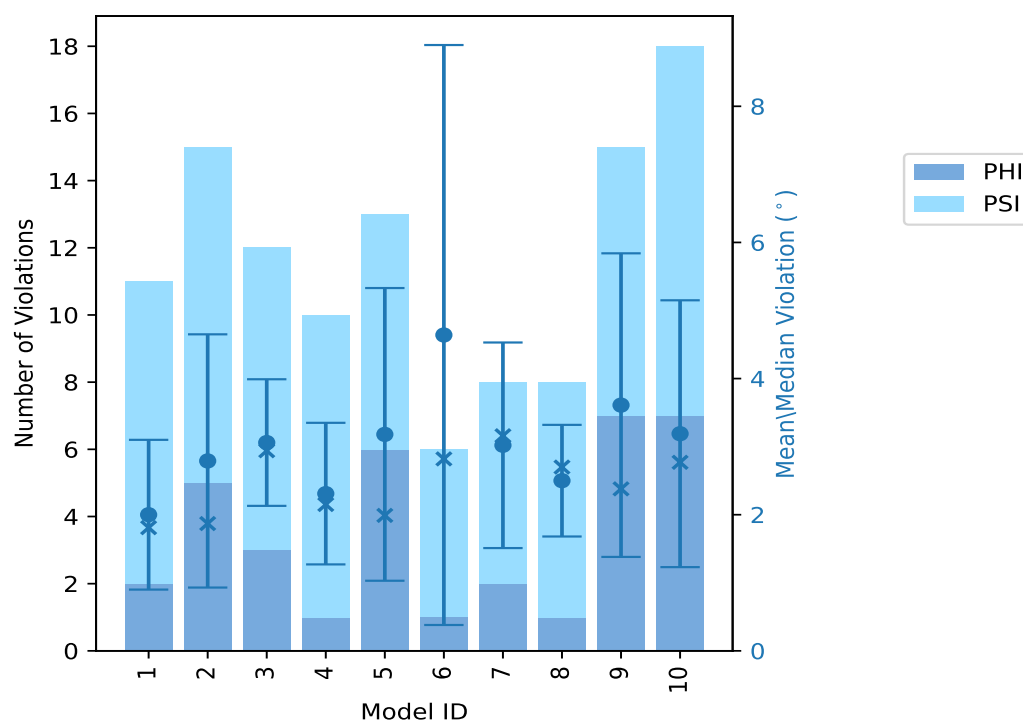
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	2	9	11	2.0	5.17	1.1	1.81
2	5	10	15	2.79	6.75	1.86	1.87
3	3	9	12	3.06	5.31	0.93	2.94
4	1	9	10	2.31	4.22	1.04	2.15
5	6	7	13	3.18	8.46	2.15	1.99
6	1	5	6	4.64	13.56	4.26	2.82
7	2	6	8	3.02	6.12	1.51	3.16
8	1	7	8	2.5	3.56	0.82	2.7
9	7	8	15	3.61	7.68	2.23	2.38
10	7	11	18	3.19	8.76	1.96	2.77

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



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

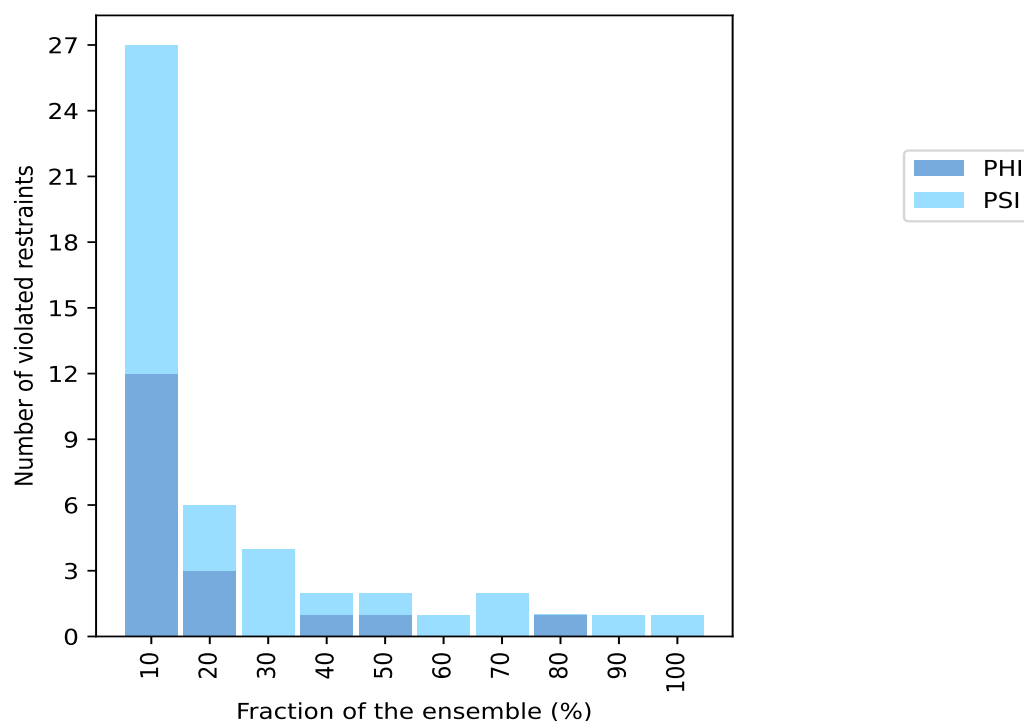
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
12	15	27	1	10.0
3	3	6	2	20.0
0	4	4	3	30.0
1	1	2	4	40.0
1	1	2	5	50.0
0	1	1	6	60.0
0	2	2	7	70.0
1	0	1	8	80.0
0	1	1	9	90.0
0	1	1	10	100.0

¹ Number of models with violations

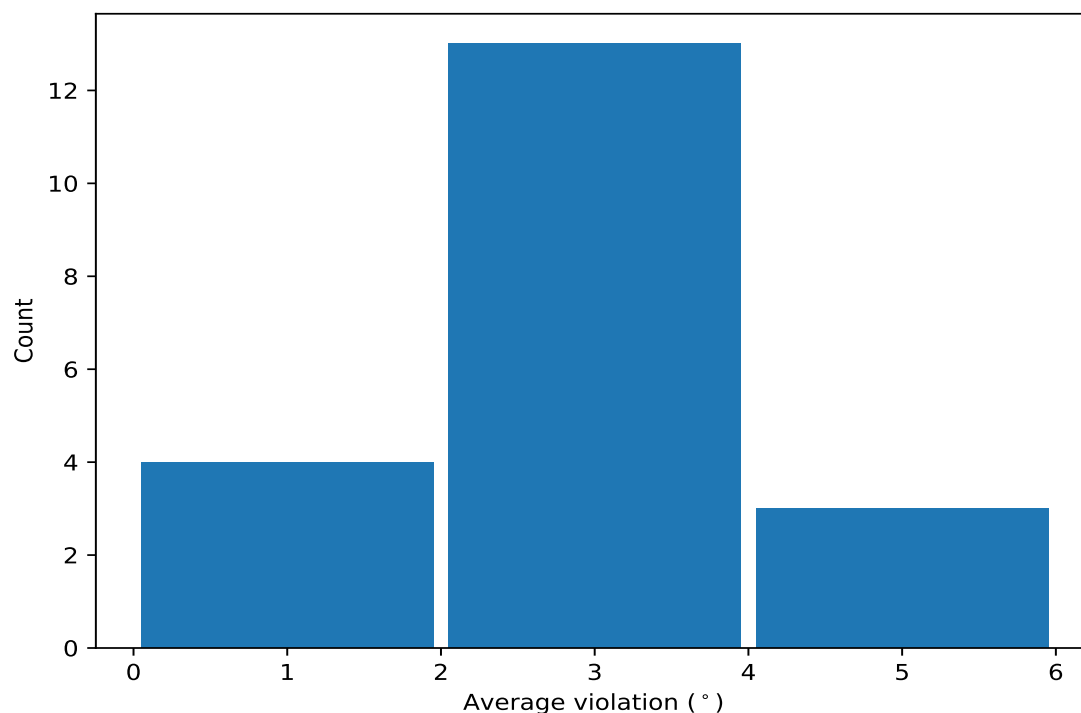
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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 [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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,218)	2:50:B:ALA:N	2:50:B:ALA:CA	2:50:B:ALA:C	2:51:B:VAL:N	10	2.36	0.83	2.13
(1,82)	1:121:A:LEU:N	1:121:A:LEU:CA	1:121:A:LEU:C	1:122:A:LYS:N	9	5.59	2.13	5.27
(1,123)	1:147:A:MET:C	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	8	3.52	0.94	3.61
(1,124)	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	1:149:A:LYS:N	7	3.58	1.7	2.93
(1,74)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:C	1:118:A:LYS:N	7	2.15	0.55	1.94
(1,90)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:HIS:N	6	2.87	0.91	3.16
(1,320)	2:50:C:ALA:N	2:50:C:ALA:CA	2:50:C:ALA:C	2:51:C:VAL:N	5	3.2	2.07	3.15
(1,225)	2:53:B:GLY:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	5	2.67	1.16	2.22
(1,117)	1:144:A:ILE:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	4	2.78	1.08	2.65
(1,328)	2:54:C:ILE:N	2:54:C:ILE:CA	2:54:C:ILE:C	2:55:C:LEU:N	4	2.22	1.05	1.81
(1,94)	1:128:A:ASP:N	1:128:A:ASP:CA	1:128:A:ASP:C	1:129:A:ASN:N	3	2.18	0.47	1.9
(1,156)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:ILE:N	3	2.01	0.45	2.21
(1,84)	1:123:A:GLY:N	1:123:A:GLY:CA	1:123:A:GLY:C	1:124:A:LYS:N	3	1.64	0.87	1.05

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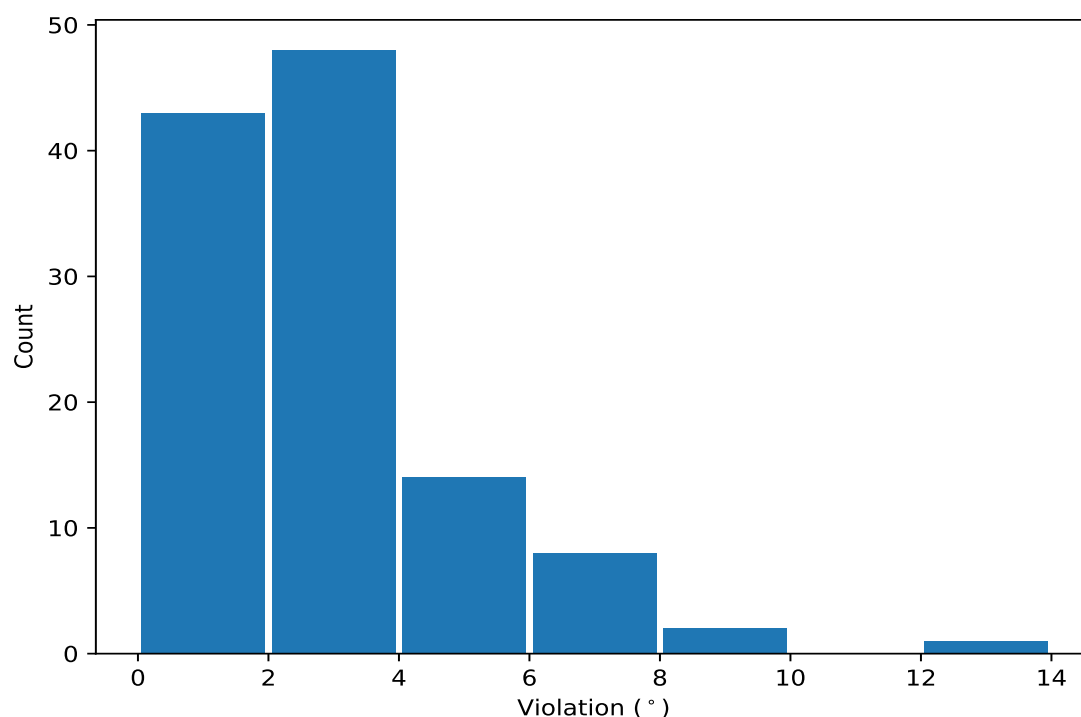
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,106)	1:135:A:LEU:N	1:135:A:LEU:CA	1:135:A:LEU:C	1:136:A:LYS:N	3	1.13	0.05	1.14
(1,327)	2:53:C:GLY:C	2:54:C:ILE:N	2:54:C:ILE:CA	2:54:C:ILE:C	2	5.57	1.32	5.57
(1,91)	1:126:A:LEU:C	1:127:A:HIS:N	1:127:A:HIS:CA	1:127:A:HIS:C	2	5.42	0.88	5.42
(1,32)	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	1:96:A:ASP:N	2	2.82	0.15	2.82
(1,318)	2:49:C:GLU:N	2:49:C:GLU:CA	2:49:C:GLU:C	2:50:C:ALA:N	2	2.23	0.15	2.23
(1,72)	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	1:117:A:ILE:N	2	1.58	0.53	1.58
(1,209)	2:45:B:GLY:C	2:46:B:PHE:N	2:46:B:PHE:CA	2:46:B:PHE:C	2	1.14	0.02	1.14

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 (°)
(1,81)	1:120:A:LEU:C	1:121:A:LEU:N	1:121:A:LEU:CA	1:121:A:LEU:C	6	13.56

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,82)	1:121:A:LEU:N	1:121:A:LEU:CA	1:121:A:LEU:C	1:122:A:LYS:N	10	8.76
(1,82)	1:121:A:LEU:N	1:121:A:LEU:CA	1:121:A:LEU:C	1:122:A:LYS:N	5	8.46
(1,330)	2:55:C:LEU:N	2:55:C:LEU:CA	2:55:C:LEU:C	2:56:C:GLY:N	9	7.68
(1,82)	1:121:A:LEU:N	1:121:A:LEU:CA	1:121:A:LEU:C	1:122:A:LYS:N	9	7.06
(1,327)	2:53:C:GLY:C	2:54:C:ILE:N	2:54:C:ILE:CA	2:54:C:ILE:C	10	6.89
(1,320)	2:50:C:ALA:N	2:50:C:ALA:CA	2:50:C:ALA:C	2:51:C:VAL:N	9	6.86
(1,124)	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	1:149:A:LYS:N	2	6.75
(1,91)	1:126:A:LEU:C	1:127:A:HIS:N	1:127:A:HIS:CA	1:127:A:HIS:C	5	6.3
(1,323)	2:51:C:VAL:C	2:52:C:SER:N	2:52:C:SER:CA	2:52:C:SER:C	9	6.27
(1,82)	1:121:A:LEU:N	1:121:A:LEU:CA	1:121:A:LEU:C	1:122:A:LYS:N	7	6.12
(1,114)	1:143:A:THR:N	1:143:A:THR:CA	1:143:A:THR:C	1:144:A:ILE:N	2	5.82
(1,80)	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	1:121:A:LEU:N	6	5.74
(1,124)	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	1:149:A:LYS:N	3	5.31
(1,82)	1:121:A:LEU:N	1:121:A:LEU:CA	1:121:A:LEU:C	1:122:A:LYS:N	2	5.27
(1,82)	1:121:A:LEU:N	1:121:A:LEU:CA	1:121:A:LEU:C	1:122:A:LYS:N	1	5.17
(1,123)	1:147:A:MET:C	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	2	4.78
(1,225)	2:53:B:GLY:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	5	4.7
(1,91)	1:126:A:LEU:C	1:127:A:HIS:N	1:127:A:HIS:CA	1:127:A:HIS:C	9	4.53
(1,123)	1:147:A:MET:C	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	10	4.45
(1,327)	2:53:C:GLY:C	2:54:C:ILE:N	2:54:C:ILE:CA	2:54:C:ILE:C	5	4.25
(1,218)	2:50:B:ALA:N	2:50:B:ALA:CA	2:50:B:ALA:C	2:51:B:VAL:N	4	4.22
(1,117)	1:144:A:ILE:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	10	4.2
(1,123)	1:147:A:MET:C	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	3	4.06
(1,321)	2:50:C:ALA:C	2:51:C:VAL:N	2:51:C:VAL:CA	2:51:C:VAL:C	9	4.03
(1,328)	2:54:C:ILE:N	2:54:C:ILE:CA	2:54:C:ILE:C	2:55:C:LEU:N	10	3.98
(1,90)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:HIS:N	7	3.91
(1,82)	1:121:A:LEU:N	1:121:A:LEU:CA	1:121:A:LEU:C	1:122:A:LYS:N	3	3.89
(1,123)	1:147:A:MET:C	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	4	3.82
(1,215)	2:48:B:ARG:C	2:49:B:GLU:N	2:49:B:GLU:CA	2:49:B:GLU:C	5	3.69
(1,124)	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	1:149:A:LYS:N	10	3.58
(1,320)	2:50:C:ALA:N	2:50:C:ALA:CA	2:50:C:ALA:C	2:51:C:VAL:N	8	3.56
(1,90)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:HIS:N	10	3.51
(1,82)	1:121:A:LEU:N	1:121:A:LEU:CA	1:121:A:LEU:C	1:122:A:LYS:N	8	3.47
(1,117)	1:144:A:ILE:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	7	3.43
(1,90)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:HIS:N	6	3.43
(1,123)	1:147:A:MET:C	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	7	3.4
(1,123)	1:147:A:MET:C	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	9	3.2
(1,225)	2:53:B:GLY:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	10	3.16
(1,320)	2:50:C:ALA:N	2:50:C:ALA:CA	2:50:C:ALA:C	2:51:C:VAL:N	3	3.15
(1,74)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:C	1:118:A:LYS:N	3	2.99
(1,218)	2:50:B:ALA:N	2:50:B:ALA:CA	2:50:B:ALA:C	2:51:B:VAL:N	2	2.98
(1,218)	2:50:B:ALA:N	2:50:B:ALA:CA	2:50:B:ALA:C	2:51:B:VAL:N	3	2.98
(1,32)	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	1:96:A:ASP:N	5	2.97
(1,124)	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	1:149:A:LYS:N	7	2.93
(1,74)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:C	1:118:A:LYS:N	4	2.92
(1,90)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:HIS:N	3	2.89
(1,22)	1:90:A:HIS:N	1:90:A:HIS:CA	1:90:A:HIS:C	1:91:A:ASP:N	3	2.89
(1,84)	1:123:A:GLY:N	1:123:A:GLY:CA	1:123:A:GLY:C	1:124:A:LYS:N	2	2.87
(1,123)	1:147:A:MET:C	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	8	2.84
(1,94)	1:128:A:ASP:N	1:128:A:ASP:CA	1:128:A:ASP:C	1:129:A:ASN:N	10	2.84
(1,124)	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	1:149:A:LYS:N	4	2.76

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,218)	2:50:B:ALA:N	2:50:B:ALA:CA	2:50:B:ALA:C	2:51:B:VAL:N	8	2.73
(1,20)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:HIS:N	10	2.7
(1,32)	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	1:96:A:ASP:N	8	2.68
(1,317)	2:48:C:ARG:C	2:49:C:GLU:N	2:49:C:GLU:CA	2:49:C:GLU:C	10	2.61
(1,119)	1:145:A:THR:C	1:146:A:VAL:N	1:146:A:VAL:CA	1:146:A:VAL:C	3	2.56
(1,156)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:ILE:N	1	2.43
(1,318)	2:49:C:GLU:N	2:49:C:GLU:CA	2:49:C:GLU:C	2:50:C:ALA:N	9	2.38
(1,316)	2:48:C:ARG:N	2:48:C:ARG:CA	2:48:C:ARG:C	2:49:C:GLU:N	3	2.33
(1,124)	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	1:149:A:LYS:N	9	2.33
(1,90)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:HIS:N	2	2.3
(1,225)	2:53:B:GLY:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	9	2.22
(1,74)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:C	1:118:A:LYS:N	6	2.22
(1,258)	2:18:C:SER:N	2:18:C:SER:CA	2:18:C:SER:C	2:19:C:ILE:N	4	2.21
(1,156)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:ILE:N	10	2.21
(1,218)	2:50:B:ALA:N	2:50:B:ALA:CA	2:50:B:ALA:C	2:51:B:VAL:N	9	2.14
(1,218)	2:50:B:ALA:N	2:50:B:ALA:CA	2:50:B:ALA:C	2:51:B:VAL:N	1	2.12
(1,172)	2:27:B:GLU:N	2:27:B:GLU:CA	2:27:B:GLU:C	2:28:B:ASP:N	1	2.12
(1,72)	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	1:117:A:ILE:N	8	2.11
(1,82)	1:121:A:LEU:N	1:121:A:LEU:CA	1:121:A:LEU:C	1:122:A:LYS:N	4	2.09
(1,318)	2:49:C:GLU:N	2:49:C:GLU:CA	2:49:C:GLU:C	2:50:C:ALA:N	10	2.08
(1,328)	2:54:C:ILE:N	2:54:C:ILE:CA	2:54:C:ILE:C	2:55:C:LEU:N	1	2.04
(1,218)	2:50:B:ALA:N	2:50:B:ALA:CA	2:50:B:ALA:C	2:51:B:VAL:N	5	1.99
(1,74)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:C	1:118:A:LYS:N	5	1.94
(1,94)	1:128:A:ASP:N	1:128:A:ASP:CA	1:128:A:ASP:C	1:129:A:ASN:N	3	1.9
(1,117)	1:144:A:ILE:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	2	1.87
(1,225)	2:53:B:GLY:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	3	1.83
(1,74)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:C	1:118:A:LYS:N	7	1.83
(1,94)	1:128:A:ASP:N	1:128:A:ASP:CA	1:128:A:ASP:C	1:129:A:ASN:N	1	1.81
(1,218)	2:50:B:ALA:N	2:50:B:ALA:CA	2:50:B:ALA:C	2:51:B:VAL:N	6	1.7
(1,157)	2:18:B:SER:C	2:19:B:ILE:N	2:19:B:ILE:CA	2:19:B:ILE:C	5	1.67
(1,69)	1:114:A:ILE:C	1:115:A:SER:N	1:115:A:SER:CA	1:115:A:SER:C	9	1.65
(1,228)	2:55:B:LEU:N	2:55:B:LEU:CA	2:55:B:LEU:C	2:56:B:GLY:N	10	1.62
(1,123)	1:147:A:MET:C	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	1	1.61
(1,117)	1:144:A:ILE:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	5	1.61
(1,74)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:C	1:118:A:LYS:N	2	1.59
(1,328)	2:54:C:ILE:N	2:54:C:ILE:CA	2:54:C:ILE:C	2:55:C:LEU:N	5	1.58
(1,74)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:C	1:118:A:LYS:N	9	1.56
(1,116)	1:144:A:ILE:N	1:144:A:ILE:CA	1:144:A:ILE:C	1:145:A:THR:N	2	1.5
(1,218)	2:50:B:ALA:N	2:50:B:ALA:CA	2:50:B:ALA:C	2:51:B:VAL:N	7	1.49
(1,225)	2:53:B:GLY:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	1	1.45
(1,124)	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	1:149:A:LYS:N	8	1.43
(1,320)	2:50:C:ALA:N	2:50:C:ALA:CA	2:50:C:ALA:C	2:51:C:VAL:N	2	1.42
(1,156)	2:18:B:SER:N	2:18:B:SER:CA	2:18:B:SER:C	2:19:B:ILE:N	4	1.39
(1,87)	1:124:A:LYS:C	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	2	1.34
(1,65)	1:112:A:SER:C	1:113:A:HIS:N	1:113:A:HIS:CA	1:113:A:HIS:C	9	1.29
(1,328)	2:54:C:ILE:N	2:54:C:ILE:CA	2:54:C:ILE:C	2:55:C:LEU:N	4	1.28
(1,218)	2:50:B:ALA:N	2:50:B:ALA:CA	2:50:B:ALA:C	2:51:B:VAL:N	10	1.28
(1,73)	1:116:A:GLU:C	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:C	10	1.25
(1,16)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:ILE:N	1	1.24
(1,88)	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	1:126:A:LEU:N	4	1.23
(1,106)	1:135:A:LEU:N	1:135:A:LEU:CA	1:135:A:LEU:C	1:136:A:LYS:N	5	1.19

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,90)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:HIS:N	4	1.18
(1,12)	1:79:A:LYS:N	1:79:A:LYS:CA	1:79:A:LYS:C	1:80:A:LYS:N	6	1.17
(1,209)	2:45:B:GLY:C	2:46:B:PHE:N	2:46:B:PHE:CA	2:46:B:PHE:C	10	1.16
(1,106)	1:135:A:LEU:N	1:135:A:LEU:CA	1:135:A:LEU:C	1:136:A:LYS:N	8	1.14
(1,265)	2:21:C:GLU:C	2:22:C:LYS:N	2:22:C:LYS:CA	2:22:C:LYS:C	2	1.13
(1,209)	2:45:B:GLY:C	2:46:B:PHE:N	2:46:B:PHE:CA	2:46:B:PHE:C	2	1.11
(1,26)	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	1:93:A:SER:N	10	1.1
(1,106)	1:135:A:LEU:N	1:135:A:LEU:CA	1:135:A:LEU:C	1:136:A:LYS:N	2	1.06
(1,84)	1:123:A:GLY:N	1:123:A:GLY:CA	1:123:A:GLY:C	1:124:A:LYS:N	7	1.05
(1,72)	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	1:117:A:ILE:N	5	1.05
(1,320)	2:50:C:ALA:N	2:50:C:ALA:CA	2:50:C:ALA:C	2:51:C:VAL:N	1	1.01
(1,264)	2:21:C:GLU:N	2:21:C:GLU:CA	2:21:C:GLU:C	2:22:C:LYS:N	1	1.01
(1,84)	1:123:A:GLY:N	1:123:A:GLY:CA	1:123:A:GLY:C	1:124:A:LYS:N	9	1.0