



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 03:00 PM UTC

PDB ID : 2LXX / pdb_00002lxx
BMRB ID : 18701
Title : Solution structure of cofilin like UNC-60B protein from *Caenorhabditis elegans*
Authors : Shukla, V.; Yadav, R.; Kabra, A.; Jain, A.; Kumar, D.; Ono, S.; Arora, A.
Deposited on : 2012-09-04

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

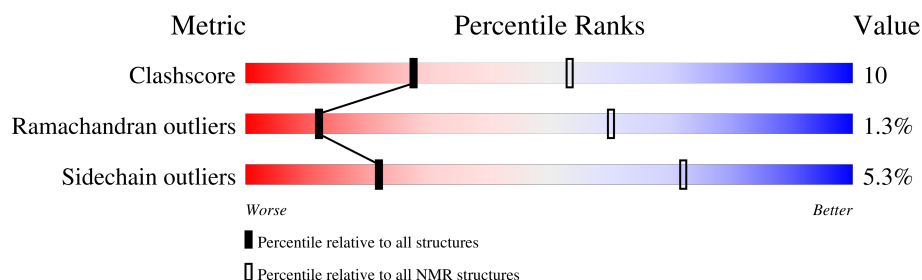
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 87%.

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	152	

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 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:1-A:152 (152)	1.10	3

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

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

The models can be grouped into 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2396 atoms, of which 1203 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Actin-depolymerizing factor 2, isoform c.

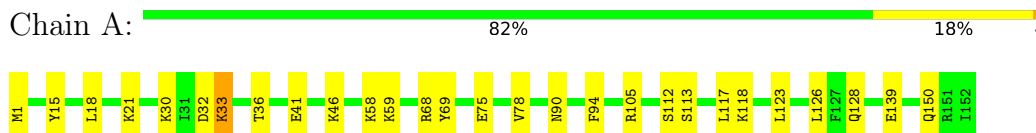
Mol	Chain	Residues	Atoms						Trace
1	A	152	Total	C	H	N	O	S	0
			2396	744	1203	207	234	8	

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: Actin-depolymerizing factor 2, isoform c

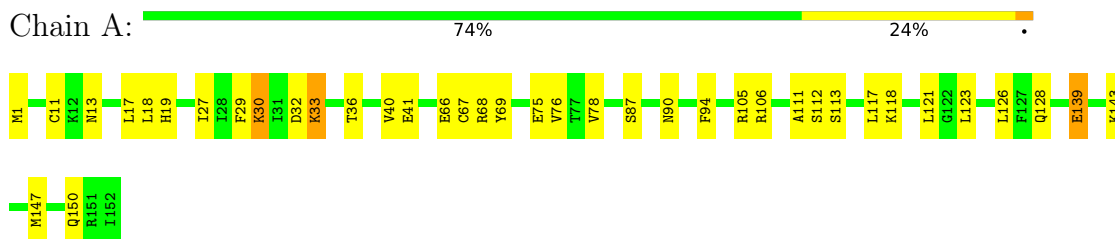


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

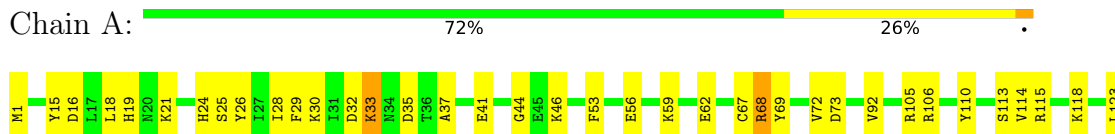
4.2.1 Score per residue for model 1

- Molecule 1: Actin-depolymerizing factor 2, isoform c



4.2.2 Score per residue for model 2

- Molecule 1: Actin-depolymerizing factor 2, isoform c

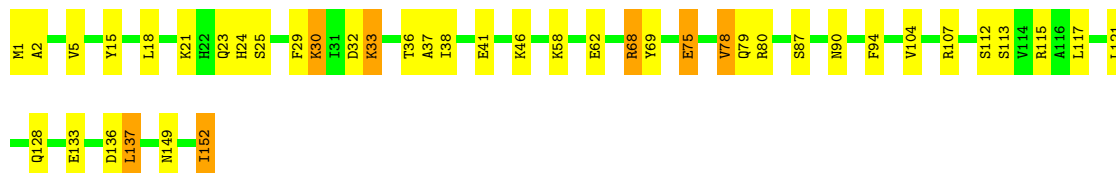




4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Actin-depolymerizing factor 2, isoform c

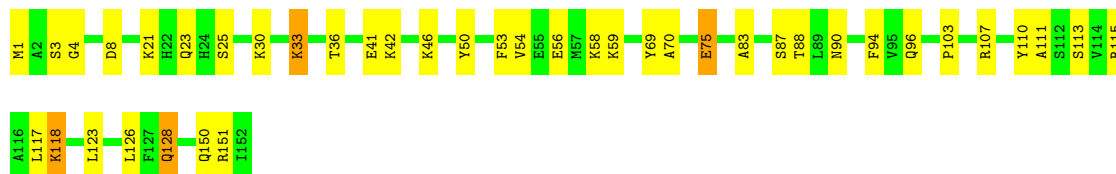
Chain A: 72% 23% 5%



4.2.4 Score per residue for model 4

- Molecule 1: Actin-depolymerizing factor 2, isoform c

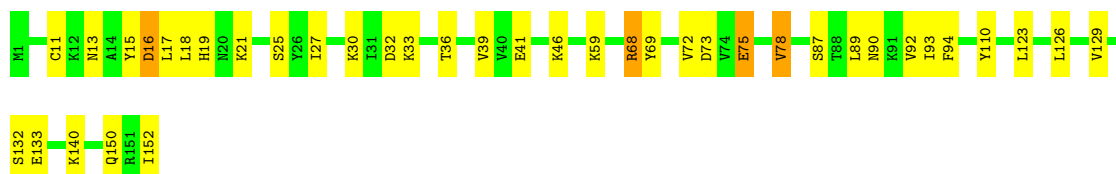
Chain A: 73% 24% .



4.2.5 Score per residue for model 5

- Molecule 1: Actin-depolymerizing factor 2, isoform c

Chain A: 74% 23% .



4.2.6 Score per residue for model 6

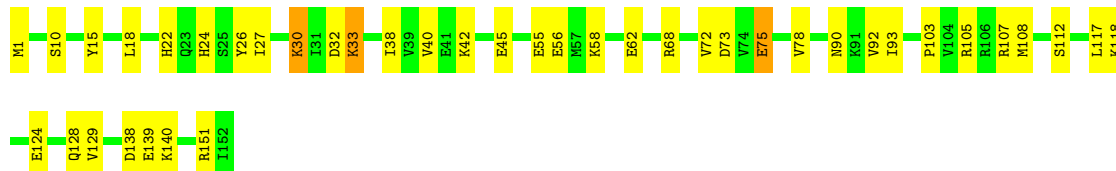
- Molecule 1: Actin-depolymerizing factor 2, isoform c

Chain A: 78% 18% .



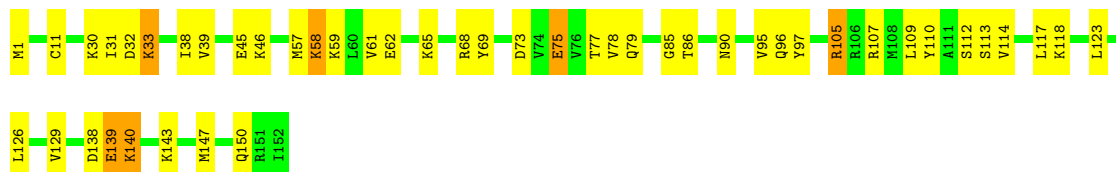
4.2.7 Score per residue for model 7

- Molecule 1: Actin-depolymerizing factor 2, isoform c



4.2.8 Score per residue for model 8

- Molecule 1: Actin-depolymerizing factor 2, isoform c



4.2.9 Score per residue for model 9

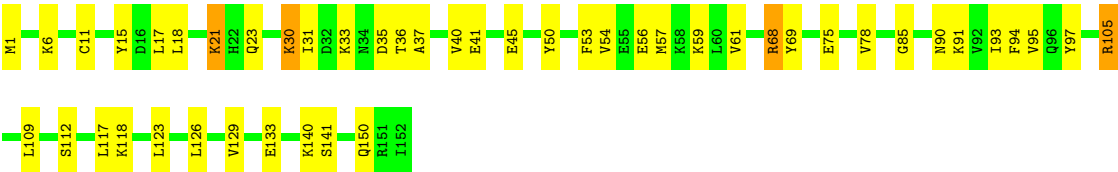
- Molecule 1: Actin-depolymerizing factor 2, isoform c



4.2.10 Score per residue for model 10

- Molecule 1: Actin-depolymerizing factor 2, isoform c





5 Refinement protocol and experimental data overview

The models were refined using the following method: *Water refinement*.

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
CYANA	structure calculation	3.0
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1795
Number of shifts mapped to atoms	1795
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1193	1203	1200	23±4
All	All	11930	12030	12000	233

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:MET:HA	1:A:112:SER:HA	0.94	1.36	10	5
1:A:25:SER:HB2	1:A:46:LYS:HA	0.85	1.49	3	3
1:A:56:GLU:HA	1:A:59:LYS:HE2	0.78	1.52	10	4
1:A:30:LYS:HD3	1:A:32:ASP:HB2	0.76	1.58	2	1
1:A:33:LYS:HE2	1:A:35:ASP:HB3	0.73	1.57	2	1
1:A:30:LYS:HB3	1:A:68:ARG:HD2	0.72	1.61	3	2
1:A:30:LYS:HB2	1:A:41:GLU:HB2	0.71	1.61	4	1
1:A:32:ASP:O	1:A:33:LYS:HG2	0.67	1.89	3	5
1:A:96:GLN:HE22	1:A:114:VAL:HG22	0.67	1.49	8	1
1:A:33:LYS:HD3	1:A:37:ALA:HB3	0.67	1.66	3	2
1:A:61:VAL:HG22	1:A:68:ARG:HH21	0.66	1.50	10	1
1:A:16:ASP:HA	1:A:19:HIS:HB3	0.66	1.68	2	2
1:A:75:GLU:HB3	1:A:90:ASN:HB3	0.65	1.67	3	2
1:A:1:MET:HB3	1:A:115:ARG:HB2	0.65	1.68	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:ASP:HB2	1:A:92:VAL:HB	0.65	1.69	9	2
1:A:137:LEU:H	1:A:137:LEU:HD13	0.63	1.52	3	1
1:A:30:LYS:HG2	1:A:41:GLU:HB2	0.63	1.71	2	1
1:A:18:LEU:HB3	1:A:24:HIS:HB2	0.63	1.70	7	3
1:A:75:GLU:HA	1:A:90:ASN:HA	0.62	1.70	4	6
1:A:21:LYS:HE2	1:A:21:LYS:HA	0.61	1.70	4	1
1:A:80:ARG:HH22	1:A:148:SER:HA	0.60	1.56	9	1
1:A:42:LYS:HE2	1:A:56:GLU:HG3	0.60	1.73	7	1
1:A:118:LYS:HA	1:A:123:LEU:HD12	0.59	1.74	9	2
1:A:105:ARG:HD2	1:A:105:ARG:H	0.59	1.57	10	3
1:A:78:VAL:HG23	1:A:87:SER:HB3	0.59	1.74	1	1
1:A:38:ILE:HD13	1:A:117:LEU:HD23	0.59	1.74	7	1
1:A:91:LYS:HG3	1:A:150:GLN:HG2	0.58	1.75	9	2
1:A:126:LEU:HD21	1:A:150:GLN:HA	0.58	1.75	10	1
1:A:123:LEU:HA	1:A:126:LEU:HD23	0.58	1.74	8	5
1:A:25:SER:OG	1:A:46:LYS:HA	0.57	1.99	4	2
1:A:15:TYR:O	1:A:18:LEU:HG	0.57	1.99	9	6
1:A:103:PRO:O	1:A:107:ARG:HG3	0.57	2.00	7	2
1:A:29:PHE:HB2	1:A:69:TYR:HB2	0.57	1.76	3	3
1:A:17:LEU:O	1:A:21:LYS:HB2	0.57	1.99	9	1
1:A:95:VAL:HA	1:A:129:VAL:O	0.57	2.00	10	2
1:A:80:ARG:NH2	1:A:148:SER:HA	0.57	2.13	9	1
1:A:69:TYR:HB2	1:A:94:PHE:CZ	0.57	2.35	5	1
1:A:27:ILE:HD11	1:A:40:VAL:HG22	0.56	1.77	1	2
1:A:57:MET:HE2	1:A:61:VAL:HG21	0.56	1.76	8	1
1:A:67:CYS:SG	1:A:106:ARG:HD3	0.56	2.41	1	2
1:A:83:ALA:HB3	1:A:87:SER:HB2	0.56	1.75	4	1
1:A:6:LYS:O	1:A:37:ALA:HA	0.56	2.01	10	2
1:A:5:VAL:HG13	1:A:36:THR:HB	0.56	1.76	6	1
1:A:79:GLN:O	1:A:80:ARG:HD2	0.55	2.01	3	1
1:A:77:THR:OG1	1:A:86:THR:HB	0.55	2.01	8	1
1:A:75:GLU:HB3	1:A:90:ASN:CG	0.55	2.26	7	1
1:A:18:LEU:O	1:A:22:HIS:HA	0.55	2.01	6	2
1:A:38:ILE:HD13	1:A:117:LEU:HB3	0.55	1.77	3	1
1:A:6:LYS:N	1:A:6:LYS:HD2	0.55	2.17	9	1
1:A:69:TYR:HB3	1:A:94:PHE:CZ	0.54	2.37	10	2
1:A:141:SER:O	1:A:145:ASP:HB2	0.54	2.03	2	1
1:A:151:ARG:O	1:A:151:ARG:HD3	0.54	2.01	7	2
1:A:11:CYS:SG	1:A:39:VAL:HA	0.54	2.43	5	2
1:A:33:LYS:HG3	1:A:35:ASP:H	0.54	1.62	6	2
1:A:31:ILE:HD13	1:A:109:LEU:HB3	0.54	1.79	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:MET:HA	1:A:111:ALA:O	0.53	2.04	1	1
1:A:151:ARG:HD3	1:A:151:ARG:O	0.52	2.04	6	1
1:A:93:ILE:HD11	1:A:129:VAL:HG23	0.52	1.81	5	2
1:A:17:LEU:O	1:A:21:LYS:HB3	0.52	2.05	10	1
1:A:73:ASP:HA	1:A:92:VAL:HA	0.52	1.80	5	2
1:A:11:CYS:HB2	1:A:29:PHE:HE1	0.52	1.65	1	1
1:A:68:ARG:HA	1:A:68:ARG:HE	0.51	1.66	5	1
1:A:107:ARG:HA	1:A:110:TYR:HB3	0.51	1.81	4	1
1:A:94:PHE:O	1:A:128:GLN:HA	0.51	2.06	4	1
1:A:69:TYR:HB3	1:A:96:GLN:HA	0.50	1.82	8	1
1:A:1:MET:HG2	1:A:111:ALA:HB1	0.50	1.81	6	2
1:A:66:GLU:HB3	1:A:68:ARG:NH1	0.50	2.21	1	1
1:A:13:ASN:O	1:A:17:LEU:HG	0.50	2.07	5	2
1:A:30:LYS:HG3	1:A:41:GLU:HB2	0.49	1.83	10	2
1:A:117:LEU:HD12	1:A:118:LYS:N	0.49	2.23	7	5
1:A:113:SER:O	1:A:117:LEU:HG	0.49	2.08	4	5
1:A:104:VAL:HA	1:A:107:ARG:HG2	0.48	1.85	3	1
1:A:140:LYS:HD2	1:A:141:SER:N	0.48	2.24	10	1
1:A:76:VAL:HB	1:A:150:GLN:OE1	0.48	2.09	1	1
1:A:133:GLU:HB3	1:A:136:ASP:HB2	0.48	1.85	3	1
1:A:46:LYS:H	1:A:46:LYS:HD3	0.48	1.69	6	1
1:A:68:ARG:N	1:A:68:ARG:HD3	0.48	2.24	9	1
1:A:118:LYS:NZ	1:A:124:GLU:HA	0.48	2.24	7	1
1:A:93:ILE:HB	1:A:126:LEU:HD13	0.47	1.86	10	1
1:A:25:SER:CB	1:A:46:LYS:HA	0.47	2.38	2	1
1:A:53:PHE:HZ	1:A:70:ALA:HB1	0.47	1.69	4	1
1:A:1:MET:C	1:A:112:SER:HA	0.47	2.33	1	1
1:A:30:LYS:HD2	1:A:41:GLU:HB2	0.47	1.86	3	1
1:A:58:LYS:O	1:A:62:GLU:HG3	0.47	2.10	7	2
1:A:5:VAL:HG21	1:A:113:SER:HB2	0.47	1.87	3	1
1:A:117:LEU:O	1:A:121:LEU:HB2	0.47	2.09	3	1
1:A:41:GLU:O	1:A:42:LYS:HD2	0.47	2.10	4	1
1:A:28:ILE:HG23	1:A:68:ARG:HB3	0.47	1.86	2	1
1:A:1:MET:CA	1:A:112:SER:HA	0.47	2.24	10	3
1:A:25:SER:O	1:A:72:VAL:HA	0.47	2.10	2	1
1:A:28:ILE:CG2	1:A:68:ARG:HB3	0.47	2.40	2	1
1:A:94:PHE:HB3	1:A:128:GLN:HG2	0.46	1.86	6	1
1:A:57:MET:O	1:A:61:VAL:HG23	0.46	2.11	9	2
1:A:78:VAL:O	1:A:87:SER:HB2	0.46	2.10	5	1
1:A:50:TYR:O	1:A:54:VAL:HG23	0.46	2.11	10	2
1:A:55:GLU:HA	1:A:58:LYS:HB3	0.46	1.88	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:GLY:HA3	1:A:53:PHE:HE1	0.46	1.71	2	1
1:A:107:ARG:HA	1:A:110:TYR:CE2	0.45	2.46	8	1
1:A:139:GLU:O	1:A:143:LYS:HB3	0.45	2.11	8	1
1:A:142:VAL:HG12	1:A:146:LEU:HD23	0.45	1.87	9	1
1:A:105:ARG:HD2	1:A:105:ARG:N	0.45	2.26	1	2
1:A:78:VAL:HG12	1:A:79:GLN:H	0.45	1.70	9	1
1:A:41:GLU:C	1:A:42:LYS:HD2	0.45	2.36	4	1
1:A:21:LYS:O	1:A:21:LYS:HD3	0.45	2.12	5	1
1:A:138:ASP:HB3	1:A:140:LYS:CD	0.45	2.40	8	1
1:A:152:ILE:HD12	1:A:152:ILE:OXT	0.45	2.11	3	1
1:A:11:CYS:HB2	1:A:29:PHE:CE1	0.45	2.47	6	1
1:A:50:TYR:HA	1:A:53:PHE:HB3	0.44	1.88	9	2
1:A:33:LYS:HG3	1:A:35:ASP:O	0.44	2.12	9	1
1:A:137:LEU:O	1:A:137:LEU:HD13	0.44	2.13	9	1
1:A:134:MET:O	1:A:137:LEU:HG	0.43	2.13	6	1
1:A:26:TYR:HB3	1:A:72:VAL:HG23	0.43	1.90	7	1
1:A:105:ARG:O	1:A:109:LEU:HG	0.43	2.13	8	1
1:A:44:GLY:HA3	1:A:53:PHE:CE1	0.43	2.48	2	1
1:A:30:LYS:HE3	1:A:41:GLU:OE2	0.43	2.13	2	1
1:A:21:LYS:HD3	1:A:21:LYS:O	0.43	2.13	2	1
1:A:45:GLU:OE1	1:A:46:LYS:HG2	0.43	2.14	8	1
1:A:97:TYR:CE2	1:A:99:PRO:HG3	0.43	2.48	9	1
1:A:59:LYS:HA	1:A:62:GLU:OE2	0.43	2.14	2	1
1:A:147:MET:HA	1:A:150:GLN:OE1	0.43	2.13	1	2
1:A:32:ASP:O	1:A:33:LYS:HB3	0.43	2.13	2	1
1:A:69:TYR:OH	1:A:113:SER:HB3	0.43	2.13	3	2
1:A:75:GLU:HB2	1:A:88:THR:HG22	0.43	1.90	4	1
1:A:79:GLN:HA	1:A:85:GLY:O	0.43	2.14	8	1
1:A:149:ASN:HA	1:A:152:ILE:CG1	0.42	2.44	3	1
1:A:138:ASP:HB3	1:A:140:LYS:CE	0.42	2.44	7	1
1:A:68:ARG:HD2	1:A:97:TYR:HB2	0.42	1.90	10	1
1:A:18:LEU:HD12	1:A:19:HIS:N	0.42	2.29	1	1
1:A:78:VAL:O	1:A:87:SER:N	0.42	2.52	3	1
1:A:146:LEU:O	1:A:150:GLN:HG3	0.42	2.14	2	1
1:A:89:LEU:HB2	1:A:150:GLN:NE2	0.42	2.29	5	1
1:A:110:TYR:O	1:A:114:VAL:HG23	0.42	2.12	2	1
1:A:21:LYS:CG	1:A:23:GLN:HG3	0.42	2.45	10	1
1:A:94:PHE:HD2	1:A:128:GLN:HG3	0.42	1.74	3	1
1:A:105:ARG:HD3	1:A:105:ARG:H	0.42	1.74	2	1
1:A:26:TYR:HD1	1:A:72:VAL:HB	0.42	1.73	2	1
1:A:139:GLU:HB2	1:A:143:LYS:HB2	0.42	1.91	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:LEU:HA	1:A:121:LEU:HD13	0.41	1.90	1	1
1:A:11:CYS:HA	1:A:40:VAL:HG23	0.41	1.92	10	1
1:A:75:GLU:H	1:A:75:GLU:CD	0.41	2.23	4	2
1:A:139:GLU:HB2	1:A:143:LYS:CB	0.41	2.45	6	1
1:A:105:ARG:O	1:A:108:MET:HG2	0.41	2.14	7	1
1:A:32:ASP:HB3	1:A:39:VAL:CG1	0.41	2.45	9	1
1:A:90:ASN:O	1:A:91:LYS:HD2	0.41	2.15	6	1
1:A:68:ARG:O	1:A:97:TYR:HB2	0.41	2.14	8	1
1:A:115:ARG:C	1:A:115:ARG:HD3	0.41	2.41	3	1
1:A:114:VAL:O	1:A:118:LYS:HB2	0.41	2.15	2	1
1:A:30:LYS:HD3	1:A:41:GLU:OE2	0.41	2.16	5	1
1:A:69:TYR:CE1	1:A:96:GLN:HB3	0.41	2.50	4	1
1:A:25:SER:HB2	1:A:46:LYS:CA	0.40	2.42	2	1
1:A:54:VAL:O	1:A:58:LYS:HG3	0.40	2.16	4	1
1:A:94:PHE:HE2	1:A:117:LEU:HD13	0.40	1.77	4	1
1:A:58:LYS:HD3	1:A:59:LYS:N	0.40	2.31	8	1
1:A:31:ILE:HD12	1:A:38:ILE:HG13	0.40	1.92	8	1
1:A:91:LYS:HG2	1:A:150:GLN:HG2	0.40	1.94	6	1
1:A:67:CYS:O	1:A:68:ARG:HD2	0.40	2.17	1	1
1:A:21:LYS:HE3	1:A:21:LYS:HA	0.40	1.93	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	150/152 (99%)	137±3 (91±2%)	11±3 (7±2%)	2±1 (1±1%)	12	60
All	All	1500/1520 (99%)	1369 (91%)	112 (7%)	19 (1%)	12	60

All 7 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	33	LYS	8
1	A	36	THR	6

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Mol	Chain	Res	Type	Models (Total)
1	A	2	ALA	1
1	A	3	SER	1
1	A	4	GLY	1
1	A	150	GLN	1
1	A	85	GLY	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	133/133 (100%)	126±3 (95±2%)	7±3 (5±2%)	22	72
All	All	1330/1330 (100%)	1260 (95%)	70 (5%)	22	72

All 38 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	78	VAL	6
1	A	30	LYS	5
1	A	75	GLU	5
1	A	68	ARG	4
1	A	133	GLU	4
1	A	128	GLN	3
1	A	139	GLU	3
1	A	105	ARG	3
1	A	118	LYS	2
1	A	151	ARG	2
1	A	21	LYS	2
1	A	23	GLN	2
1	A	152	ILE	2
1	A	140	LYS	2
1	A	45	GLU	2
1	A	145	ASP	1
1	A	137	LEU	1
1	A	8	ASP	1
1	A	33	LYS	1
1	A	115	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	16	ASP	1
1	A	27	ILE	1
1	A	59	LYS	1
1	A	72	VAL	1
1	A	110	TYR	1
1	A	132	SER	1
1	A	46	LYS	1
1	A	52	GLU	1
1	A	69	TYR	1
1	A	90	ASN	1
1	A	94	PHE	1
1	A	10	SER	1
1	A	58	LYS	1
1	A	62	GLU	1
1	A	65	LYS	1
1	A	73	ASP	1
1	A	13	ASN	1
1	A	63	ASP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 87% 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	1795
Number of shifts mapped to atoms	1795
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	150	-0.37 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	144	-0.13 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	147	0.08 ± 0.06	None needed (< 0.5 ppm)
^{15}N	144	0.37 ± 0.26	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 87%, i.e. 1794 atoms were assigned a chemical shift out of a possible 2067. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	739/758 (97%)	298/306 (97%)	297/304 (98%)	144/148 (97%)
Sidechain	971/1191 (82%)	664/771 (86%)	307/371 (83%)	0/49 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	84/118 (71%)	42/56 (75%)	42/56 (75%)	0/6 (0%)
Overall	1794/2067 (87%)	1004/1133 (89%)	646/731 (88%)	144/203 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1794 atoms were assigned a chemical shift out of a possible 2067. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	739/758 (97%)	298/306 (97%)	297/304 (98%)	144/148 (97%)
Sidechain	971/1191 (82%)	664/771 (86%)	307/371 (83%)	0/49 (0%)
Aromatic	84/118 (71%)	42/56 (75%)	42/56 (75%)	0/6 (0%)
Overall	1794/2067 (87%)	1004/1133 (89%)	646/731 (88%)	144/203 (71%)

7.1.4 Statistically unusual chemical shifts ⓘ

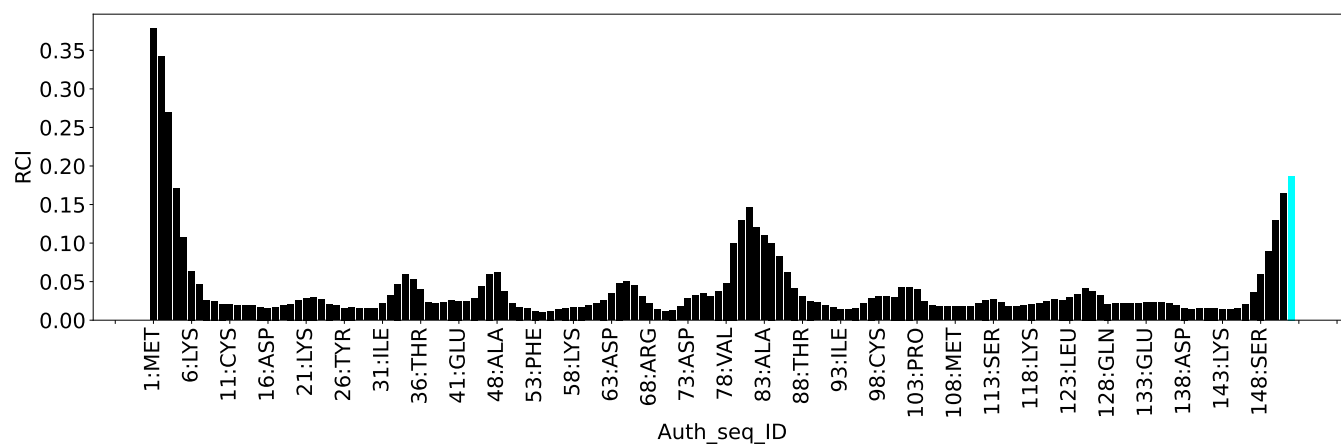
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	28	ILE	CG2	28.79	10.93 – 24.12	8.5
1	A	28	ILE	CG1	17.45	19.24 – 36.26	-6.0
1	A	26	TYR	CD1	125.46	125.84 – 139.60	-5.3

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:



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	1909
Intra-residue ($ i-j =0$)	252
Sequential ($ i-j =1$)	546
Medium range ($ i-j >1$ and $ i-j <5$)	551
Long range ($ i-j \geq 5$)	500
Inter-chain	0
Hydrogen bond restraints	60
Disulfide bond restraints	0
Total dihedral-angle restraints	241
Number of unmapped restraints	0
Number of restraints per residue	14.1
Number of long range restraints per residue ¹	3.6

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)	64.1	0.2
0.2-0.5 (Medium)	133.2	0.5
>0.5 (Large)	147.7	2.93

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)	15.8	4.66
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

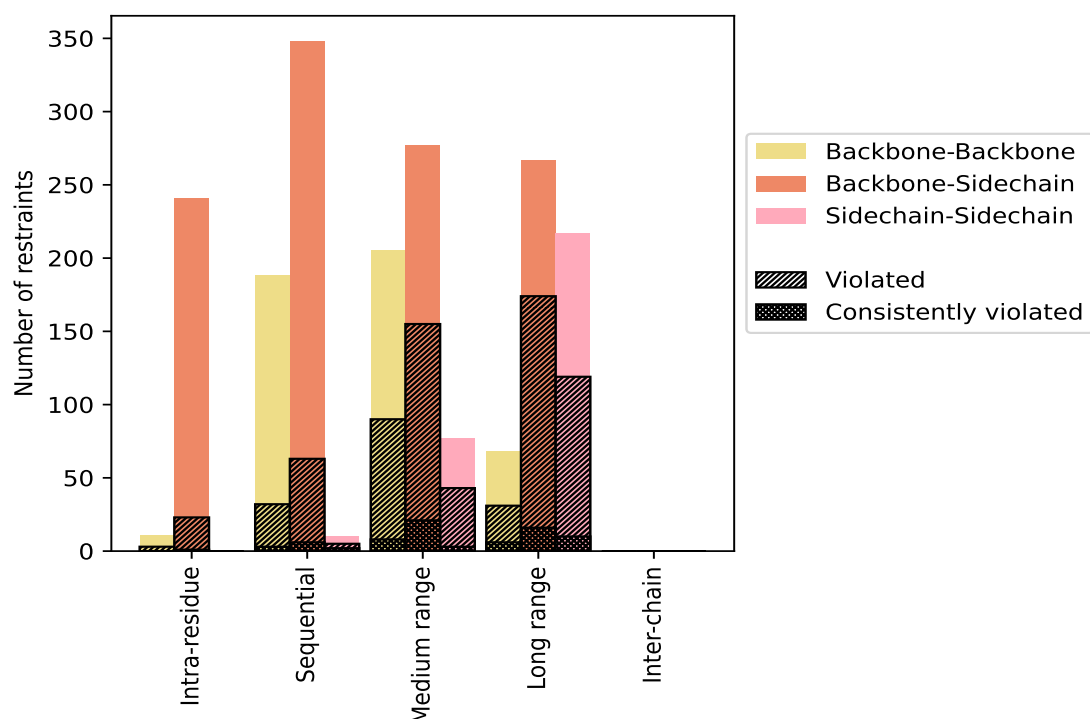
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	252	13.2	26	10.3	1.4	1	0.4	0.1
Backbone-Backbone	11	0.6	3	27.3	0.2	0	0.0	0.0
Backbone-Sidechain	241	12.6	23	9.5	1.2	1	0.4	0.1
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	546	28.6	100	18.3	5.2	11	2.0	0.6
Backbone-Backbone	188	9.8	32	17.0	1.7	3	1.6	0.2
Backbone-Sidechain	348	18.2	63	18.1	3.3	6	1.7	0.3
Sidechain-Sidechain	10	0.5	5	50.0	0.3	2	20.0	0.1
Medium range ($i-j >1$ & $i-j <5$)	551	28.9	283	51.4	14.8	32	5.8	1.7
Backbone-Backbone	205	10.7	90	43.9	4.7	8	3.9	0.4
Backbone-Sidechain	269	14.1	150	55.8	7.9	21	7.8	1.1
Sidechain-Sidechain	77	4.0	43	55.8	2.3	3	3.9	0.2
Long range ($i-j \geq 5$)	500	26.2	308	61.6	16.1	32	6.4	1.7
Backbone-Backbone	68	3.6	31	45.6	1.6	6	8.8	0.3
Backbone-Sidechain	215	11.3	158	73.5	8.3	16	7.4	0.8
Sidechain-Sidechain	217	11.4	119	54.8	6.2	10	4.6	0.5
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	60	3.1	21	35.0	1.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1909	100.0	738	38.7	38.7	76	4.0	4.0
Backbone-Backbone	472	24.7	156	33.1	8.2	17	3.6	0.9
Backbone-Sidechain	1133	59.4	415	36.6	21.7	44	3.9	2.3
Sidechain-Sidechain	304	15.9	167	54.9	8.7	15	4.9	0.8

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

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



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

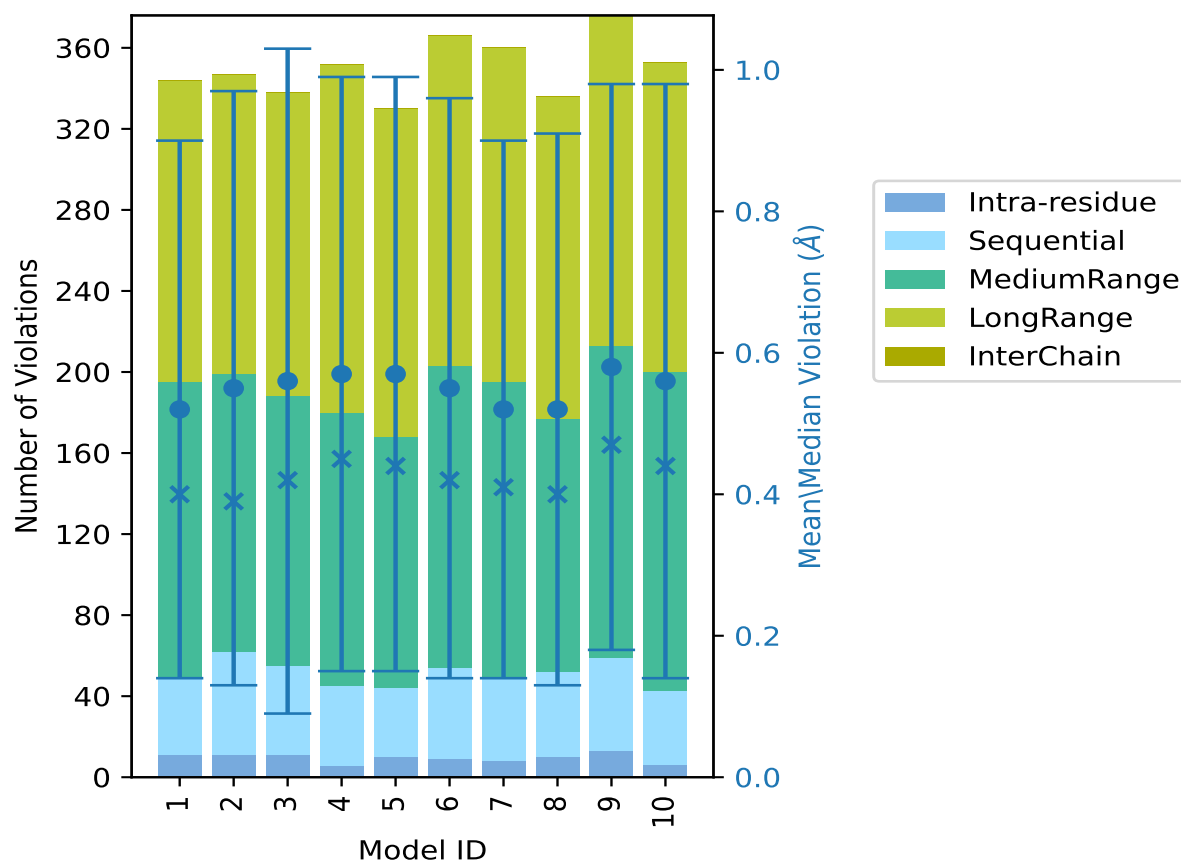
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	11	38	146	149	0	344	0.52	1.93	0.38	0.4
2	11	51	137	148	0	347	0.55	2.16	0.42	0.39
3	11	44	133	150	0	338	0.56	2.93	0.47	0.42
4	6	39	135	172	0	352	0.57	1.98	0.42	0.45
5	10	34	124	162	0	330	0.57	2.47	0.42	0.44
6	9	45	149	163	0	366	0.55	2.38	0.41	0.42
7	8	41	146	165	0	360	0.52	2.58	0.38	0.41
8	10	42	125	159	0	336	0.52	1.91	0.39	0.4
9	13	46	154	163	0	376	0.58	1.99	0.4	0.47
10	6	37	157	153	0	353	0.56	2.61	0.42	0.44

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, 1132(IR:226, SQ:446, MR:268, LR:192, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
9	27	48	62	0	146	1	10.0
3	16	46	30	0	95	2	20.0
1	12	25	32	0	70	3	30.0

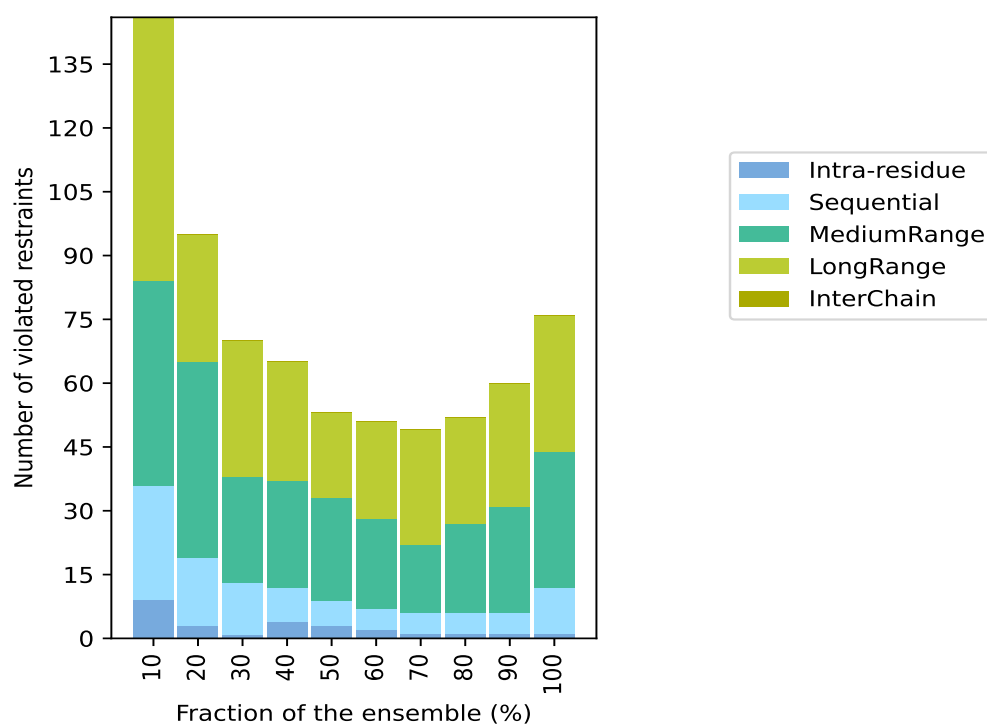
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
4	8	25	28	0	65	4	40.0
3	6	24	20	0	53	5	50.0
2	5	21	23	0	51	6	60.0
1	5	16	27	0	49	7	70.0
1	5	21	25	0	52	8	80.0
1	5	25	29	0	60	9	90.0
1	11	32	32	0	76	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 ⓘ

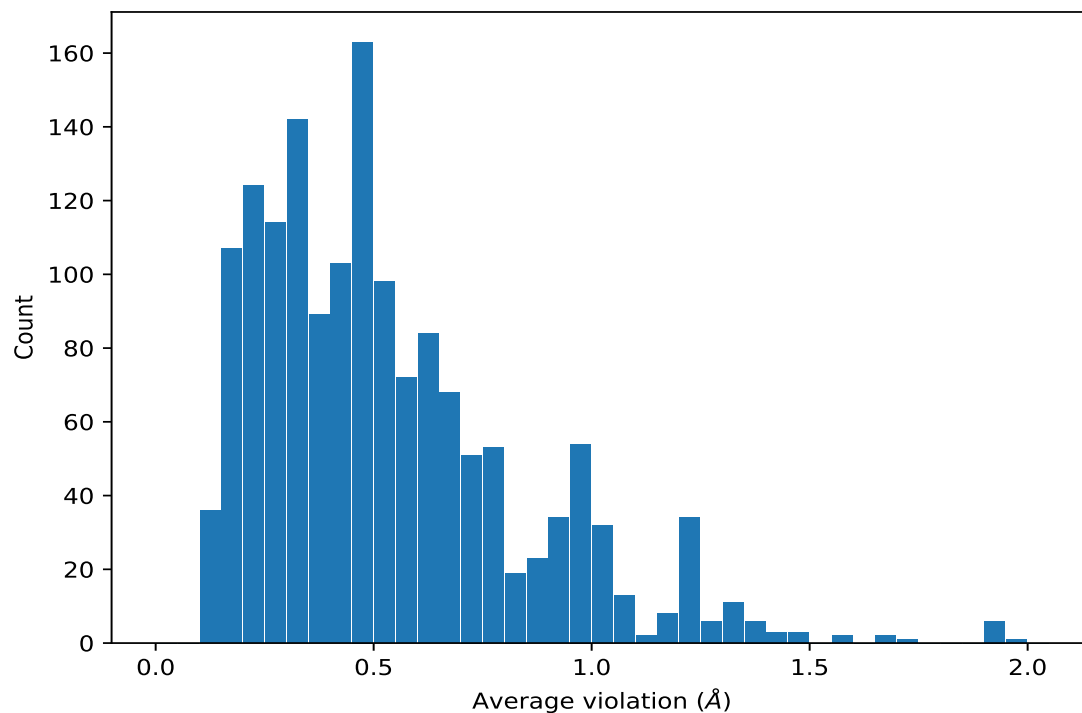


9.4 Most violated distance restraints in the ensemble ⓘ

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)
(1,170)	1:11:A:CYS:H	1:40:A:VAL:HB	10	1.98	0.19	1.95
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB2	10	1.68	0.22	1.62
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB3	10	1.68	0.22	1.62
(1,169)	1:11:A:CYS:H	1:40:A:VAL:HA	10	1.59	0.15	1.62
(1,1084)	1:93:A:ILE:HA	1:146:A:LEU:HB2	10	1.46	0.27	1.48
(1,163)	1:10:A:SER:HB2	1:40:A:VAL:HB	10	1.39	0.29	1.35
(1,163)	1:10:A:SER:HB3	1:40:A:VAL:HB	10	1.39	0.29	1.35
(1,1653)	1:140:A:LYS:HE2	1:142:A:VAL:H	10	1.33	0.33	1.46
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB2	10	1.31	0.53	1.16
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB3	10	1.31	0.53	1.16
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB2	10	1.31	0.53	1.16
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB3	10	1.31	0.53	1.16
(1,76)	1:7:A:VAL:HB	1:38:A:ILE:HB	10	1.3	0.54	1.57
(1,897)	1:75:A:GLU:HG3	1:89:A:LEU:H	10	1.28	0.38	1.32
(1,894)	1:75:A:GLU:HG3	1:76:A:VAL:H	10	1.24	0.26	1.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,994)	1:80:A:ARG:HG2	1:86:A:THR:HA	10	1.21	0.42	1.38
(1,994)	1:80:A:ARG:HG3	1:86:A:THR:HA	10	1.21	0.42	1.38
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB2	10	1.21	0.44	1.17
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB3	10	1.21	0.44	1.17
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB2	10	1.21	0.44	1.17
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB3	10	1.21	0.44	1.17
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB2	10	1.21	0.44	1.17
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB3	10	1.21	0.44	1.17
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB2	10	1.21	0.44	1.17
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB3	10	1.21	0.44	1.17
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB2	10	1.21	0.44	1.17
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB3	10	1.21	0.44	1.17
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB2	10	1.21	0.44	1.17
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB3	10	1.21	0.44	1.17
(1,316)	1:18:A:LEU:HD11	1:123:A:LEU:HG	10	1.16	0.3	1.25
(1,316)	1:18:A:LEU:HD12	1:123:A:LEU:HG	10	1.16	0.3	1.25
(1,316)	1:18:A:LEU:HD13	1:123:A:LEU:HG	10	1.16	0.3	1.25
(1,205)	1:12:A:LYS:HD3	1:14:A:ALA:H	10	1.05	0.02	1.05
(1,207)	1:12:A:LYS:HD3	1:15:A:TYR:HA	10	1.05	0.11	1.1
(1,891)	1:75:A:GLU:HG2	1:89:A:LEU:H	10	1.03	0.3	1.12
(1,1443)	1:118:A:LYS:HE3	1:119:A:ALA:H	10	0.96	0.24	0.92
(1,524)	1:33:A:LYS:HG2	1:36:A:THR:HB	10	0.95	0.27	1.03
(1,94)	1:7:A:VAL:HG21	1:38:A:ILE:HB	10	0.94	0.38	1.1
(1,94)	1:7:A:VAL:HG22	1:38:A:ILE:HB	10	0.94	0.38	1.1
(1,94)	1:7:A:VAL:HG23	1:38:A:ILE:HB	10	0.94	0.38	1.1
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB2	10	0.93	0.25	0.97
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB3	10	0.93	0.25	0.97
(1,1067)	1:92:A:VAL:H	1:127:A:PHE:H	10	0.91	0.36	0.98
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	10	0.88	0.41	0.79
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	10	0.88	0.41	0.79
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG2	10	0.88	0.2	0.94
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG3	10	0.88	0.2	0.94
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG2	10	0.88	0.2	0.94
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG3	10	0.88	0.2	0.94
(1,1670)	1:141:A:SER:HB3	1:145:A:ASP:HA	10	0.83	0.04	0.83
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG21	10	0.82	0.31	0.84
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG22	10	0.82	0.31	0.84
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG23	10	0.82	0.31	0.84
(1,1664)	1:141:A:SER:HA	1:143:A:LYS:H	10	0.8	0.13	0.81
(1,72)	1:7:A:VAL:HB	1:117:A:LEU:HA	10	0.79	0.38	0.8
(1,1442)	1:118:A:LYS:HE2	1:121:A:LEU:H	10	0.77	0.07	0.8
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB2	10	0.77	0.08	0.78

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB3	10	0.77	0.08	0.78
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB2	10	0.77	0.08	0.78
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB3	10	0.77	0.08	0.78
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB2	10	0.7	0.3	0.79
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB3	10	0.7	0.3	0.79
(1,1344)	1:111:A:ALA:HA	1:115:A:ARG:H	10	0.7	0.27	0.64
(1,1726)	1:144:A:SER:HB3	1:146:A:LEU:H	10	0.68	0.12	0.68
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	10	0.66	0.29	0.68
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	10	0.66	0.29	0.68
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	10	0.66	0.29	0.68
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	10	0.66	0.29	0.68
(1,1299)	1:108:A:MET:HB2	1:112:A:SER:H	10	0.65	0.22	0.64
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB2	10	0.65	0.27	0.61
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB3	10	0.65	0.27	0.61
(1,137)	1:8:A:ASP:HB2	1:9:A:PRO:HA	10	0.61	0.06	0.6
(1,137)	1:8:A:ASP:HB3	1:9:A:PRO:HA	10	0.61	0.06	0.6
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG2	10	0.59	0.22	0.58
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG3	10	0.59	0.22	0.58
(1,1709)	1:143:A:LYS:HB2	1:147:A:MET:H	10	0.59	0.17	0.64
(1,1718)	1:144:A:SER:H	1:146:A:LEU:H	10	0.58	0.16	0.51
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB1	10	0.57	0.28	0.53
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB2	10	0.57	0.28	0.53
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB3	10	0.57	0.28	0.53
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB1	10	0.57	0.28	0.53
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB2	10	0.57	0.28	0.53
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB3	10	0.57	0.28	0.53
(1,327)	1:18:A:LEU:HD21	1:73:A:ASP:HA	10	0.56	0.34	0.43
(1,327)	1:18:A:LEU:HD22	1:73:A:ASP:HA	10	0.56	0.34	0.43
(1,327)	1:18:A:LEU:HD23	1:73:A:ASP:HA	10	0.56	0.34	0.43
(1,1378)	1:114:A:VAL:HB	1:118:A:LYS:H	10	0.56	0.24	0.48
(1,1333)	1:110:A:TYR:HA	1:114:A:VAL:H	10	0.55	0.23	0.59
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD2	10	0.54	0.3	0.52
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD3	10	0.54	0.3	0.52
(1,158)	1:10:A:SER:HB3	1:12:A:LYS:H	10	0.53	0.12	0.51
(1,1316)	1:109:A:LEU:HA	1:113:A:SER:H	10	0.53	0.23	0.58
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG21	10	0.52	0.18	0.59
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG22	10	0.52	0.18	0.59
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG23	10	0.52	0.18	0.59
(1,73)	1:7:A:VAL:HB	1:120:A:SER:HA	10	0.5	0.09	0.52
(1,206)	1:12:A:LYS:HD3	1:15:A:TYR:H	10	0.5	0.06	0.52
(2,1)	1:1:A:MET:HA	1:114:A:VAL:HA	10	0.49	0.09	0.53
(1,1777)	1:149:A:ASN:HB2	1:151:A:ARG:H	10	0.48	0.13	0.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1777)	1:149:A:ASN:HB3	1:151:A:ARG:H	10	0.48	0.13	0.46
(1,1117)	1:94:A:PHE:HA	1:128:A:GLN:HA	10	0.48	0.13	0.44
(1,1719)	1:144:A:SER:HA	1:146:A:LEU:H	10	0.47	0.11	0.47
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG11	10	0.45	0.15	0.46
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG12	10	0.45	0.15	0.46
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG13	10	0.45	0.15	0.46
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG21	10	0.45	0.15	0.46
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG22	10	0.45	0.15	0.46
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG23	10	0.45	0.15	0.46
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG11	10	0.45	0.15	0.46
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG12	10	0.45	0.15	0.46
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG13	10	0.45	0.15	0.46
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG21	10	0.45	0.15	0.46
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG22	10	0.45	0.15	0.46
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG23	10	0.45	0.15	0.46
(1,83)	1:7:A:VAL:HG11	1:120:A:SER:HA	10	0.44	0.24	0.51
(1,83)	1:7:A:VAL:HG12	1:120:A:SER:HA	10	0.44	0.24	0.51
(1,83)	1:7:A:VAL:HG13	1:120:A:SER:HA	10	0.44	0.24	0.51
(1,1165)	1:97:A:TYR:HA	1:131:A:ALA:HA	10	0.42	0.1	0.43
(1,1725)	1:144:A:SER:HB3	1:145:A:ASP:H	10	0.41	0.1	0.42
(1,1174)	1:99:A:PRO:HA	1:102:A:ALA:H	10	0.41	0.15	0.41
(1,214)	1:12:A:LYS:HG3	1:15:A:TYR:H	10	0.41	0.08	0.39
(1,159)	1:10:A:SER:HB3	1:13:A:ASN:H	10	0.41	0.2	0.33
(1,1658)	1:140:A:LYS:HB2	1:142:A:VAL:H	10	0.41	0.08	0.4
(1,1658)	1:140:A:LYS:HB3	1:142:A:VAL:H	10	0.41	0.08	0.4
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG11	10	0.4	0.19	0.4
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG12	10	0.4	0.19	0.4
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG13	10	0.4	0.19	0.4
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG21	10	0.4	0.19	0.4
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG22	10	0.4	0.19	0.4
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG23	10	0.4	0.19	0.4
(1,1669)	1:141:A:SER:HB3	1:143:A:LYS:H	10	0.39	0.1	0.44
(1,883)	1:75:A:GLU:HB3	1:76:A:VAL:H	10	0.37	0.09	0.4
(1,226)	1:13:A:ASN:HB2	1:14:A:ALA:H	10	0.35	0.07	0.38
(1,1700)	1:143:A:LYS:H	1:145:A:ASP:H	10	0.35	0.08	0.38
(1,277)	1:16:A:ASP:HB2	1:18:A:LEU:H	10	0.33	0.23	0.24
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	10	0.31	0.07	0.3
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	10	0.31	0.07	0.3
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	10	0.31	0.07	0.3
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG11	10	0.31	0.07	0.3
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG12	10	0.31	0.07	0.3
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG13	10	0.31	0.07	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	10	0.31	0.07	0.3
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	10	0.31	0.07	0.3
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	10	0.31	0.07	0.3
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD2	10	0.31	0.09	0.3
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD3	10	0.31	0.09	0.3
(2,6)	1:12:A:LYS:HG2	1:15:A:TYR:H	10	0.3	0.07	0.3
(1,1426)	1:117:A:LEU:HB2	1:119:A:ALA:H	10	0.28	0.1	0.26
(1,1699)	1:143:A:LYS:H	1:144:A:SER:H	10	0.28	0.05	0.26
(1,1114)	1:94:A:PHE:H	1:129:A:VAL:H	10	0.27	0.12	0.24
(1,1729)	1:145:A:ASP:H	1:146:A:LEU:H	10	0.24	0.11	0.26
(1,944)	1:78:A:VAL:H	1:79:A:GLN:H	10	0.24	0.05	0.25
(1,213)	1:12:A:LYS:HG3	1:14:A:ALA:H	10	0.2	0.05	0.2
(1,1074)	1:92:A:VAL:HG11	1:125:A:SER:HA	9	1.93	0.34	1.87
(1,1074)	1:92:A:VAL:HG12	1:125:A:SER:HA	9	1.93	0.34	1.87
(1,1074)	1:92:A:VAL:HG13	1:125:A:SER:HA	9	1.93	0.34	1.87
(1,1074)	1:92:A:VAL:HG21	1:125:A:SER:HA	9	1.93	0.34	1.87
(1,1074)	1:92:A:VAL:HG22	1:125:A:SER:HA	9	1.93	0.34	1.87
(1,1074)	1:92:A:VAL:HG23	1:125:A:SER:HA	9	1.93	0.34	1.87
(1,889)	1:75:A:GLU:HG2	1:88:A:THR:HB	9	1.55	0.81	1.53
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG21	9	1.34	0.43	1.5
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG22	9	1.34	0.43	1.5
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG23	9	1.34	0.43	1.5
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD11	9	1.29	0.5	1.14
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD12	9	1.29	0.5	1.14
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD13	9	1.29	0.5	1.14
(1,969)	1:79:A:GLN:HA	1:86:A:THR:HA	9	1.27	0.26	1.22
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD11	9	1.22	0.39	1.41
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD12	9	1.22	0.39	1.41
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD13	9	1.22	0.39	1.41
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD21	9	1.22	0.39	1.41
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD22	9	1.22	0.39	1.41
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD23	9	1.22	0.39	1.41
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD11	9	1.22	0.39	1.41
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD12	9	1.22	0.39	1.41
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD13	9	1.22	0.39	1.41
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD21	9	1.22	0.39	1.41
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD22	9	1.22	0.39	1.41
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD23	9	1.22	0.39	1.41
(1,945)	1:78:A:VAL:H	1:86:A:THR:HB	9	1.21	0.56	0.99
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE2	9	1.21	0.66	1.25
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE3	9	1.21	0.66	1.25
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE2	9	1.21	0.66	1.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE3	9	1.21	0.66	1.25
(1,609)	1:49:A:PRO:HG2	1:51:A:ALA:H	9	1.05	0.36	1.01
(1,609)	1:49:A:PRO:HG3	1:51:A:ALA:H	9	1.05	0.36	1.01
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG21	9	1.0	0.33	1.08
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG22	9	1.0	0.33	1.08
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG23	9	1.0	0.33	1.08
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG21	9	1.0	0.33	1.08
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG22	9	1.0	0.33	1.08
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG23	9	1.0	0.33	1.08
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG21	9	1.0	0.33	1.08
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG22	9	1.0	0.33	1.08
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG23	9	1.0	0.33	1.08
(1,684)	1:54:A:VAL:HG11	1:138:A:ASP:H	9	0.99	0.46	0.99
(1,684)	1:54:A:VAL:HG12	1:138:A:ASP:H	9	0.99	0.46	0.99
(1,684)	1:54:A:VAL:HG13	1:138:A:ASP:H	9	0.99	0.46	0.99
(1,684)	1:54:A:VAL:HG21	1:138:A:ASP:H	9	0.99	0.46	0.99
(1,684)	1:54:A:VAL:HG22	1:138:A:ASP:H	9	0.99	0.46	0.99
(1,684)	1:54:A:VAL:HG23	1:138:A:ASP:H	9	0.99	0.46	0.99
(1,970)	1:79:A:GLN:HA	1:86:A:THR:HB	9	0.97	0.22	1.07
(1,907)	1:76:A:VAL:H	1:88:A:THR:HB	9	0.97	0.45	0.88
(1,685)	1:54:A:VAL:HG11	1:138:A:ASP:HA	9	0.95	0.43	0.89
(1,685)	1:54:A:VAL:HG12	1:138:A:ASP:HA	9	0.95	0.43	0.89
(1,685)	1:54:A:VAL:HG13	1:138:A:ASP:HA	9	0.95	0.43	0.89
(1,685)	1:54:A:VAL:HG21	1:138:A:ASP:HA	9	0.95	0.43	0.89
(1,685)	1:54:A:VAL:HG22	1:138:A:ASP:HA	9	0.95	0.43	0.89
(1,685)	1:54:A:VAL:HG23	1:138:A:ASP:HA	9	0.95	0.43	0.89
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD11	9	0.94	0.45	0.91
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD12	9	0.94	0.45	0.91
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD13	9	0.94	0.45	0.91
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD11	9	0.94	0.45	0.91
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD12	9	0.94	0.45	0.91
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD13	9	0.94	0.45	0.91
(1,1773)	1:149:A:ASN:HB3	1:151:A:ARG:HA	9	0.94	0.27	1.03
(1,1790)	1:150:A:GLN:HB3	1:152:A:ILE:H	9	0.93	0.58	0.72
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG2	9	0.91	0.47	0.93
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG3	9	0.91	0.47	0.93
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG21	9	0.91	0.25	0.9
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG22	9	0.91	0.25	0.9
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG23	9	0.91	0.25	0.9
(1,1286)	1:107:A:ARG:HD2	1:111:A:ALA:HA	9	0.9	0.47	0.75
(1,1286)	1:107:A:ARG:HD3	1:111:A:ALA:HA	9	0.9	0.47	0.75
(1,736)	1:57:A:MET:HB2	1:60:A:LEU:HG	9	0.88	0.61	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,736)	1:57:A:MET:HB3	1:60:A:LEU:HG	9	0.88	0.61	0.5
(1,1576)	1:134:A:MET:HA	1:138:A:ASP:H	9	0.88	0.33	0.93
(1,511)	1:31:A:ILE:HG21	1:109:A:LEU:HG	9	0.85	0.43	0.98
(1,511)	1:31:A:ILE:HG22	1:109:A:LEU:HG	9	0.85	0.43	0.98
(1,511)	1:31:A:ILE:HG23	1:109:A:LEU:HG	9	0.85	0.43	0.98
(1,528)	1:33:A:LYS:HG3	1:36:A:THR:HB	9	0.82	0.36	1.0
(1,935)	1:77:A:THR:HB	1:87:A:SER:H	9	0.8	0.34	0.79
(1,498)	1:31:A:ILE:HG13	1:38:A:ILE:HA	9	0.8	0.22	0.84
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG21	9	0.78	0.23	0.9
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG22	9	0.78	0.23	0.9
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG23	9	0.78	0.23	0.9
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG21	9	0.77	0.32	0.86
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG22	9	0.77	0.32	0.86
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG23	9	0.77	0.32	0.86
(1,237)	1:14:A:ALA:HA	1:18:A:LEU:H	9	0.75	0.37	0.71
(1,516)	1:32:A:ASP:HB2	1:37:A:ALA:H	9	0.73	0.36	0.73
(1,499)	1:31:A:ILE:HG13	1:38:A:ILE:HB	9	0.68	0.34	0.73
(1,737)	1:57:A:MET:HG2	1:60:A:LEU:HG	9	0.68	0.34	0.69
(1,737)	1:57:A:MET:HG3	1:60:A:LEU:HG	9	0.68	0.34	0.69
(1,123)	1:8:A:ASP:HB2	1:39:A:VAL:HA	9	0.68	0.39	0.49
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB2	9	0.66	0.29	0.52
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB3	9	0.66	0.29	0.52
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB2	9	0.66	0.29	0.52
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB3	9	0.66	0.29	0.52
(1,1778)	1:149:A:ASN:HB2	1:151:A:ARG:HA	9	0.66	0.23	0.68
(1,1778)	1:149:A:ASN:HB3	1:151:A:ARG:HA	9	0.66	0.23	0.68
(1,1172)	1:98:A:CYS:HB2	1:107:A:ARG:HA	9	0.63	0.29	0.61
(1,1172)	1:98:A:CYS:HB3	1:107:A:ARG:HA	9	0.63	0.29	0.61
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB2	9	0.62	0.27	0.8
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB3	9	0.62	0.27	0.8
(1,102)	1:7:A:VAL:HG11	1:120:A:SER:HA	9	0.59	0.27	0.73
(1,102)	1:7:A:VAL:HG12	1:120:A:SER:HA	9	0.59	0.27	0.73
(1,102)	1:7:A:VAL:HG13	1:120:A:SER:HA	9	0.59	0.27	0.73
(1,102)	1:7:A:VAL:HG21	1:120:A:SER:HA	9	0.59	0.27	0.73
(1,102)	1:7:A:VAL:HG22	1:120:A:SER:HA	9	0.59	0.27	0.73
(1,102)	1:7:A:VAL:HG23	1:120:A:SER:HA	9	0.59	0.27	0.73
(1,887)	1:75:A:GLU:HB3	1:89:A:LEU:H	9	0.57	0.31	0.6
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD11	9	0.53	0.2	0.49
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD12	9	0.53	0.2	0.49
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD13	9	0.53	0.2	0.49
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD21	9	0.53	0.2	0.49
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD22	9	0.53	0.2	0.49

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD23	9	0.53	0.2	0.49
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD11	9	0.53	0.36	0.37
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD12	9	0.53	0.36	0.37
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD13	9	0.53	0.36	0.37
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD21	9	0.53	0.36	0.37
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD22	9	0.53	0.36	0.37
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD23	9	0.53	0.36	0.37
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD11	9	0.53	0.36	0.37
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD12	9	0.53	0.36	0.37
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD13	9	0.53	0.36	0.37
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD21	9	0.53	0.36	0.37
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD22	9	0.53	0.36	0.37
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD23	9	0.53	0.36	0.37
(1,1555)	1:132:A:SER:H	1:136:A:ASP:HA	9	0.52	0.44	0.38
(1,1145)	1:95:A:VAL:HG11	1:131:A:ALA:HA	9	0.51	0.3	0.52
(1,1145)	1:95:A:VAL:HG12	1:131:A:ALA:HA	9	0.51	0.3	0.52
(1,1145)	1:95:A:VAL:HG13	1:131:A:ALA:HA	9	0.51	0.3	0.52
(1,1145)	1:95:A:VAL:HG21	1:131:A:ALA:HA	9	0.51	0.3	0.52
(1,1145)	1:95:A:VAL:HG22	1:131:A:ALA:HA	9	0.51	0.3	0.52
(1,1145)	1:95:A:VAL:HG23	1:131:A:ALA:HA	9	0.51	0.3	0.52
(1,892)	1:75:A:GLU:HG2	1:90:A:ASN:HA	9	0.46	0.14	0.46
(1,888)	1:75:A:GLU:HG2	1:76:A:VAL:H	9	0.46	0.19	0.43
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG2	9	0.46	0.24	0.37
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG3	9	0.46	0.24	0.37
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG2	9	0.46	0.24	0.37
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG3	9	0.46	0.24	0.37
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG2	9	0.46	0.24	0.37
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG3	9	0.46	0.24	0.37
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG2	9	0.46	0.24	0.37
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG3	9	0.46	0.24	0.37
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG2	9	0.46	0.24	0.37
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG3	9	0.46	0.24	0.37
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG2	9	0.46	0.24	0.37
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG3	9	0.46	0.24	0.37
(1,1441)	1:118:A:LYS:HE2	1:119:A:ALA:H	9	0.44	0.27	0.33
(2,34)	1:114:A:VAL:HA	1:117:A:LEU:HA	9	0.42	0.14	0.51
(1,669)	1:54:A:VAL:HA	1:56:A:GLU:H	9	0.4	0.09	0.4
(1,654)	1:53:A:PHE:HA	1:55:A:GLU:H	9	0.4	0.11	0.39
(1,1027)	1:86:A:THR:HB	1:87:A:SER:H	9	0.39	0.2	0.37
(1,947)	1:78:A:VAL:H	1:87:A:SER:H	9	0.39	0.16	0.36
(1,162)	1:10:A:SER:HB2	1:13:A:ASN:H	9	0.34	0.15	0.25
(1,162)	1:10:A:SER:HB3	1:13:A:ASN:H	9	0.34	0.15	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	9	0.33	0.02	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	9	0.33	0.02	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	9	0.33	0.02	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	9	0.33	0.02	0.32
(1,1769)	1:149:A:ASN:H	1:150:A:GLN:H	9	0.29	0.09	0.27
(1,675)	1:54:A:VAL:HB	1:56:A:GLU:H	9	0.25	0.1	0.24
(1,227)	1:13:A:ASN:HB2	1:15:A:TYR:H	9	0.25	0.08	0.24
(1,1429)	1:117:A:LEU:HB3	1:119:A:ALA:H	9	0.24	0.12	0.2
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG2	9	0.24	0.08	0.23
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG3	9	0.24	0.08	0.23
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG2	9	0.24	0.08	0.23
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG3	9	0.24	0.08	0.23
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG2	9	0.24	0.08	0.23
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG3	9	0.24	0.08	0.23
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG2	9	0.24	0.08	0.23
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG3	9	0.24	0.08	0.23
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG2	9	0.24	0.08	0.23
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG3	9	0.24	0.08	0.23
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG2	9	0.24	0.08	0.23
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG3	9	0.24	0.08	0.23
(1,1717)	1:144:A:SER:H	1:145:A:ASP:H	9	0.21	0.05	0.22
(1,491)	1:31:A:ILE:HG12	1:109:A:LEU:HA	8	1.49	0.4	1.71
(1,1788)	1:150:A:GLN:HB2	1:152:A:ILE:H	8	1.18	0.49	1.31
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB1	8	1.07	0.49	1.12
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB2	8	1.07	0.49	1.12
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB3	8	1.07	0.49	1.12
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD11	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD12	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD13	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD21	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD22	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD23	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD11	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD12	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD13	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD21	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD22	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD23	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD11	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD12	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD13	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD21	8	0.95	0.27	0.9

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD22	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD23	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD11	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD12	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD13	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD21	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD22	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD23	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD11	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD12	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD13	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD21	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD22	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD23	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD11	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD12	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD13	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD21	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD22	8	0.95	0.27	0.9
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD23	8	0.95	0.27	0.9
(1,75)	1:7:A:VAL:HB	1:38:A:ILE:H	8	0.85	0.29	0.99
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	8	0.78	0.35	0.77
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	8	0.78	0.35	0.77
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	8	0.78	0.35	0.77
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	8	0.78	0.35	0.77
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD2	8	0.75	0.33	0.8
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD3	8	0.75	0.33	0.8
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD2	8	0.75	0.33	0.8
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD3	8	0.75	0.33	0.8
(1,527)	1:33:A:LYS:HG3	1:36:A:THR:HA	8	0.75	0.32	0.8
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	8	0.72	0.45	0.59
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	8	0.72	0.45	0.59
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG2	8	0.71	0.21	0.78
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG3	8	0.71	0.21	0.78
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD11	8	0.7	0.3	0.76
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD12	8	0.7	0.3	0.76
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD13	8	0.7	0.3	0.76
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD21	8	0.7	0.3	0.76
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD22	8	0.7	0.3	0.76
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD23	8	0.7	0.3	0.76
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG2	8	0.67	0.16	0.72
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG3	8	0.67	0.16	0.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG2	8	0.67	0.16	0.72
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG3	8	0.67	0.16	0.72
(1,31)	1:5:A:VAL:HB	1:36:A:THR:HB	8	0.64	0.45	0.44
(1,611)	1:49:A:PRO:HG2	1:52:A:GLU:H	8	0.64	0.24	0.59
(1,611)	1:49:A:PRO:HG3	1:52:A:GLU:H	8	0.64	0.24	0.59
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD2	8	0.64	0.27	0.58
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD3	8	0.64	0.27	0.58
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD2	8	0.64	0.27	0.58
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD3	8	0.64	0.27	0.58
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD2	8	0.64	0.27	0.58
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD3	8	0.64	0.27	0.58
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD2	8	0.64	0.27	0.58
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD3	8	0.64	0.27	0.58
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD2	8	0.64	0.27	0.58
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD3	8	0.64	0.27	0.58
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD2	8	0.64	0.27	0.58
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD3	8	0.64	0.27	0.58
(1,884)	1:75:A:GLU:HB3	1:88:A:THR:HA	8	0.64	0.26	0.75
(1,1651)	1:140:A:LYS:HD3	1:142:A:VAL:H	8	0.64	0.17	0.68
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB1	8	0.63	0.41	0.59
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB2	8	0.63	0.41	0.59
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB3	8	0.63	0.41	0.59
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB1	8	0.63	0.41	0.59
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB2	8	0.63	0.41	0.59
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB3	8	0.63	0.41	0.59
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG21	8	0.61	0.14	0.64
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG22	8	0.61	0.14	0.64
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG23	8	0.61	0.14	0.64
(1,705)	1:55:A:GLU:HA	1:59:A:LYS:HB3	8	0.6	0.25	0.59
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE2	8	0.54	0.41	0.4
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE3	8	0.54	0.41	0.4
(1,93)	1:7:A:VAL:HG21	1:38:A:ILE:H	8	0.52	0.09	0.54
(1,93)	1:7:A:VAL:HG22	1:38:A:ILE:H	8	0.52	0.09	0.54
(1,93)	1:7:A:VAL:HG23	1:38:A:ILE:H	8	0.52	0.09	0.54
(1,452)	1:28:A:ILE:HD11	1:71:A:ALA:H	8	0.52	0.24	0.46
(1,452)	1:28:A:ILE:HD12	1:71:A:ALA:H	8	0.52	0.24	0.46
(1,452)	1:28:A:ILE:HD13	1:71:A:ALA:H	8	0.52	0.24	0.46
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB1	8	0.51	0.26	0.57
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB2	8	0.51	0.26	0.57
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB3	8	0.51	0.26	0.57
(1,898)	1:75:A:GLU:HG3	1:90:A:ASN:HA	8	0.5	0.16	0.52
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB2	8	0.48	0.18	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB3	8	0.48	0.18	0.45
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB2	8	0.48	0.18	0.45
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB3	8	0.48	0.18	0.45
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB2	8	0.48	0.18	0.45
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB3	8	0.48	0.18	0.45
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB2	8	0.48	0.18	0.45
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB3	8	0.48	0.18	0.45
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB2	8	0.48	0.18	0.45
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB3	8	0.48	0.18	0.45
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB2	8	0.48	0.18	0.45
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB3	8	0.48	0.18	0.45
(1,480)	1:30:A:LYS:HB2	1:41:A:GLU:HA	8	0.47	0.28	0.38
(1,480)	1:30:A:LYS:HB3	1:41:A:GLU:HA	8	0.47	0.28	0.38
(1,124)	1:8:A:ASP:HB2	1:39:A:VAL:HB	8	0.45	0.23	0.48
(2,2)	1:2:A:ALA:HB1	1:112:A:SER:H	8	0.43	0.1	0.47
(2,2)	1:2:A:ALA:HB2	1:112:A:SER:H	8	0.43	0.1	0.47
(2,2)	1:2:A:ALA:HB3	1:112:A:SER:H	8	0.43	0.1	0.47
(2,3)	1:5:A:VAL:HB	1:117:A:LEU:HG	8	0.43	0.08	0.44
(1,1218)	1:104:A:VAL:HA	1:106:A:ARG:H	8	0.38	0.19	0.34
(1,1086)	1:93:A:ILE:HB	1:127:A:PHE:H	8	0.36	0.09	0.35
(3,59)	1:143:A:LYS:O	1:147:A:MET:H	8	0.36	0.13	0.36
(1,1186)	1:99:A:PRO:HG2	1:132:A:SER:HA	8	0.36	0.17	0.31
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG11	8	0.33	0.11	0.36
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG12	8	0.33	0.11	0.36
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG13	8	0.33	0.11	0.36
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG21	8	0.33	0.11	0.36
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG22	8	0.33	0.11	0.36
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG23	8	0.33	0.11	0.36
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG11	8	0.33	0.11	0.36
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG12	8	0.33	0.11	0.36
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG13	8	0.33	0.11	0.36
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG21	8	0.33	0.11	0.36
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG22	8	0.33	0.11	0.36
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG23	8	0.33	0.11	0.36
(1,302)	1:17:A:LEU:HD21	1:19:A:HIS:H	8	0.33	0.15	0.3
(1,302)	1:17:A:LEU:HD22	1:19:A:HIS:H	8	0.33	0.15	0.3
(1,302)	1:17:A:LEU:HD23	1:19:A:HIS:H	8	0.33	0.15	0.3
(1,1756)	1:147:A:MET:HA	1:149:A:ASN:H	8	0.32	0.15	0.3
(1,1665)	1:141:A:SER:HA	1:144:A:SER:H	8	0.31	0.18	0.28
(1,1757)	1:147:A:MET:HA	1:150:A:GLN:H	8	0.3	0.15	0.3
(1,1092)	1:93:A:ILE:HG12	1:127:A:PHE:H	8	0.29	0.11	0.32
(1,156)	1:10:A:SER:HB2	1:13:A:ASN:H	8	0.28	0.15	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,280)	1:16:A:ASP:HB3	1:18:A:LEU:H	8	0.27	0.07	0.26
(1,1358)	1:113:A:SER:H	1:115:A:ARG:H	8	0.27	0.19	0.18
(1,1652)	1:140:A:LYS:HE2	1:141:A:SER:H	8	0.26	0.09	0.24
(1,723)	1:56:A:GLU:HG2	1:57:A:MET:H	8	0.25	0.08	0.24
(1,1030)	1:87:A:SER:H	1:88:A:THR:H	8	0.22	0.08	0.19
(1,677)	1:54:A:VAL:HB	1:58:A:LYS:H	8	0.22	0.03	0.21
(2,27)	1:78:A:VAL:HB	1:87:A:SER:HA	8	0.21	0.05	0.2
(1,426)	1:28:A:ILE:H	1:42:A:LYS:HA	8	0.19	0.07	0.2
(1,725)	1:56:A:GLU:HG3	1:57:A:MET:H	8	0.19	0.08	0.2
(1,1747)	1:146:A:LEU:HB2	1:147:A:MET:H	8	0.19	0.05	0.18
(1,1747)	1:146:A:LEU:HB3	1:147:A:MET:H	8	0.19	0.05	0.18
(1,283)	1:16:A:ASP:HB2	1:18:A:LEU:H	8	0.18	0.06	0.17
(1,283)	1:16:A:ASP:HB3	1:18:A:LEU:H	8	0.18	0.06	0.17
(1,963)	1:79:A:GLN:H	1:79:A:GLN:HA	8	0.16	0.03	0.16
(1,592)	1:45:A:GLU:HB3	1:48:A:ALA:HA	7	1.73	0.22	1.82
(1,959)	1:78:A:VAL:HG21	1:87:A:SER:HA	7	1.16	0.22	1.2
(1,959)	1:78:A:VAL:HG22	1:87:A:SER:HA	7	1.16	0.22	1.2
(1,959)	1:78:A:VAL:HG23	1:87:A:SER:HA	7	1.16	0.22	1.2
(1,351)	1:21:A:LYS:HE2	1:22:A:HIS:H	7	1.07	0.16	1.13
(1,351)	1:21:A:LYS:HE3	1:22:A:HIS:H	7	1.07	0.16	1.13
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD11	7	1.03	0.51	1.05
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD12	7	1.03	0.51	1.05
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD13	7	1.03	0.51	1.05
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD21	7	1.03	0.51	1.05
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD22	7	1.03	0.51	1.05
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD23	7	1.03	0.51	1.05
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD11	7	1.03	0.51	1.05
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD12	7	1.03	0.51	1.05
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD13	7	1.03	0.51	1.05
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD21	7	1.03	0.51	1.05
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD22	7	1.03	0.51	1.05
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD23	7	1.03	0.51	1.05
(1,755)	1:58:A:LYS:HD2	1:60:A:LEU:H	7	0.99	0.45	1.05
(1,1589)	1:135:A:SER:HA	1:140:A:LYS:HE2	7	0.95	0.32	1.01
(1,978)	1:79:A:GLN:HG2	1:85:A:GLY:H	7	0.91	0.48	0.76
(1,113)	1:8:A:ASP:H	1:37:A:ALA:HA	7	0.87	0.21	0.75
(1,429)	1:28:A:ILE:H	1:42:A:LYS:HG2	7	0.85	0.47	0.83
(1,429)	1:28:A:ILE:H	1:42:A:LYS:HG3	7	0.85	0.47	0.83
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG21	7	0.84	0.24	0.92
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG22	7	0.84	0.24	0.92
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG23	7	0.84	0.24	0.92
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG21	7	0.8	0.37	1.04

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG22	7	0.8	0.37	1.04
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG23	7	0.8	0.37	1.04
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD11	7	0.76	0.25	0.73
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD12	7	0.76	0.25	0.73
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD13	7	0.76	0.25	0.73
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD21	7	0.76	0.25	0.73
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD22	7	0.76	0.25	0.73
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD23	7	0.76	0.25	0.73
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD11	7	0.76	0.25	0.73
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD12	7	0.76	0.25	0.73
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD13	7	0.76	0.25	0.73
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD21	7	0.76	0.25	0.73
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD22	7	0.76	0.25	0.73
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD23	7	0.76	0.25	0.73
(1,968)	1:79:A:GLN:HA	1:85:A:GLY:H	7	0.74	0.16	0.67
(1,1189)	1:99:A:PRO:HG3	1:102:A:ALA:HA	7	0.69	0.39	0.62
(1,91)	1:7:A:VAL:HG21	1:120:A:SER:HA	7	0.68	0.3	0.79
(1,91)	1:7:A:VAL:HG22	1:120:A:SER:HA	7	0.68	0.3	0.79
(1,91)	1:7:A:VAL:HG23	1:120:A:SER:HA	7	0.68	0.3	0.79
(1,434)	1:28:A:ILE:HB	1:41:A:GLU:HA	7	0.61	0.18	0.57
(1,117)	1:8:A:ASP:H	1:39:A:VAL:HB	7	0.6	0.26	0.61
(1,454)	1:28:A:ILE:HG12	1:41:A:GLU:HG2	7	0.58	0.17	0.54
(1,454)	1:28:A:ILE:HG12	1:41:A:GLU:HG3	7	0.58	0.17	0.54
(1,454)	1:28:A:ILE:HG13	1:41:A:GLU:HG2	7	0.58	0.17	0.54
(1,454)	1:28:A:ILE:HG13	1:41:A:GLU:HG3	7	0.58	0.17	0.54
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD11	7	0.57	0.33	0.39
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD12	7	0.57	0.33	0.39
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD13	7	0.57	0.33	0.39
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD21	7	0.57	0.33	0.39
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD22	7	0.57	0.33	0.39
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD23	7	0.57	0.33	0.39
(1,1107)	1:93:A:ILE:HG21	1:146:A:LEU:HA	7	0.57	0.35	0.46
(1,1107)	1:93:A:ILE:HG22	1:146:A:LEU:HA	7	0.57	0.35	0.46
(1,1107)	1:93:A:ILE:HG23	1:146:A:LEU:HA	7	0.57	0.35	0.46
(1,507)	1:31:A:ILE:HG12	1:109:A:LEU:HB2	7	0.54	0.13	0.55
(1,507)	1:31:A:ILE:HG12	1:109:A:LEU:HB3	7	0.54	0.13	0.55
(1,507)	1:31:A:ILE:HG13	1:109:A:LEU:HB2	7	0.54	0.13	0.55
(1,507)	1:31:A:ILE:HG13	1:109:A:LEU:HB3	7	0.54	0.13	0.55
(1,1580)	1:134:A:MET:HB2	1:136:A:ASP:H	7	0.52	0.21	0.44
(1,1580)	1:134:A:MET:HB3	1:136:A:ASP:H	7	0.52	0.21	0.44
(3,3)	1:8:A:ASP:H	1:38:A:ILE:O	7	0.52	0.21	0.42
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG11	7	0.51	0.34	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG12	7	0.51	0.34	0.36
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG13	7	0.51	0.34	0.36
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG21	7	0.51	0.34	0.36
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG22	7	0.51	0.34	0.36
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG23	7	0.51	0.34	0.36
(1,135)	1:8:A:ASP:HB2	1:39:A:VAL:HB	7	0.5	0.19	0.52
(1,135)	1:8:A:ASP:HB3	1:39:A:VAL:HB	7	0.5	0.19	0.52
(1,335)	1:19:A:HIS:HA	1:21:A:LYS:H	7	0.5	0.28	0.35
(1,1594)	1:135:A:SER:HB2	1:140:A:LYS:HG2	7	0.5	0.19	0.46
(1,1594)	1:135:A:SER:HB2	1:140:A:LYS:HG3	7	0.5	0.19	0.46
(1,1594)	1:135:A:SER:HB3	1:140:A:LYS:HG2	7	0.5	0.19	0.46
(1,1594)	1:135:A:SER:HB3	1:140:A:LYS:HG3	7	0.5	0.19	0.46
(1,909)	1:76:A:VAL:H	1:89:A:LEU:H	7	0.49	0.2	0.5
(1,33)	1:5:A:VAL:HB	1:7:A:VAL:HA	7	0.45	0.16	0.42
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG11	7	0.44	0.2	0.42
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG12	7	0.44	0.2	0.42
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG13	7	0.44	0.2	0.42
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG21	7	0.44	0.2	0.42
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG22	7	0.44	0.2	0.42
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG23	7	0.44	0.2	0.42
(1,1224)	1:104:A:VAL:HB	1:106:A:ARG:H	7	0.43	0.2	0.45
(1,1579)	1:134:A:MET:HB2	1:135:A:SER:H	7	0.42	0.07	0.4
(1,1579)	1:134:A:MET:HB3	1:135:A:SER:H	7	0.42	0.07	0.4
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG21	7	0.39	0.2	0.27
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG22	7	0.39	0.2	0.27
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG23	7	0.39	0.2	0.27
(1,608)	1:49:A:PRO:HG2	1:50:A:TYR:H	7	0.39	0.09	0.36
(1,608)	1:49:A:PRO:HG3	1:50:A:TYR:H	7	0.39	0.09	0.36
(1,116)	1:8:A:ASP:H	1:39:A:VAL:HA	7	0.38	0.2	0.31
(1,108)	1:7:A:VAL:HG11	1:38:A:ILE:HB	7	0.35	0.1	0.38
(1,108)	1:7:A:VAL:HG12	1:38:A:ILE:HB	7	0.35	0.1	0.38
(1,108)	1:7:A:VAL:HG13	1:38:A:ILE:HB	7	0.35	0.1	0.38
(1,108)	1:7:A:VAL:HG21	1:38:A:ILE:HB	7	0.35	0.1	0.38
(1,108)	1:7:A:VAL:HG22	1:38:A:ILE:HB	7	0.35	0.1	0.38
(1,108)	1:7:A:VAL:HG23	1:38:A:ILE:HB	7	0.35	0.1	0.38
(2,31)	1:97:A:TYR:HB2	1:131:A:ALA:HA	7	0.33	0.16	0.33
(2,31)	1:97:A:TYR:HB3	1:131:A:ALA:HA	7	0.33	0.16	0.33
(1,724)	1:56:A:GLU:HG2	1:58:A:LYS:H	7	0.32	0.15	0.32
(1,590)	1:45:A:GLU:HB2	1:48:A:ALA:HA	7	0.32	0.15	0.23
(1,494)	1:31:A:ILE:HG12	1:38:A:ILE:HA	7	0.3	0.13	0.23
(1,575)	1:42:A:LYS:HB2	1:43:A:VAL:H	7	0.3	0.09	0.3
(1,575)	1:42:A:LYS:HB3	1:43:A:VAL:H	7	0.3	0.09	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1382)	1:114:A:VAL:HG21	1:116:A:ALA:H	7	0.28	0.07	0.29
(1,1382)	1:114:A:VAL:HG22	1:116:A:ALA:H	7	0.28	0.07	0.29
(1,1382)	1:114:A:VAL:HG23	1:116:A:ALA:H	7	0.28	0.07	0.29
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB1	7	0.27	0.1	0.33
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB2	7	0.27	0.1	0.33
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB3	7	0.27	0.1	0.33
(1,1293)	1:108:A:MET:HA	1:110:A:TYR:H	7	0.25	0.17	0.15
(1,1659)	1:140:A:LYS:HB2	1:143:A:LYS:H	7	0.25	0.08	0.25
(1,1659)	1:140:A:LYS:HB3	1:143:A:LYS:H	7	0.25	0.08	0.25
(1,161)	1:10:A:SER:HB2	1:12:A:LYS:H	7	0.24	0.1	0.22
(1,161)	1:10:A:SER:HB3	1:12:A:LYS:H	7	0.24	0.1	0.22
(1,682)	1:54:A:VAL:HG21	1:57:A:MET:H	7	0.23	0.06	0.25
(1,682)	1:54:A:VAL:HG22	1:57:A:MET:H	7	0.23	0.06	0.25
(1,682)	1:54:A:VAL:HG23	1:57:A:MET:H	7	0.23	0.06	0.25
(3,4)	1:8:A:ASP:N	1:38:A:ILE:O	7	0.21	0.09	0.21
(1,689)	1:54:A:VAL:HG11	1:57:A:MET:H	7	0.21	0.06	0.2
(1,689)	1:54:A:VAL:HG12	1:57:A:MET:H	7	0.21	0.06	0.2
(1,689)	1:54:A:VAL:HG13	1:57:A:MET:H	7	0.21	0.06	0.2
(1,689)	1:54:A:VAL:HG21	1:57:A:MET:H	7	0.21	0.06	0.2
(1,689)	1:54:A:VAL:HG22	1:57:A:MET:H	7	0.21	0.06	0.2
(1,689)	1:54:A:VAL:HG23	1:57:A:MET:H	7	0.21	0.06	0.2
(1,615)	1:50:A:TYR:HA	1:51:A:ALA:H	7	0.15	0.03	0.15
(1,1794)	1:151:A:ARG:H	1:151:A:ARG:HA	7	0.15	0.02	0.15
(1,757)	1:58:A:LYS:HD3	1:60:A:LEU:H	6	1.47	0.25	1.55
(1,895)	1:75:A:GLU:HG3	1:88:A:THR:HB	6	1.34	0.64	1.28
(1,1021)	1:85:A:GLY:H	1:86:A:THR:H	6	1.06	0.45	1.13
(1,692)	1:54:A:VAL:HG11	1:58:A:LYS:HE2	6	0.9	0.45	0.88
(1,692)	1:54:A:VAL:HG11	1:58:A:LYS:HE3	6	0.9	0.45	0.88
(1,692)	1:54:A:VAL:HG12	1:58:A:LYS:HE2	6	0.9	0.45	0.88
(1,692)	1:54:A:VAL:HG12	1:58:A:LYS:HE3	6	0.9	0.45	0.88
(1,692)	1:54:A:VAL:HG13	1:58:A:LYS:HE2	6	0.9	0.45	0.88
(1,692)	1:54:A:VAL:HG13	1:58:A:LYS:HE3	6	0.9	0.45	0.88
(1,692)	1:54:A:VAL:HG21	1:58:A:LYS:HE2	6	0.9	0.45	0.88
(1,692)	1:54:A:VAL:HG21	1:58:A:LYS:HE3	6	0.9	0.45	0.88
(1,692)	1:54:A:VAL:HG22	1:58:A:LYS:HE2	6	0.9	0.45	0.88
(1,692)	1:54:A:VAL:HG22	1:58:A:LYS:HE3	6	0.9	0.45	0.88
(1,692)	1:54:A:VAL:HG23	1:58:A:LYS:HE2	6	0.9	0.45	0.88
(1,692)	1:54:A:VAL:HG23	1:58:A:LYS:HE3	6	0.9	0.45	0.88
(1,523)	1:33:A:LYS:HG2	1:36:A:THR:HA	6	0.88	0.24	0.81
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD11	6	0.85	0.58	1.0
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD12	6	0.85	0.58	1.0
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD13	6	0.85	0.58	1.0

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD21	6	0.85	0.58	1.0
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD22	6	0.85	0.58	1.0
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD23	6	0.85	0.58	1.0
(1,1285)	1:107:A:ARG:HD2	1:108:A:MET:H	6	0.82	0.15	0.82
(1,1285)	1:107:A:ARG:HD3	1:108:A:MET:H	6	0.82	0.15	0.82
(1,1285)	1:107:A:ARG:HD2	1:108:A:MET:H	6	0.82	0.15	0.82
(1,1285)	1:107:A:ARG:HD3	1:108:A:MET:H	6	0.82	0.15	0.82
(1,962)	1:78:A:VAL:HG11	1:87:A:SER:HB2	6	0.7	0.22	0.77
(1,962)	1:78:A:VAL:HG11	1:87:A:SER:HB3	6	0.7	0.22	0.77
(1,962)	1:78:A:VAL:HG12	1:87:A:SER:HB2	6	0.7	0.22	0.77
(1,962)	1:78:A:VAL:HG12	1:87:A:SER:HB3	6	0.7	0.22	0.77
(1,962)	1:78:A:VAL:HG13	1:87:A:SER:HB2	6	0.7	0.22	0.77
(1,962)	1:78:A:VAL:HG13	1:87:A:SER:HB3	6	0.7	0.22	0.77
(1,962)	1:78:A:VAL:HG21	1:87:A:SER:HB2	6	0.7	0.22	0.77
(1,962)	1:78:A:VAL:HG21	1:87:A:SER:HB3	6	0.7	0.22	0.77
(1,962)	1:78:A:VAL:HG22	1:87:A:SER:HB2	6	0.7	0.22	0.77
(1,962)	1:78:A:VAL:HG22	1:87:A:SER:HB3	6	0.7	0.22	0.77
(1,962)	1:78:A:VAL:HG23	1:87:A:SER:HB2	6	0.7	0.22	0.77
(1,962)	1:78:A:VAL:HG23	1:87:A:SER:HB3	6	0.7	0.22	0.77
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG11	6	0.7	0.3	0.62
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG12	6	0.7	0.3	0.62
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG13	6	0.7	0.3	0.62
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG21	6	0.7	0.3	0.62
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG22	6	0.7	0.3	0.62
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG23	6	0.7	0.3	0.62
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG11	6	0.7	0.3	0.62
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG12	6	0.7	0.3	0.62
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG13	6	0.7	0.3	0.62
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG21	6	0.7	0.3	0.62
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG22	6	0.7	0.3	0.62
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG23	6	0.7	0.3	0.62
(1,1744)	1:146:A:LEU:HA	1:150:A:GLN:HA	6	0.7	0.16	0.73
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD11	6	0.64	0.29	0.62
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD12	6	0.64	0.29	0.62
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD13	6	0.64	0.29	0.62
(1,225)	1:13:A:ASN:HA	1:17:A:LEU:H	6	0.61	0.25	0.57
(1,439)	1:28:A:ILE:HB	1:42:A:LYS:HD2	6	0.6	0.22	0.7
(1,439)	1:28:A:ILE:HB	1:42:A:LYS:HD3	6	0.6	0.22	0.7
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG11	6	0.6	0.25	0.6
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG12	6	0.6	0.25	0.6
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG13	6	0.6	0.25	0.6
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG21	6	0.6	0.25	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG22	6	0.6	0.25	0.6
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG23	6	0.6	0.25	0.6
(1,1721)	1:144:A:SER:HA	1:148:A:SER:H	6	0.55	0.31	0.46
(2,28)	1:79:A:GLN:HB3	1:85:A:GLY:H	6	0.53	0.01	0.53
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB1	6	0.52	0.22	0.43
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB2	6	0.52	0.22	0.43
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB3	6	0.52	0.22	0.43
(1,1325)	1:109:A:LEU:HD11	1:112:A:SER:HB2	6	0.49	0.29	0.4
(1,1325)	1:109:A:LEU:HD11	1:112:A:SER:HB3	6	0.49	0.29	0.4
(1,1325)	1:109:A:LEU:HD12	1:112:A:SER:HB2	6	0.49	0.29	0.4
(1,1325)	1:109:A:LEU:HD12	1:112:A:SER:HB3	6	0.49	0.29	0.4
(1,1325)	1:109:A:LEU:HD13	1:112:A:SER:HB2	6	0.49	0.29	0.4
(1,1325)	1:109:A:LEU:HD13	1:112:A:SER:HB3	6	0.49	0.29	0.4
(1,1325)	1:109:A:LEU:HD21	1:112:A:SER:HB2	6	0.49	0.29	0.4
(1,1325)	1:109:A:LEU:HD21	1:112:A:SER:HB3	6	0.49	0.29	0.4
(1,1325)	1:109:A:LEU:HD22	1:112:A:SER:HB2	6	0.49	0.29	0.4
(1,1325)	1:109:A:LEU:HD22	1:112:A:SER:HB3	6	0.49	0.29	0.4
(1,1325)	1:109:A:LEU:HD23	1:112:A:SER:HB2	6	0.49	0.29	0.4
(1,1325)	1:109:A:LEU:HD23	1:112:A:SER:HB3	6	0.49	0.29	0.4
(1,577)	1:42:A:LYS:HB2	1:53:A:PHE:HA	6	0.48	0.24	0.57
(1,577)	1:42:A:LYS:HB3	1:53:A:PHE:HA	6	0.48	0.24	0.57
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD11	6	0.47	0.14	0.45
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD12	6	0.47	0.14	0.45
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD13	6	0.47	0.14	0.45
(1,1550)	1:131:A:ALA:HA	1:136:A:ASP:HA	6	0.46	0.27	0.36
(1,659)	1:53:A:PHE:HB2	1:56:A:GLU:H	6	0.41	0.18	0.35
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB1	6	0.4	0.23	0.34
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB2	6	0.4	0.23	0.34
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB3	6	0.4	0.23	0.34
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB1	6	0.4	0.23	0.34
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB2	6	0.4	0.23	0.34
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB3	6	0.4	0.23	0.34
(1,1082)	1:93:A:ILE:HA	1:127:A:PHE:HA	6	0.39	0.12	0.38
(1,453)	1:28:A:ILE:HG12	1:41:A:GLU:HB2	6	0.38	0.17	0.3
(1,453)	1:28:A:ILE:HG12	1:41:A:GLU:HB3	6	0.38	0.17	0.3
(1,453)	1:28:A:ILE:HG13	1:41:A:GLU:HB2	6	0.38	0.17	0.3
(1,453)	1:28:A:ILE:HG13	1:41:A:GLU:HB3	6	0.38	0.17	0.3
(1,1587)	1:135:A:SER:HA	1:138:A:ASP:H	6	0.37	0.16	0.4
(1,65)	1:7:A:VAL:HA	1:37:A:ALA:HA	6	0.36	0.18	0.36
(1,1436)	1:118:A:LYS:H	1:118:A:LYS:HE2	6	0.35	0.04	0.36
(1,1436)	1:118:A:LYS:H	1:118:A:LYS:HE3	6	0.35	0.04	0.36
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG11	6	0.35	0.05	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG12	6	0.35	0.05	0.36
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG13	6	0.35	0.05	0.36
(1,256)	1:15:A:TYR:HB2	1:121:A:LEU:HG	6	0.33	0.16	0.3
(1,985)	1:80:A:ARG:H	1:80:A:ARG:HG2	6	0.32	0.2	0.28
(1,985)	1:80:A:ARG:H	1:80:A:ARG:HG3	6	0.32	0.2	0.28
(1,4)	1:1:A:MET:HA	1:114:A:VAL:HB	6	0.32	0.15	0.24
(1,822)	1:70:A:ALA:H	1:94:A:PHE:HA	6	0.32	0.15	0.32
(1,515)	1:31:A:ILE:HG21	1:37:A:ALA:H	6	0.32	0.07	0.32
(1,515)	1:31:A:ILE:HG22	1:37:A:ALA:H	6	0.32	0.07	0.32
(1,515)	1:31:A:ILE:HG23	1:37:A:ALA:H	6	0.32	0.07	0.32
(1,1016)	1:84:A:GLU:HA	1:85:A:GLY:H	6	0.3	0.05	0.3
(1,402)	1:27:A:ILE:HB	1:43:A:VAL:HA	6	0.3	0.22	0.17
(1,1703)	1:143:A:LYS:HA	1:146:A:LEU:HA	6	0.3	0.16	0.26
(1,1322)	1:109:A:LEU:HD21	1:113:A:SER:H	6	0.29	0.15	0.27
(1,1322)	1:109:A:LEU:HD22	1:113:A:SER:H	6	0.29	0.15	0.27
(1,1322)	1:109:A:LEU:HD23	1:113:A:SER:H	6	0.29	0.15	0.27
(1,366)	1:25:A:SER:H	1:73:A:ASP:H	6	0.28	0.17	0.26
(1,1298)	1:108:A:MET:HB2	1:110:A:TYR:H	6	0.28	0.2	0.17
(1,1208)	1:103:A:PRO:HA	1:107:A:ARG:H	6	0.27	0.18	0.24
(1,1233)	1:104:A:VAL:HG21	1:106:A:ARG:H	6	0.26	0.14	0.2
(1,1233)	1:104:A:VAL:HG22	1:106:A:ARG:H	6	0.26	0.14	0.2
(1,1233)	1:104:A:VAL:HG23	1:106:A:ARG:H	6	0.26	0.14	0.2
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG11	6	0.25	0.09	0.24
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG12	6	0.25	0.09	0.24
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG13	6	0.25	0.09	0.24
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG21	6	0.25	0.09	0.24
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG22	6	0.25	0.09	0.24
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG23	6	0.25	0.09	0.24
(1,1313)	1:109:A:LEU:HA	1:111:A:ALA:H	6	0.23	0.05	0.22
(1,1740)	1:146:A:LEU:H	1:148:A:SER:H	6	0.22	0.09	0.22
(1,1366)	1:113:A:SER:HB3	1:116:A:ALA:H	6	0.2	0.09	0.2
(1,1627)	1:139:A:GLU:HA	1:143:A:LYS:HE2	6	0.19	0.03	0.2
(1,1627)	1:139:A:GLU:HA	1:143:A:LYS:HE3	6	0.19	0.03	0.2
(1,676)	1:54:A:VAL:HB	1:57:A:MET:H	6	0.18	0.07	0.16
(1,683)	1:54:A:VAL:HG21	1:58:A:LYS:H	6	0.18	0.05	0.16
(1,683)	1:54:A:VAL:HG22	1:58:A:LYS:H	6	0.18	0.05	0.16
(1,683)	1:54:A:VAL:HG23	1:58:A:LYS:H	6	0.18	0.05	0.16
(2,16)	1:27:A:ILE:HG21	1:43:A:VAL:H	6	0.16	0.01	0.16
(2,16)	1:27:A:ILE:HG22	1:43:A:VAL:H	6	0.16	0.01	0.16
(2,16)	1:27:A:ILE:HG23	1:43:A:VAL:H	6	0.16	0.01	0.16
(1,905)	1:76:A:VAL:H	1:77:A:THR:H	6	0.16	0.04	0.15
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG21	5	1.43	0.26	1.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG22	5	1.43	0.26	1.43
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG23	5	1.43	0.26	1.43
(1,14)	1:3:A:SER:H	1:113:A:SER:HA	5	0.81	0.11	0.87
(1,1241)	1:104:A:VAL:HG11	1:107:A:ARG:HB2	5	0.79	0.4	0.64
(1,1241)	1:104:A:VAL:HG11	1:107:A:ARG:HB3	5	0.79	0.4	0.64
(1,1241)	1:104:A:VAL:HG12	1:107:A:ARG:HB2	5	0.79	0.4	0.64
(1,1241)	1:104:A:VAL:HG12	1:107:A:ARG:HB3	5	0.79	0.4	0.64
(1,1241)	1:104:A:VAL:HG13	1:107:A:ARG:HB2	5	0.79	0.4	0.64
(1,1241)	1:104:A:VAL:HG13	1:107:A:ARG:HB3	5	0.79	0.4	0.64
(1,1241)	1:104:A:VAL:HG21	1:107:A:ARG:HB2	5	0.79	0.4	0.64
(1,1241)	1:104:A:VAL:HG21	1:107:A:ARG:HB3	5	0.79	0.4	0.64
(1,1241)	1:104:A:VAL:HG22	1:107:A:ARG:HB2	5	0.79	0.4	0.64
(1,1241)	1:104:A:VAL:HG22	1:107:A:ARG:HB3	5	0.79	0.4	0.64
(1,1241)	1:104:A:VAL:HG23	1:107:A:ARG:HB2	5	0.79	0.4	0.64
(1,1241)	1:104:A:VAL:HG23	1:107:A:ARG:HB3	5	0.79	0.4	0.64
(1,385)	1:26:A:TYR:HB2	1:72:A:VAL:HA	5	0.78	0.4	0.77
(1,385)	1:26:A:TYR:HB3	1:72:A:VAL:HA	5	0.78	0.4	0.77
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD11	5	0.77	0.31	0.62
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD12	5	0.77	0.31	0.62
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD13	5	0.77	0.31	0.62
(1,382)	1:26:A:TYR:HB3	1:72:A:VAL:HA	5	0.72	0.39	0.85
(1,518)	1:32:A:ASP:HB3	1:37:A:ALA:H	5	0.71	0.49	0.58
(1,1122)	1:94:A:PHE:HB2	1:118:A:LYS:HE2	5	0.68	0.28	0.65
(1,1122)	1:94:A:PHE:HB2	1:118:A:LYS:HE3	5	0.68	0.28	0.65
(1,1122)	1:94:A:PHE:HB3	1:118:A:LYS:HE2	5	0.68	0.28	0.65
(1,1122)	1:94:A:PHE:HB3	1:118:A:LYS:HE3	5	0.68	0.28	0.65
(1,987)	1:80:A:ARG:H	1:85:A:GLY:H	5	0.66	0.22	0.63
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG21	5	0.65	0.22	0.58
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG22	5	0.65	0.22	0.58
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG23	5	0.65	0.22	0.58
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG21	5	0.65	0.22	0.58
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG22	5	0.65	0.22	0.58
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG23	5	0.65	0.22	0.58
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB1	5	0.65	0.31	0.7
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB2	5	0.65	0.31	0.7
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB3	5	0.65	0.31	0.7
(1,1173)	1:98:A:CYS:HB2	1:107:A:ARG:HD2	5	0.6	0.24	0.7
(1,1173)	1:98:A:CYS:HB2	1:107:A:ARG:HD3	5	0.6	0.24	0.7
(1,1173)	1:98:A:CYS:HB3	1:107:A:ARG:HD2	5	0.6	0.24	0.7
(1,1173)	1:98:A:CYS:HB3	1:107:A:ARG:HD3	5	0.6	0.24	0.7
(1,1187)	1:99:A:PRO:HG2	1:132:A:SER:HB3	5	0.58	0.2	0.52
(1,112)	1:8:A:ASP:H	1:11:A:CYS:HB2	5	0.57	0.32	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,112)	1:8:A:ASP:H	1:11:A:CYS:HB3	5	0.57	0.32	0.56
(1,97)	1:7:A:VAL:HG11	1:116:A:ALA:H	5	0.56	0.22	0.68
(1,97)	1:7:A:VAL:HG12	1:116:A:ALA:H	5	0.56	0.22	0.68
(1,97)	1:7:A:VAL:HG13	1:116:A:ALA:H	5	0.56	0.22	0.68
(1,97)	1:7:A:VAL:HG21	1:116:A:ALA:H	5	0.56	0.22	0.68
(1,97)	1:7:A:VAL:HG22	1:116:A:ALA:H	5	0.56	0.22	0.68
(1,97)	1:7:A:VAL:HG23	1:116:A:ALA:H	5	0.56	0.22	0.68
(1,1240)	1:104:A:VAL:HG11	1:107:A:ARG:HA	5	0.53	0.26	0.47
(1,1240)	1:104:A:VAL:HG12	1:107:A:ARG:HA	5	0.53	0.26	0.47
(1,1240)	1:104:A:VAL:HG13	1:107:A:ARG:HA	5	0.53	0.26	0.47
(1,1240)	1:104:A:VAL:HG21	1:107:A:ARG:HA	5	0.53	0.26	0.47
(1,1240)	1:104:A:VAL:HG22	1:107:A:ARG:HA	5	0.53	0.26	0.47
(1,1240)	1:104:A:VAL:HG23	1:107:A:ARG:HA	5	0.53	0.26	0.47
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD11	5	0.5	0.18	0.42
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD12	5	0.5	0.18	0.42
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD13	5	0.5	0.18	0.42
(1,885)	1:75:A:GLU:HB3	1:88:A:THR:HB	5	0.49	0.31	0.32
(3,10)	1:26:A:TYR:N	1:44:A:GLY:O	5	0.48	0.17	0.44
(1,1803)	1:151:A:ARG:HG2	1:152:A:ILE:H	5	0.45	0.06	0.43
(1,1803)	1:151:A:ARG:HG3	1:152:A:ILE:H	5	0.45	0.06	0.43
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG21	5	0.44	0.24	0.4
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG22	5	0.44	0.24	0.4
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG23	5	0.44	0.24	0.4
(1,1398)	1:115:A:ARG:HA	1:119:A:ALA:H	5	0.44	0.16	0.4
(1,331)	1:18:A:LEU:HD11	1:92:A:VAL:HA	5	0.43	0.2	0.46
(1,331)	1:18:A:LEU:HD12	1:92:A:VAL:HA	5	0.43	0.2	0.46
(1,331)	1:18:A:LEU:HD13	1:92:A:VAL:HA	5	0.43	0.2	0.46
(1,331)	1:18:A:LEU:HD21	1:92:A:VAL:HA	5	0.43	0.2	0.46
(1,331)	1:18:A:LEU:HD22	1:92:A:VAL:HA	5	0.43	0.2	0.46
(1,331)	1:18:A:LEU:HD23	1:92:A:VAL:HA	5	0.43	0.2	0.46
(1,466)	1:29:A:PHE:HB3	1:41:A:GLU:H	5	0.42	0.33	0.23
(1,1410)	1:116:A:ALA:HA	1:120:A:SER:H	5	0.41	0.2	0.38
(3,9)	1:26:A:TYR:H	1:44:A:GLY:O	5	0.4	0.26	0.35
(1,1065)	1:91:A:LYS:HE3	1:150:A:GLN:H	5	0.4	0.26	0.28
(1,1234)	1:104:A:VAL:HG21	1:107:A:ARG:H	5	0.39	0.22	0.31
(1,1234)	1:104:A:VAL:HG22	1:107:A:ARG:H	5	0.39	0.22	0.31
(1,1234)	1:104:A:VAL:HG23	1:107:A:ARG:H	5	0.39	0.22	0.31
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG11	5	0.38	0.18	0.32
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG12	5	0.38	0.18	0.32
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG13	5	0.38	0.18	0.32
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG21	5	0.38	0.18	0.32
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG22	5	0.38	0.18	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG23	5	0.38	0.18	0.32
(1,255)	1:15:A:TYR:HA	1:19:A:HIS:H	5	0.38	0.31	0.27
(1,1118)	1:94:A:PHE:HA	1:128:A:GLN:HB2	5	0.36	0.06	0.35
(1,1178)	1:99:A:PRO:HB2	1:102:A:ALA:HA	5	0.36	0.23	0.37
(2,35)	1:118:A:LYS:HE3	1:128:A:GLN:HA	5	0.34	0.16	0.3
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB1	5	0.34	0.15	0.36
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB2	5	0.34	0.15	0.36
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB3	5	0.34	0.15	0.36
(1,1364)	1:113:A:SER:HB2	1:116:A:ALA:H	5	0.33	0.09	0.3
(1,671)	1:54:A:VAL:HA	1:57:A:MET:HA	5	0.33	0.06	0.33
(1,800)	1:64:A:GLY:H	1:65:A:LYS:H	5	0.31	0.13	0.39
(1,1597)	1:136:A:ASP:H	1:138:A:ASP:H	5	0.3	0.08	0.27
(1,599)	1:49:A:PRO:HA	1:52:A:GLU:H	5	0.3	0.14	0.2
(1,655)	1:53:A:PHE:HA	1:56:A:GLU:H	5	0.3	0.17	0.24
(1,664)	1:53:A:PHE:HB2	1:57:A:MET:H	5	0.3	0.11	0.26
(1,664)	1:53:A:PHE:HB3	1:57:A:MET:H	5	0.3	0.11	0.26
(1,181)	1:11:A:CYS:HB3	1:13:A:ASN:H	5	0.27	0.08	0.3
(1,629)	1:51:A:ALA:HA	1:54:A:VAL:HA	5	0.26	0.1	0.25
(3,60)	1:143:A:LYS:O	1:147:A:MET:N	5	0.26	0.07	0.25
(1,1052)	1:89:A:LEU:HD21	1:90:A:ASN:H	5	0.26	0.06	0.24
(1,1052)	1:89:A:LEU:HD22	1:90:A:ASN:H	5	0.26	0.06	0.24
(1,1052)	1:89:A:LEU:HD23	1:90:A:ASN:H	5	0.26	0.06	0.24
(1,178)	1:11:A:CYS:HB2	1:13:A:ASN:H	5	0.25	0.08	0.26
(1,751)	1:58:A:LYS:HB2	1:60:A:LEU:H	5	0.24	0.11	0.21
(1,948)	1:78:A:VAL:HA	1:79:A:GLN:H	5	0.23	0.02	0.24
(1,294)	1:17:A:LEU:HA	1:21:A:LYS:HD2	5	0.22	0.08	0.18
(1,294)	1:17:A:LEU:HA	1:21:A:LYS:HD3	5	0.22	0.08	0.18
(1,1033)	1:88:A:THR:H	1:88:A:THR:HB	5	0.21	0.06	0.19
(1,1288)	1:107:A:ARG:HG2	1:109:A:LEU:H	5	0.19	0.05	0.22
(1,1288)	1:107:A:ARG:HG3	1:109:A:LEU:H	5	0.19	0.05	0.22
(1,437)	1:28:A:ILE:HB	1:42:A:LYS:HA	5	0.18	0.02	0.18
(1,1014)	1:84:A:GLU:H	1:84:A:GLU:HB2	5	0.16	0.04	0.15
(1,1014)	1:84:A:GLU:H	1:84:A:GLU:HB3	5	0.16	0.04	0.15
(1,1024)	1:86:A:THR:H	1:86:A:THR:HB	5	0.16	0.02	0.14
(1,1536)	1:128:A:GLN:HB2	1:129:A:VAL:H	5	0.14	0.02	0.13
(1,1536)	1:128:A:GLN:HB3	1:129:A:VAL:H	5	0.14	0.02	0.13
(1,1330)	1:110:A:TYR:HA	1:111:A:ALA:H	5	0.1	0.0	0.1
(1,379)	1:26:A:TYR:HB2	1:72:A:VAL:HA	4	1.33	0.6	1.6
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB1	4	1.02	0.28	1.08
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB2	4	1.02	0.28	1.08
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB3	4	1.02	0.28	1.08
(1,519)	1:32:A:ASP:HB2	1:37:A:ALA:HB1	4	1.02	0.28	1.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,519)	1:32:A:ASP:HB2	1:37:A:ALA:HB2	4	1.02	0.28	1.08
(1,519)	1:32:A:ASP:HB2	1:37:A:ALA:HB3	4	1.02	0.28	1.08
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB1	4	1.02	0.28	1.08
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB2	4	1.02	0.28	1.08
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB3	4	1.02	0.28	1.08
(1,1196)	1:100:A:ASP:HA	1:132:A:SER:HB3	4	0.77	0.2	0.88
(1,292)	1:17:A:LEU:HA	1:21:A:LYS:H	4	0.74	0.56	0.72
(1,1220)	1:104:A:VAL:HA	1:107:A:ARG:HB2	4	0.74	0.22	0.73
(1,1220)	1:104:A:VAL:HA	1:107:A:ARG:HB3	4	0.74	0.22	0.73
(1,1774)	1:149:A:ASN:HB3	1:152:A:ILE:HD11	4	0.72	0.33	0.7
(1,1774)	1:149:A:ASN:HB3	1:152:A:ILE:HD12	4	0.72	0.33	0.7
(1,1774)	1:149:A:ASN:HB3	1:152:A:ILE:HD13	4	0.72	0.33	0.7
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG11	4	0.68	0.23	0.66
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG12	4	0.68	0.23	0.66
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG13	4	0.68	0.23	0.66
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG21	4	0.68	0.23	0.66
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG22	4	0.68	0.23	0.66
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG23	4	0.68	0.23	0.66
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG11	4	0.68	0.23	0.66
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG12	4	0.68	0.23	0.66
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG13	4	0.68	0.23	0.66
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG21	4	0.68	0.23	0.66
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG22	4	0.68	0.23	0.66
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG23	4	0.68	0.23	0.66
(1,1185)	1:99:A:PRO:HG2	1:102:A:ALA:HA	4	0.66	0.25	0.65
(1,55)	1:6:A:LYS:HE2	1:7:A:VAL:H	4	0.63	0.15	0.68
(1,55)	1:6:A:LYS:HE3	1:7:A:VAL:H	4	0.63	0.15	0.68
(1,1281)	1:107:A:ARG:HA	1:110:A:TYR:HA	4	0.62	0.36	0.44
(1,699)	1:55:A:GLU:HA	1:58:A:LYS:HD2	4	0.62	0.39	0.66
(1,699)	1:55:A:GLU:HA	1:58:A:LYS:HD3	4	0.62	0.39	0.66
(1,700)	1:55:A:GLU:HA	1:58:A:LYS:HE2	4	0.56	0.31	0.42
(1,700)	1:55:A:GLU:HA	1:58:A:LYS:HE3	4	0.56	0.31	0.42
(1,790)	1:61:A:VAL:HG11	1:66:A:GLU:HG2	4	0.56	0.2	0.64
(1,790)	1:61:A:VAL:HG11	1:66:A:GLU:HG3	4	0.56	0.2	0.64
(1,790)	1:61:A:VAL:HG12	1:66:A:GLU:HG2	4	0.56	0.2	0.64
(1,790)	1:61:A:VAL:HG12	1:66:A:GLU:HG3	4	0.56	0.2	0.64
(1,790)	1:61:A:VAL:HG13	1:66:A:GLU:HG2	4	0.56	0.2	0.64
(1,790)	1:61:A:VAL:HG13	1:66:A:GLU:HG3	4	0.56	0.2	0.64
(1,790)	1:61:A:VAL:HG21	1:66:A:GLU:HG2	4	0.56	0.2	0.64
(1,790)	1:61:A:VAL:HG21	1:66:A:GLU:HG3	4	0.56	0.2	0.64
(1,790)	1:61:A:VAL:HG22	1:66:A:GLU:HG2	4	0.56	0.2	0.64
(1,790)	1:61:A:VAL:HG22	1:66:A:GLU:HG3	4	0.56	0.2	0.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,790)	1:61:A:VAL:HG23	1:66:A:GLU:HG2	4	0.56	0.2	0.64
(1,790)	1:61:A:VAL:HG23	1:66:A:GLU:HG3	4	0.56	0.2	0.64
(1,440)	1:28:A:ILE:HB	1:70:A:ALA:HB1	4	0.55	0.31	0.53
(1,440)	1:28:A:ILE:HB	1:70:A:ALA:HB2	4	0.55	0.31	0.53
(1,440)	1:28:A:ILE:HB	1:70:A:ALA:HB3	4	0.55	0.31	0.53
(1,756)	1:58:A:LYS:HD3	1:59:A:LYS:H	4	0.55	0.29	0.5
(1,1808)	1:152:A:ILE:H	1:152:A:ILE:HG12	4	0.53	0.41	0.36
(1,1808)	1:152:A:ILE:H	1:152:A:ILE:HG13	4	0.53	0.41	0.36
(1,1780)	1:149:A:ASN:HB2	1:152:A:ILE:HD11	4	0.51	0.28	0.48
(1,1780)	1:149:A:ASN:HB2	1:152:A:ILE:HD12	4	0.51	0.28	0.48
(1,1780)	1:149:A:ASN:HB2	1:152:A:ILE:HD13	4	0.51	0.28	0.48
(1,1780)	1:149:A:ASN:HB3	1:152:A:ILE:HD11	4	0.51	0.28	0.48
(1,1780)	1:149:A:ASN:HB3	1:152:A:ILE:HD12	4	0.51	0.28	0.48
(1,1780)	1:149:A:ASN:HB3	1:152:A:ILE:HD13	4	0.51	0.28	0.48
(1,48)	1:6:A:LYS:H	1:6:A:LYS:HE2	4	0.5	0.2	0.56
(1,48)	1:6:A:LYS:H	1:6:A:LYS:HE3	4	0.5	0.2	0.56
(1,606)	1:49:A:PRO:HB3	1:52:A:GLU:H	4	0.49	0.23	0.48
(1,509)	1:31:A:ILE:HG21	1:109:A:LEU:H	4	0.49	0.26	0.48
(1,509)	1:31:A:ILE:HG22	1:109:A:LEU:H	4	0.49	0.26	0.48
(1,509)	1:31:A:ILE:HG23	1:109:A:LEU:H	4	0.49	0.26	0.48
(1,820)	1:69:A:TYR:HA	1:96:A:GLN:HG2	4	0.48	0.16	0.48
(1,820)	1:69:A:TYR:HA	1:96:A:GLN:HG3	4	0.48	0.16	0.48
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB1	4	0.48	0.2	0.52
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB2	4	0.48	0.2	0.52
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB3	4	0.48	0.2	0.52
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB1	4	0.48	0.2	0.52
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB2	4	0.48	0.2	0.52
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB3	4	0.48	0.2	0.52
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB1	4	0.48	0.2	0.52
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB2	4	0.48	0.2	0.52
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB3	4	0.48	0.2	0.52
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB1	4	0.48	0.2	0.52
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB2	4	0.48	0.2	0.52
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB3	4	0.48	0.2	0.52
(1,27)	1:5:A:VAL:HA	1:36:A:THR:HA	4	0.46	0.12	0.46
(1,973)	1:79:A:GLN:HB2	1:85:A:GLY:H	4	0.46	0.1	0.5
(1,960)	1:78:A:VAL:HG21	1:87:A:SER:HB2	4	0.46	0.1	0.44
(1,960)	1:78:A:VAL:HG22	1:87:A:SER:HB2	4	0.46	0.1	0.44
(1,960)	1:78:A:VAL:HG23	1:87:A:SER:HB2	4	0.46	0.1	0.44
(1,960)	1:78:A:VAL:HG21	1:87:A:SER:HB3	4	0.46	0.1	0.44
(1,960)	1:78:A:VAL:HG22	1:87:A:SER:HB3	4	0.46	0.1	0.44
(1,960)	1:78:A:VAL:HG23	1:87:A:SER:HB3	4	0.46	0.1	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1775)	1:149:A:ASN:HB3	1:152:A:ILE:HG21	4	0.46	0.31	0.42
(1,1775)	1:149:A:ASN:HB3	1:152:A:ILE:HG22	4	0.46	0.31	0.42
(1,1775)	1:149:A:ASN:HB3	1:152:A:ILE:HG23	4	0.46	0.31	0.42
(1,1799)	1:151:A:ARG:H	1:152:A:ILE:H	4	0.45	0.16	0.48
(1,428)	1:28:A:ILE:H	1:42:A:LYS:HD2	4	0.43	0.13	0.41
(1,428)	1:28:A:ILE:H	1:42:A:LYS:HD3	4	0.43	0.13	0.41
(1,607)	1:49:A:PRO:HG2	1:51:A:ALA:HB1	4	0.43	0.24	0.36
(1,607)	1:49:A:PRO:HG2	1:51:A:ALA:HB2	4	0.43	0.24	0.36
(1,607)	1:49:A:PRO:HG2	1:51:A:ALA:HB3	4	0.43	0.24	0.36
(1,607)	1:49:A:PRO:HG3	1:51:A:ALA:HB1	4	0.43	0.24	0.36
(1,607)	1:49:A:PRO:HG3	1:51:A:ALA:HB2	4	0.43	0.24	0.36
(1,607)	1:49:A:PRO:HG3	1:51:A:ALA:HB3	4	0.43	0.24	0.36
(1,1235)	1:104:A:VAL:HG21	1:108:A:MET:H	4	0.42	0.04	0.43
(1,1235)	1:104:A:VAL:HG22	1:108:A:MET:H	4	0.42	0.04	0.43
(1,1235)	1:104:A:VAL:HG23	1:108:A:MET:H	4	0.42	0.04	0.43
(1,1397)	1:115:A:ARG:HA	1:118:A:LYS:HD2	4	0.41	0.11	0.42
(1,1397)	1:115:A:ARG:HA	1:118:A:LYS:HD3	4	0.41	0.11	0.42
(1,64)	1:7:A:VAL:HA	1:117:A:LEU:HA	4	0.4	0.18	0.42
(1,323)	1:18:A:LEU:HD21	1:71:A:ALA:HA	4	0.4	0.17	0.44
(1,323)	1:18:A:LEU:HD22	1:71:A:ALA:HA	4	0.4	0.17	0.44
(1,323)	1:18:A:LEU:HD23	1:71:A:ALA:HA	4	0.4	0.17	0.44
(1,902)	1:75:A:GLU:HG2	1:90:A:ASN:HB2	4	0.4	0.34	0.27
(1,902)	1:75:A:GLU:HG2	1:90:A:ASN:HB3	4	0.4	0.34	0.27
(1,902)	1:75:A:GLU:HG3	1:90:A:ASN:HB2	4	0.4	0.34	0.27
(1,902)	1:75:A:GLU:HG3	1:90:A:ASN:HB3	4	0.4	0.34	0.27
(1,741)	1:58:A:LYS:H	1:58:A:LYS:HD2	4	0.4	0.11	0.34
(1,741)	1:58:A:LYS:H	1:58:A:LYS:HD3	4	0.4	0.11	0.34
(1,784)	1:61:A:VAL:HG11	1:66:A:GLU:HG2	4	0.37	0.21	0.36
(1,784)	1:61:A:VAL:HG12	1:66:A:GLU:HG2	4	0.37	0.21	0.36
(1,784)	1:61:A:VAL:HG13	1:66:A:GLU:HG2	4	0.37	0.21	0.36
(1,784)	1:61:A:VAL:HG11	1:66:A:GLU:HG3	4	0.37	0.21	0.36
(1,784)	1:61:A:VAL:HG12	1:66:A:GLU:HG3	4	0.37	0.21	0.36
(1,784)	1:61:A:VAL:HG13	1:66:A:GLU:HG3	4	0.37	0.21	0.36
(1,129)	1:8:A:ASP:HB3	1:39:A:VAL:HB	4	0.36	0.16	0.39
(1,1099)	1:93:A:ILE:HD11	1:142:A:VAL:HA	4	0.34	0.06	0.34
(1,1099)	1:93:A:ILE:HD12	1:142:A:VAL:HA	4	0.34	0.06	0.34
(1,1099)	1:93:A:ILE:HD13	1:142:A:VAL:HA	4	0.34	0.06	0.34
(1,1061)	1:91:A:LYS:HA	1:150:A:GLN:HG2	4	0.32	0.09	0.31
(1,1061)	1:91:A:LYS:HA	1:150:A:GLN:HG3	4	0.32	0.09	0.31
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB2	4	0.31	0.17	0.24
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB2	4	0.31	0.17	0.24
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB2	4	0.31	0.17	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB3	4	0.31	0.17	0.24
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB3	4	0.31	0.17	0.24
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB3	4	0.31	0.17	0.24
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB2	4	0.31	0.17	0.24
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB3	4	0.31	0.17	0.24
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB2	4	0.31	0.17	0.24
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB3	4	0.31	0.17	0.24
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB2	4	0.31	0.17	0.24
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB3	4	0.31	0.17	0.24
(1,450)	1:28:A:ILE:HD11	1:70:A:ALA:HA	4	0.3	0.17	0.28
(1,450)	1:28:A:ILE:HD12	1:70:A:ALA:HA	4	0.3	0.17	0.28
(1,450)	1:28:A:ILE:HD13	1:70:A:ALA:HA	4	0.3	0.17	0.28
(1,111)	1:7:A:VAL:HG11	1:9:A:PRO:HA	4	0.3	0.17	0.3
(1,111)	1:7:A:VAL:HG12	1:9:A:PRO:HA	4	0.3	0.17	0.3
(1,111)	1:7:A:VAL:HG13	1:9:A:PRO:HA	4	0.3	0.17	0.3
(1,111)	1:7:A:VAL:HG21	1:9:A:PRO:HA	4	0.3	0.17	0.3
(1,111)	1:7:A:VAL:HG22	1:9:A:PRO:HA	4	0.3	0.17	0.3
(1,111)	1:7:A:VAL:HG23	1:9:A:PRO:HA	4	0.3	0.17	0.3
(1,1549)	1:131:A:ALA:H	1:136:A:ASP:HB2	4	0.3	0.11	0.29
(1,1549)	1:131:A:ALA:H	1:136:A:ASP:HB3	4	0.3	0.11	0.29
(1,281)	1:16:A:ASP:HB3	1:19:A:HIS:H	4	0.29	0.11	0.3
(2,29)	1:86:A:THR:HG21	1:88:A:THR:HA	4	0.29	0.1	0.28
(2,29)	1:86:A:THR:HG22	1:88:A:THR:HA	4	0.29	0.1	0.28
(2,29)	1:86:A:THR:HG23	1:88:A:THR:HA	4	0.29	0.1	0.28
(1,1704)	1:143:A:LYS:HA	1:146:A:LEU:HB2	4	0.29	0.19	0.22
(1,1704)	1:143:A:LYS:HA	1:146:A:LEU:HB3	4	0.29	0.19	0.22
(1,1414)	1:116:A:ALA:HB1	1:120:A:SER:H	4	0.28	0.11	0.25
(1,1414)	1:116:A:ALA:HB2	1:120:A:SER:H	4	0.28	0.11	0.25
(1,1414)	1:116:A:ALA:HB3	1:120:A:SER:H	4	0.28	0.11	0.25
(1,882)	1:75:A:GLU:HB2	1:89:A:LEU:H	4	0.27	0.02	0.28
(1,464)	1:29:A:PHE:HB2	1:41:A:GLU:H	4	0.26	0.14	0.21
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB2	4	0.24	0.13	0.21
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB3	4	0.24	0.13	0.21
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB2	4	0.24	0.13	0.21
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB3	4	0.24	0.13	0.21
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD11	4	0.24	0.06	0.25
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD12	4	0.24	0.06	0.25
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD13	4	0.24	0.06	0.25
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD21	4	0.24	0.06	0.25
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD22	4	0.24	0.06	0.25
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD23	4	0.24	0.06	0.25
(1,296)	1:17:A:LEU:HA	1:23:A:GLN:HB2	4	0.24	0.1	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,296)	1:17:A:LEU:HA	1:23:A:GLN:HB3	4	0.24	0.1	0.21
(1,107)	1:7:A:VAL:HG11	1:38:A:ILE:H	4	0.23	0.1	0.22
(1,107)	1:7:A:VAL:HG12	1:38:A:ILE:H	4	0.23	0.1	0.22
(1,107)	1:7:A:VAL:HG13	1:38:A:ILE:H	4	0.23	0.1	0.22
(1,107)	1:7:A:VAL:HG21	1:38:A:ILE:H	4	0.23	0.1	0.22
(1,107)	1:7:A:VAL:HG22	1:38:A:ILE:H	4	0.23	0.1	0.22
(1,107)	1:7:A:VAL:HG23	1:38:A:ILE:H	4	0.23	0.1	0.22
(1,1660)	1:140:A:LYS:HG2	1:142:A:VAL:H	4	0.22	0.11	0.18
(1,1660)	1:140:A:LYS:HG3	1:142:A:VAL:H	4	0.22	0.11	0.18
(1,272)	1:16:A:ASP:HA	1:18:A:LEU:H	4	0.22	0.11	0.19
(1,121)	1:8:A:ASP:HB2	1:10:A:SER:H	4	0.21	0.11	0.16
(1,636)	1:51:A:ALA:HB1	1:54:A:VAL:H	4	0.17	0.07	0.14
(1,636)	1:51:A:ALA:HB2	1:54:A:VAL:H	4	0.17	0.07	0.14
(1,636)	1:51:A:ALA:HB3	1:54:A:VAL:H	4	0.17	0.07	0.14
(1,404)	1:27:A:ILE:HB	1:71:A:ALA:HB1	4	0.16	0.05	0.14
(1,404)	1:27:A:ILE:HB	1:71:A:ALA:HB2	4	0.16	0.05	0.14
(1,404)	1:27:A:ILE:HB	1:71:A:ALA:HB3	4	0.16	0.05	0.14
(1,1514)	1:124:A:GLU:HB2	1:126:A:LEU:H	4	0.15	0.03	0.14
(1,1514)	1:124:A:GLU:HB3	1:126:A:LEU:H	4	0.15	0.03	0.14
(1,1203)	1:102:A:ALA:HB1	1:103:A:PRO:HA	4	0.14	0.04	0.12
(1,1203)	1:102:A:ALA:HB2	1:103:A:PRO:HA	4	0.14	0.04	0.12
(1,1203)	1:102:A:ALA:HB3	1:103:A:PRO:HA	4	0.14	0.04	0.12
(1,1444)	1:118:A:LYS:HG2	1:119:A:ALA:H	4	0.14	0.03	0.14
(1,1657)	1:140:A:LYS:HB2	1:141:A:SER:H	4	0.14	0.02	0.14
(1,1657)	1:140:A:LYS:HB3	1:141:A:SER:H	4	0.14	0.02	0.14
(1,1764)	1:148:A:SER:HB2	1:149:A:ASN:H	4	0.13	0.02	0.13
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD11	4	0.13	0.04	0.11
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD12	4	0.13	0.04	0.11
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD13	4	0.13	0.04	0.11
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD21	4	0.13	0.04	0.11
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD22	4	0.13	0.04	0.11
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD23	4	0.13	0.04	0.11
(1,1782)	1:150:A:GLN:H	1:150:A:GLN:HA	4	0.13	0.01	0.13
(1,732)	1:57:A:MET:HA	1:60:A:LEU:HG	3	1.26	0.23	1.28
(1,275)	1:16:A:ASP:HA	1:20:A:ASN:H	3	1.19	0.44	1.21
(1,295)	1:17:A:LEU:HA	1:21:A:LYS:HG2	3	1.14	0.15	1.24
(1,295)	1:17:A:LEU:HA	1:21:A:LYS:HG3	3	1.14	0.15	1.24
(1,502)	1:31:A:ILE:HD11	1:109:A:LEU:HA	3	1.05	0.53	0.88
(1,502)	1:31:A:ILE:HD12	1:109:A:LEU:HA	3	1.05	0.53	0.88
(1,502)	1:31:A:ILE:HD13	1:109:A:LEU:HA	3	1.05	0.53	0.88
(1,20)	1:4:A:GLY:H	1:5:A:VAL:HB	3	0.77	0.14	0.71
(1,501)	1:31:A:ILE:HD11	1:109:A:LEU:H	3	0.73	0.43	0.71

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,501)	1:31:A:ILE:HD12	1:109:A:LEU:H	3	0.73	0.43	0.71
(1,501)	1:31:A:ILE:HD13	1:109:A:LEU:H	3	0.73	0.43	0.71
(1,890)	1:75:A:GLU:HG2	1:88:A:THR:HG21	3	0.66	0.19	0.76
(1,890)	1:75:A:GLU:HG2	1:88:A:THR:HG22	3	0.66	0.19	0.76
(1,890)	1:75:A:GLU:HG2	1:88:A:THR:HG23	3	0.66	0.19	0.76
(1,580)	1:42:A:LYS:HG2	1:56:A:GLU:HG2	3	0.65	0.56	0.31
(1,580)	1:42:A:LYS:HG2	1:56:A:GLU:HG3	3	0.65	0.56	0.31
(1,580)	1:42:A:LYS:HG3	1:56:A:GLU:HG2	3	0.65	0.56	0.31
(1,580)	1:42:A:LYS:HG3	1:56:A:GLU:HG3	3	0.65	0.56	0.31
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD11	3	0.64	0.14	0.56
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD12	3	0.64	0.14	0.56
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD13	3	0.64	0.14	0.56
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD21	3	0.64	0.14	0.56
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD22	3	0.64	0.14	0.56
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD23	3	0.64	0.14	0.56
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD11	3	0.64	0.14	0.56
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD12	3	0.64	0.14	0.56
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD13	3	0.64	0.14	0.56
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD21	3	0.64	0.14	0.56
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD22	3	0.64	0.14	0.56
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD23	3	0.64	0.14	0.56
(1,387)	1:26:A:TYR:HB2	1:73:A:ASP:H	3	0.64	0.11	0.62
(1,387)	1:26:A:TYR:HB3	1:73:A:ASP:H	3	0.64	0.11	0.62
(1,1184)	1:99:A:PRO:HG2	1:100:A:ASP:H	3	0.6	0.08	0.56
(3,19)	1:29:A:PHE:O	1:69:A:TYR:H	3	0.59	0.4	0.48
(1,1566)	1:133:A:GLU:HG2	1:135:A:SER:H	3	0.57	0.05	0.56
(1,1566)	1:133:A:GLU:HG3	1:135:A:SER:H	3	0.57	0.05	0.56
(3,20)	1:29:A:PHE:O	1:69:A:TYR:N	3	0.56	0.2	0.69
(1,1064)	1:91:A:LYS:HD2	1:92:A:VAL:H	3	0.55	0.06	0.57
(1,1064)	1:91:A:LYS:HD3	1:92:A:VAL:H	3	0.55	0.06	0.57
(1,912)	1:76:A:VAL:HA	1:88:A:THR:HG21	3	0.54	0.17	0.49
(1,912)	1:76:A:VAL:HA	1:88:A:THR:HG22	3	0.54	0.17	0.49
(1,912)	1:76:A:VAL:HA	1:88:A:THR:HG23	3	0.54	0.17	0.49
(1,1779)	1:149:A:ASN:HB2	1:152:A:ILE:H	3	0.52	0.3	0.53
(1,1779)	1:149:A:ASN:HB3	1:152:A:ILE:H	3	0.52	0.3	0.53
(1,886)	1:75:A:GLU:HB3	1:88:A:THR:HG21	3	0.48	0.15	0.39
(1,886)	1:75:A:GLU:HB3	1:88:A:THR:HG22	3	0.48	0.15	0.39
(1,886)	1:75:A:GLU:HB3	1:88:A:THR:HG23	3	0.48	0.15	0.39
(1,384)	1:26:A:TYR:HB2	1:71:A:ALA:H	3	0.47	0.17	0.36
(1,384)	1:26:A:TYR:HB3	1:71:A:ALA:H	3	0.47	0.17	0.36
(3,7)	1:13:A:ASN:O	1:17:A:LEU:H	3	0.46	0.22	0.38
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD11	3	0.45	0.23	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD12	3	0.45	0.23	0.34
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD13	3	0.45	0.23	0.34
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD21	3	0.45	0.23	0.34
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD22	3	0.45	0.23	0.34
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD23	3	0.45	0.23	0.34
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD11	3	0.45	0.23	0.34
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD12	3	0.45	0.23	0.34
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD13	3	0.45	0.23	0.34
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD21	3	0.45	0.23	0.34
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD22	3	0.45	0.23	0.34
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD23	3	0.45	0.23	0.34
(1,489)	1:31:A:ILE:HA	1:38:A:ILE:HD11	3	0.45	0.12	0.42
(1,489)	1:31:A:ILE:HA	1:38:A:ILE:HD12	3	0.45	0.12	0.42
(1,489)	1:31:A:ILE:HA	1:38:A:ILE:HD13	3	0.45	0.12	0.42
(1,370)	1:25:A:SER:HB2	1:73:A:ASP:HB2	3	0.44	0.21	0.4
(1,370)	1:25:A:SER:HB2	1:73:A:ASP:HB3	3	0.44	0.21	0.4
(1,370)	1:25:A:SER:HB3	1:73:A:ASP:HB2	3	0.44	0.21	0.4
(1,370)	1:25:A:SER:HB3	1:73:A:ASP:HB3	3	0.44	0.21	0.4
(1,1581)	1:134:A:MET:HG2	1:135:A:SER:H	3	0.43	0.01	0.42
(1,1581)	1:134:A:MET:HG3	1:135:A:SER:H	3	0.43	0.01	0.42
(1,521)	1:33:A:LYS:HE2	1:35:A:ASP:H	3	0.41	0.21	0.39
(1,521)	1:33:A:LYS:HE3	1:35:A:ASP:H	3	0.41	0.21	0.39
(1,921)	1:76:A:VAL:HG11	1:143:A:LYS:HG2	3	0.39	0.21	0.29
(1,921)	1:76:A:VAL:HG11	1:143:A:LYS:HG3	3	0.39	0.21	0.29
(1,921)	1:76:A:VAL:HG12	1:143:A:LYS:HG2	3	0.39	0.21	0.29
(1,921)	1:76:A:VAL:HG12	1:143:A:LYS:HG3	3	0.39	0.21	0.29
(1,921)	1:76:A:VAL:HG13	1:143:A:LYS:HG2	3	0.39	0.21	0.29
(1,921)	1:76:A:VAL:HG13	1:143:A:LYS:HG3	3	0.39	0.21	0.29
(1,921)	1:76:A:VAL:HG21	1:143:A:LYS:HG2	3	0.39	0.21	0.29
(1,921)	1:76:A:VAL:HG21	1:143:A:LYS:HG3	3	0.39	0.21	0.29
(1,921)	1:76:A:VAL:HG22	1:143:A:LYS:HG2	3	0.39	0.21	0.29
(1,921)	1:76:A:VAL:HG22	1:143:A:LYS:HG3	3	0.39	0.21	0.29
(1,921)	1:76:A:VAL:HG23	1:143:A:LYS:HG2	3	0.39	0.21	0.29
(1,921)	1:76:A:VAL:HG23	1:143:A:LYS:HG3	3	0.39	0.21	0.29
(1,57)	1:6:A:LYS:HB2	1:37:A:ALA:HA	3	0.38	0.34	0.14
(1,57)	1:6:A:LYS:HB3	1:37:A:ALA:HA	3	0.38	0.34	0.14
(1,1440)	1:118:A:LYS:HD2	1:119:A:ALA:H	3	0.38	0.09	0.32
(1,1440)	1:118:A:LYS:HD3	1:119:A:ALA:H	3	0.38	0.09	0.32
(1,749)	1:58:A:LYS:HA	1:62:A:GLU:H	3	0.36	0.19	0.24
(1,1466)	1:120:A:SER:HB3	1:122:A:GLY:H	3	0.35	0.29	0.18
(1,579)	1:42:A:LYS:HG2	1:56:A:GLU:HB2	3	0.35	0.24	0.28
(1,579)	1:42:A:LYS:HG2	1:56:A:GLU:HB3	3	0.35	0.24	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,579)	1:42:A:LYS:HG3	1:56:A:GLU:HB2	3	0.35	0.24	0.28
(1,579)	1:42:A:LYS:HG3	1:56:A:GLU:HB3	3	0.35	0.24	0.28
(1,597)	1:49:A:PRO:HA	1:51:A:ALA:H	3	0.34	0.09	0.29
(3,8)	1:13:A:ASN:O	1:17:A:LEU:N	3	0.34	0.22	0.26
(3,27)	1:68:A:ARG:O	1:97:A:TYR:H	3	0.33	0.15	0.38
(1,704)	1:55:A:GLU:HA	1:59:A:LYS:H	3	0.32	0.0	0.32
(1,874)	1:75:A:GLU:HA	1:88:A:THR:HG21	3	0.32	0.21	0.18
(1,874)	1:75:A:GLU:HA	1:88:A:THR:HG22	3	0.32	0.21	0.18
(1,874)	1:75:A:GLU:HA	1:88:A:THR:HG23	3	0.32	0.21	0.18
(1,1207)	1:103:A:PRO:HA	1:106:A:ARG:H	3	0.32	0.09	0.37
(1,598)	1:49:A:PRO:HA	1:51:A:ALA:HB1	3	0.31	0.11	0.27
(1,598)	1:49:A:PRO:HA	1:51:A:ALA:HB2	3	0.31	0.11	0.27
(1,598)	1:49:A:PRO:HA	1:51:A:ALA:HB3	3	0.31	0.11	0.27
(1,264)	1:15:A:TYR:HB3	1:27:A:ILE:HD11	3	0.31	0.11	0.26
(1,264)	1:15:A:TYR:HB3	1:27:A:ILE:HD12	3	0.31	0.11	0.26
(1,264)	1:15:A:TYR:HB3	1:27:A:ILE:HD13	3	0.31	0.11	0.26
(1,334)	1:19:A:HIS:H	1:21:A:LYS:H	3	0.31	0.13	0.28
(1,1239)	1:104:A:VAL:HG11	1:107:A:ARG:H	3	0.31	0.13	0.38
(1,1239)	1:104:A:VAL:HG12	1:107:A:ARG:H	3	0.31	0.13	0.38
(1,1239)	1:104:A:VAL:HG13	1:107:A:ARG:H	3	0.31	0.13	0.38
(1,1239)	1:104:A:VAL:HG21	1:107:A:ARG:H	3	0.31	0.13	0.38
(1,1239)	1:104:A:VAL:HG22	1:107:A:ARG:H	3	0.31	0.13	0.38
(1,1239)	1:104:A:VAL:HG23	1:107:A:ARG:H	3	0.31	0.13	0.38
(1,1109)	1:94:A:PHE:H	1:127:A:PHE:H	3	0.29	0.08	0.34
(1,657)	1:53:A:PHE:HA	1:57:A:MET:H	3	0.29	0.14	0.27
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD11	3	0.28	0.01	0.28
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD12	3	0.28	0.01	0.28
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD13	3	0.28	0.01	0.28
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD21	3	0.28	0.01	0.28
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD22	3	0.28	0.01	0.28
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD23	3	0.28	0.01	0.28
(1,953)	1:78:A:VAL:HB	1:87:A:SER:HB2	3	0.28	0.08	0.27
(1,953)	1:78:A:VAL:HB	1:87:A:SER:HB3	3	0.28	0.08	0.27
(1,1314)	1:109:A:LEU:HA	1:112:A:SER:H	3	0.28	0.11	0.23
(1,1547)	1:130:A:GLN:HG2	1:131:A:ALA:H	3	0.28	0.12	0.35
(1,1547)	1:130:A:GLN:HG3	1:131:A:ALA:H	3	0.28	0.12	0.35
(1,16)	1:3:A:SER:H	1:4:A:GLY:H	3	0.28	0.1	0.34
(2,5)	1:12:A:LYS:HG2	1:121:A:LEU:HD21	3	0.28	0.06	0.31
(2,5)	1:12:A:LYS:HG2	1:121:A:LEU:HD22	3	0.28	0.06	0.31
(2,5)	1:12:A:LYS:HG2	1:121:A:LEU:HD23	3	0.28	0.06	0.31
(1,1373)	1:114:A:VAL:HA	1:117:A:LEU:HB2	3	0.27	0.14	0.28
(1,1373)	1:114:A:VAL:HA	1:117:A:LEU:HB3	3	0.27	0.14	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1453)	1:119:A:ALA:HA	1:122:A:GLY:H	3	0.26	0.14	0.18
(1,1190)	1:99:A:PRO:HG3	1:132:A:SER:HA	3	0.25	0.06	0.24
(1,243)	1:14:A:ALA:HB1	1:27:A:ILE:HB	3	0.24	0.05	0.26
(1,243)	1:14:A:ALA:HB2	1:27:A:ILE:HB	3	0.24	0.05	0.26
(1,243)	1:14:A:ALA:HB3	1:27:A:ILE:HB	3	0.24	0.05	0.26
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG11	3	0.24	0.13	0.16
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG12	3	0.24	0.13	0.16
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG13	3	0.24	0.13	0.16
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG21	3	0.24	0.13	0.16
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG22	3	0.24	0.13	0.16
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG23	3	0.24	0.13	0.16
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG11	3	0.24	0.13	0.16
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG12	3	0.24	0.13	0.16
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG13	3	0.24	0.13	0.16
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG21	3	0.24	0.13	0.16
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG22	3	0.24	0.13	0.16
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG23	3	0.24	0.13	0.16
(1,1324)	1:109:A:LEU:HD11	1:112:A:SER:H	3	0.24	0.08	0.19
(1,1324)	1:109:A:LEU:HD12	1:112:A:SER:H	3	0.24	0.08	0.19
(1,1324)	1:109:A:LEU:HD13	1:112:A:SER:H	3	0.24	0.08	0.19
(1,1324)	1:109:A:LEU:HD21	1:112:A:SER:H	3	0.24	0.08	0.19
(1,1324)	1:109:A:LEU:HD22	1:112:A:SER:H	3	0.24	0.08	0.19
(1,1324)	1:109:A:LEU:HD23	1:112:A:SER:H	3	0.24	0.08	0.19
(1,1048)	1:89:A:LEU:HG	1:90:A:ASN:H	3	0.24	0.05	0.22
(1,1050)	1:89:A:LEU:HD11	1:90:A:ASN:H	3	0.24	0.0	0.24
(1,1050)	1:89:A:LEU:HD12	1:90:A:ASN:H	3	0.24	0.0	0.24
(1,1050)	1:89:A:LEU:HD13	1:90:A:ASN:H	3	0.24	0.0	0.24
(1,289)	1:17:A:LEU:H	1:23:A:GLN:HB2	3	0.23	0.04	0.24
(1,289)	1:17:A:LEU:H	1:23:A:GLN:HB3	3	0.23	0.04	0.24
(1,1097)	1:93:A:ILE:HD11	1:129:A:VAL:HA	3	0.23	0.13	0.19
(1,1097)	1:93:A:ILE:HD12	1:129:A:VAL:HA	3	0.23	0.13	0.19
(1,1097)	1:93:A:ILE:HD13	1:129:A:VAL:HA	3	0.23	0.13	0.19
(1,218)	1:12:A:LYS:HG2	1:121:A:LEU:HA	3	0.23	0.12	0.21
(1,218)	1:12:A:LYS:HG3	1:121:A:LEU:HA	3	0.23	0.12	0.21
(1,51)	1:6:A:LYS:HA	1:37:A:ALA:HA	3	0.23	0.08	0.28
(1,616)	1:50:A:TYR:HA	1:52:A:GLU:H	3	0.21	0.03	0.22
(1,1204)	1:102:A:ALA:HB1	1:103:A:PRO:HG2	3	0.21	0.06	0.18
(1,1204)	1:102:A:ALA:HB1	1:103:A:PRO:HG3	3	0.21	0.06	0.18
(1,1204)	1:102:A:ALA:HB2	1:103:A:PRO:HG2	3	0.21	0.06	0.18
(1,1204)	1:102:A:ALA:HB2	1:103:A:PRO:HG3	3	0.21	0.06	0.18
(1,1204)	1:102:A:ALA:HB3	1:103:A:PRO:HG2	3	0.21	0.06	0.18
(1,1204)	1:102:A:ALA:HB3	1:103:A:PRO:HG3	3	0.21	0.06	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,105)	1:7:A:VAL:HG11	1:37:A:ALA:HA	3	0.2	0.1	0.16
(1,105)	1:7:A:VAL:HG12	1:37:A:ALA:HA	3	0.2	0.1	0.16
(1,105)	1:7:A:VAL:HG13	1:37:A:ALA:HA	3	0.2	0.1	0.16
(1,105)	1:7:A:VAL:HG21	1:37:A:ALA:HA	3	0.2	0.1	0.16
(1,105)	1:7:A:VAL:HG22	1:37:A:ALA:HA	3	0.2	0.1	0.16
(1,105)	1:7:A:VAL:HG23	1:37:A:ALA:HA	3	0.2	0.1	0.16
(1,1405)	1:116:A:ALA:H	1:117:A:LEU:H	3	0.2	0.03	0.2
(1,708)	1:55:A:GLU:HB2	1:57:A:MET:H	3	0.19	0.04	0.16
(1,1712)	1:143:A:LYS:HB3	1:147:A:MET:H	3	0.19	0.05	0.2
(1,742)	1:58:A:LYS:H	1:58:A:LYS:HE2	3	0.18	0.05	0.15
(1,742)	1:58:A:LYS:H	1:58:A:LYS:HE3	3	0.18	0.05	0.15
(1,930)	1:77:A:THR:HA	1:78:A:VAL:HB	3	0.18	0.05	0.17
(1,1730)	1:145:A:ASP:H	1:147:A:MET:H	3	0.18	0.06	0.19
(1,1094)	1:93:A:ILE:HG13	1:127:A:PHE:H	3	0.17	0.04	0.14
(1,1433)	1:117:A:LEU:HD11	1:120:A:SER:H	3	0.16	0.05	0.16
(1,1433)	1:117:A:LEU:HD12	1:120:A:SER:H	3	0.16	0.05	0.16
(1,1433)	1:117:A:LEU:HD13	1:120:A:SER:H	3	0.16	0.05	0.16
(1,1433)	1:117:A:LEU:HD21	1:120:A:SER:H	3	0.16	0.05	0.16
(1,1433)	1:117:A:LEU:HD22	1:120:A:SER:H	3	0.16	0.05	0.16
(1,1433)	1:117:A:LEU:HD23	1:120:A:SER:H	3	0.16	0.05	0.16
(1,875)	1:75:A:GLU:HA	1:89:A:LEU:H	3	0.15	0.03	0.14
(2,11)	1:18:A:LEU:HD11	1:71:A:ALA:HA	3	0.15	0.02	0.14
(2,11)	1:18:A:LEU:HD12	1:71:A:ALA:HA	3	0.15	0.02	0.14
(2,11)	1:18:A:LEU:HD13	1:71:A:ALA:HA	3	0.15	0.02	0.14
(1,1273)	1:106:A:ARG:HB2	1:108:A:MET:H	3	0.13	0.01	0.13
(1,1273)	1:106:A:ARG:HB3	1:108:A:MET:H	3	0.13	0.01	0.13
(1,714)	1:55:A:GLU:HG2	1:58:A:LYS:HB2	2	1.37	0.11	1.37
(1,714)	1:55:A:GLU:HG2	1:58:A:LYS:HB3	2	1.37	0.11	1.37
(1,714)	1:55:A:GLU:HG3	1:58:A:LYS:HB2	2	1.37	0.11	1.37
(1,714)	1:55:A:GLU:HG3	1:58:A:LYS:HB3	2	1.37	0.11	1.37
(1,1802)	1:151:A:ARG:HD2	1:152:A:ILE:H	2	1.2	0.27	1.2
(1,1802)	1:151:A:ARG:HD3	1:152:A:ILE:H	2	1.2	0.27	1.2
(1,1609)	1:137:A:LEU:HG	1:138:A:ASP:H	2	1.03	0.06	1.03
(1,576)	1:42:A:LYS:HD2	1:43:A:VAL:H	2	0.68	0.12	0.68
(1,576)	1:42:A:LYS:HD3	1:43:A:VAL:H	2	0.68	0.12	0.68
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD11	2	0.67	0.29	0.67
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD12	2	0.67	0.29	0.67
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD13	2	0.67	0.29	0.67
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD21	2	0.67	0.29	0.67
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD22	2	0.67	0.29	0.67
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD23	2	0.67	0.29	0.67
(1,345)	1:21:A:LYS:H	1:21:A:LYS:HE2	2	0.64	0.01	0.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,345)	1:21:A:LYS:H	1:21:A:LYS:HE3	2	0.64	0.01	0.64
(1,245)	1:14:A:ALA:HB1	1:40:A:VAL:HB	2	0.62	0.22	0.62
(1,245)	1:14:A:ALA:HB2	1:40:A:VAL:HB	2	0.62	0.22	0.62
(1,245)	1:14:A:ALA:HB3	1:40:A:VAL:HB	2	0.62	0.22	0.62
(1,702)	1:55:A:GLU:HA	1:58:A:LYS:HB2	2	0.62	0.04	0.62
(1,702)	1:55:A:GLU:HA	1:58:A:LYS:HB3	2	0.62	0.04	0.62
(3,26)	1:68:A:ARG:N	1:97:A:TYR:O	2	0.61	0.17	0.61
(1,893)	1:75:A:GLU:HG2	1:90:A:ASN:HB2	2	0.6	0.3	0.6
(1,893)	1:75:A:GLU:HG2	1:90:A:ASN:HB3	2	0.6	0.3	0.6
(1,510)	1:31:A:ILE:HG21	1:109:A:LEU:HA	2	0.6	0.31	0.6
(1,510)	1:31:A:ILE:HG22	1:109:A:LEU:HA	2	0.6	0.31	0.6
(1,510)	1:31:A:ILE:HG23	1:109:A:LEU:HA	2	0.6	0.31	0.6
(1,880)	1:75:A:GLU:HB2	1:88:A:THR:HB	2	0.59	0.32	0.59
(1,1260)	1:105:A:ARG:HD2	1:106:A:ARG:H	2	0.55	0.04	0.55
(1,1260)	1:105:A:ARG:HD3	1:106:A:ARG:H	2	0.55	0.04	0.55
(1,752)	1:58:A:LYS:HB3	1:59:A:LYS:H	2	0.53	0.05	0.53
(1,321)	1:18:A:LEU:HD11	1:73:A:ASP:HA	2	0.51	0.23	0.51
(1,321)	1:18:A:LEU:HD12	1:73:A:ASP:HA	2	0.51	0.23	0.51
(1,321)	1:18:A:LEU:HD13	1:73:A:ASP:HA	2	0.51	0.23	0.51
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD11	2	0.48	0.38	0.48
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD12	2	0.48	0.38	0.48
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD13	2	0.48	0.38	0.48
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD21	2	0.48	0.38	0.48
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD22	2	0.48	0.38	0.48
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD23	2	0.48	0.38	0.48
(1,1162)	1:96:A:GLN:HG2	1:130:A:GLN:HA	2	0.48	0.18	0.48
(1,1162)	1:96:A:GLN:HG3	1:130:A:GLN:HA	2	0.48	0.18	0.48
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG11	2	0.48	0.09	0.48
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG12	2	0.48	0.09	0.48
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG13	2	0.48	0.09	0.48
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG21	2	0.48	0.09	0.48
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG22	2	0.48	0.09	0.48
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG23	2	0.48	0.09	0.48
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG11	2	0.48	0.09	0.48
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG12	2	0.48	0.09	0.48
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG13	2	0.48	0.09	0.48
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG21	2	0.48	0.09	0.48
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG22	2	0.48	0.09	0.48
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG23	2	0.48	0.09	0.48
(1,605)	1:49:A:PRO:HB3	1:51:A:ALA:HB1	2	0.48	0.13	0.48
(1,605)	1:49:A:PRO:HB3	1:51:A:ALA:HB2	2	0.48	0.13	0.48
(1,605)	1:49:A:PRO:HB3	1:51:A:ALA:HB3	2	0.48	0.13	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1574)	1:134:A:MET:HA	1:136:A:ASP:H	2	0.48	0.28	0.48
(3,25)	1:68:A:ARG:H	1:97:A:TYR:O	2	0.47	0.19	0.47
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD11	2	0.47	0.06	0.47
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD12	2	0.47	0.06	0.47
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD13	2	0.47	0.06	0.47
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD21	2	0.47	0.06	0.47
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD22	2	0.47	0.06	0.47
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD23	2	0.47	0.06	0.47
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD11	2	0.47	0.06	0.47
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD12	2	0.47	0.06	0.47
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD13	2	0.47	0.06	0.47
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD21	2	0.47	0.06	0.47
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD22	2	0.47	0.06	0.47
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD23	2	0.47	0.06	0.47
(3,37)	1:74:A:VAL:H	1:91:A:LYS:O	2	0.47	0.26	0.47
(1,28)	1:5:A:VAL:HA	1:36:A:THR:HB	2	0.46	0.08	0.46
(1,350)	1:21:A:LYS:HD3	1:22:A:HIS:H	2	0.45	0.32	0.45
(1,1315)	1:109:A:LEU:HA	1:112:A:SER:HB2	2	0.45	0.22	0.45
(1,1315)	1:109:A:LEU:HA	1:112:A:SER:HB3	2	0.45	0.22	0.45
(1,1462)	1:120:A:SER:HA	1:122:A:GLY:H	2	0.43	0.12	0.43
(1,1015)	1:84:A:GLU:H	1:85:A:GLY:H	2	0.43	0.18	0.43
(1,45)	1:6:A:LYS:H	1:37:A:ALA:HB1	2	0.42	0.22	0.42
(1,45)	1:6:A:LYS:H	1:37:A:ALA:HB2	2	0.42	0.22	0.42
(1,45)	1:6:A:LYS:H	1:37:A:ALA:HB3	2	0.42	0.22	0.42
(1,310)	1:18:A:LEU:HA	1:20:A:ASN:H	2	0.42	0.22	0.42
(1,44)	1:6:A:LYS:H	1:37:A:ALA:HA	2	0.42	0.12	0.42
(3,38)	1:74:A:VAL:N	1:91:A:LYS:O	2	0.42	0.26	0.42
(1,899)	1:75:A:GLU:HG3	1:90:A:ASN:HB2	2	0.4	0.08	0.4
(1,899)	1:75:A:GLU:HG3	1:90:A:ASN:HB3	2	0.4	0.08	0.4
(1,1356)	1:112:A:SER:HB2	1:116:A:ALA:HB1	2	0.4	0.04	0.4
(1,1356)	1:112:A:SER:HB2	1:116:A:ALA:HB2	2	0.4	0.04	0.4
(1,1356)	1:112:A:SER:HB2	1:116:A:ALA:HB3	2	0.4	0.04	0.4
(1,1356)	1:112:A:SER:HB3	1:116:A:ALA:HB1	2	0.4	0.04	0.4
(1,1356)	1:112:A:SER:HB3	1:116:A:ALA:HB2	2	0.4	0.04	0.4
(1,1356)	1:112:A:SER:HB3	1:116:A:ALA:HB3	2	0.4	0.04	0.4
(1,1649)	1:140:A:LYS:HD2	1:142:A:VAL:H	2	0.4	0.01	0.4
(1,1765)	1:148:A:SER:HB2	1:150:A:GLN:H	2	0.4	0.29	0.4
(1,697)	1:55:A:GLU:HA	1:57:A:MET:H	2	0.38	0.0	0.38
(1,703)	1:55:A:GLU:HA	1:58:A:LYS:HG2	2	0.38	0.1	0.38
(1,703)	1:55:A:GLU:HA	1:58:A:LYS:HG3	2	0.38	0.1	0.38
(1,1305)	1:108:A:MET:HG2	1:112:A:SER:H	2	0.37	0.26	0.37
(1,1305)	1:108:A:MET:HG3	1:112:A:SER:H	2	0.37	0.26	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,593)	1:45:A:GLU:HB3	1:48:A:ALA:HB1	2	0.36	0.08	0.36
(1,593)	1:45:A:GLU:HB3	1:48:A:ALA:HB2	2	0.36	0.08	0.36
(1,593)	1:45:A:GLU:HB3	1:48:A:ALA:HB3	2	0.36	0.08	0.36
(1,1205)	1:102:A:ALA:HB1	1:106:A:ARG:HD2	2	0.36	0.11	0.36
(1,1205)	1:102:A:ALA:HB1	1:106:A:ARG:HD3	2	0.36	0.11	0.36
(1,1205)	1:102:A:ALA:HB2	1:106:A:ARG:HD2	2	0.36	0.11	0.36
(1,1205)	1:102:A:ALA:HB2	1:106:A:ARG:HD3	2	0.36	0.11	0.36
(1,1205)	1:102:A:ALA:HB3	1:106:A:ARG:HD2	2	0.36	0.11	0.36
(1,1205)	1:102:A:ALA:HB3	1:106:A:ARG:HD3	2	0.36	0.11	0.36
(1,208)	1:12:A:LYS:HE2	1:122:A:GLY:H	2	0.34	0.2	0.34
(1,208)	1:12:A:LYS:HE3	1:122:A:GLY:H	2	0.34	0.2	0.34
(1,600)	1:49:A:PRO:HA	1:53:A:PHE:H	2	0.34	0.06	0.34
(1,896)	1:75:A:GLU:HG3	1:88:A:THR:HG21	2	0.34	0.12	0.34
(1,896)	1:75:A:GLU:HG3	1:88:A:THR:HG22	2	0.34	0.12	0.34
(1,896)	1:75:A:GLU:HG3	1:88:A:THR:HG23	2	0.34	0.12	0.34
(1,1762)	1:148:A:SER:H	1:150:A:GLN:H	2	0.32	0.18	0.32
(1,1375)	1:114:A:VAL:HA	1:118:A:LYS:H	2	0.32	0.09	0.32
(1,644)	1:52:A:GLU:HA	1:55:A:GLU:H	2	0.32	0.08	0.32
(1,940)	1:77:A:THR:HG21	1:87:A:SER:H	2	0.32	0.18	0.32
(1,940)	1:77:A:THR:HG22	1:87:A:SER:H	2	0.32	0.18	0.32
(1,940)	1:77:A:THR:HG23	1:87:A:SER:H	2	0.32	0.18	0.32
(1,1498)	1:123:A:LEU:H	1:125:A:SER:H	2	0.32	0.12	0.32
(1,769)	1:60:A:LEU:H	1:60:A:LEU:HG	2	0.3	0.04	0.3
(1,915)	1:76:A:VAL:HG11	1:143:A:LYS:HG2	2	0.3	0.01	0.3
(1,915)	1:76:A:VAL:HG12	1:143:A:LYS:HG2	2	0.3	0.01	0.3
(1,915)	1:76:A:VAL:HG13	1:143:A:LYS:HG2	2	0.3	0.01	0.3
(1,915)	1:76:A:VAL:HG11	1:143:A:LYS:HG3	2	0.3	0.01	0.3
(1,915)	1:76:A:VAL:HG12	1:143:A:LYS:HG3	2	0.3	0.01	0.3
(1,915)	1:76:A:VAL:HG13	1:143:A:LYS:HG3	2	0.3	0.01	0.3
(1,955)	1:78:A:VAL:HG11	1:80:A:ARG:HG2	2	0.3	0.0	0.3
(1,955)	1:78:A:VAL:HG12	1:80:A:ARG:HG2	2	0.3	0.0	0.3
(1,955)	1:78:A:VAL:HG13	1:80:A:ARG:HG2	2	0.3	0.0	0.3
(1,955)	1:78:A:VAL:HG11	1:80:A:ARG:HG3	2	0.3	0.0	0.3
(1,955)	1:78:A:VAL:HG12	1:80:A:ARG:HG3	2	0.3	0.0	0.3
(1,955)	1:78:A:VAL:HG13	1:80:A:ARG:HG3	2	0.3	0.0	0.3
(1,1419)	1:117:A:LEU:H	1:119:A:ALA:H	2	0.28	0.12	0.28
(1,1745)	1:146:A:LEU:HG	1:147:A:MET:H	2	0.28	0.13	0.28
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD11	2	0.27	0.14	0.27
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD12	2	0.27	0.14	0.27
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD13	2	0.27	0.14	0.27
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD21	2	0.27	0.14	0.27
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD22	2	0.27	0.14	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD23	2	0.27	0.14	0.27
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD11	2	0.27	0.14	0.27
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD12	2	0.27	0.14	0.27
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD13	2	0.27	0.14	0.27
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD21	2	0.27	0.14	0.27
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD22	2	0.27	0.14	0.27
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD23	2	0.27	0.14	0.27
(1,1018)	1:84:A:GLU:HG2	1:85:A:GLY:H	2	0.27	0.12	0.27
(1,1018)	1:84:A:GLU:HG3	1:85:A:GLY:H	2	0.27	0.12	0.27
(1,1180)	1:99:A:PRO:HB2	1:132:A:SER:HB2	2	0.27	0.06	0.27
(1,1180)	1:99:A:PRO:HB2	1:132:A:SER:HB3	2	0.27	0.06	0.27
(2,30)	1:91:A:LYS:HE2	1:92:A:VAL:H	2	0.26	0.04	0.26
(2,30)	1:91:A:LYS:HE3	1:92:A:VAL:H	2	0.26	0.04	0.26
(1,325)	1:18:A:LEU:HD21	1:72:A:VAL:H	2	0.26	0.11	0.26
(1,325)	1:18:A:LEU:HD22	1:72:A:VAL:H	2	0.26	0.11	0.26
(1,325)	1:18:A:LEU:HD23	1:72:A:VAL:H	2	0.26	0.11	0.26
(1,733)	1:57:A:MET:HA	1:61:A:VAL:H	2	0.26	0.11	0.26
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG11	2	0.26	0.08	0.26
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG12	2	0.26	0.08	0.26
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG13	2	0.26	0.08	0.26
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG21	2	0.26	0.08	0.26
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG22	2	0.26	0.08	0.26
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG23	2	0.26	0.08	0.26
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG11	2	0.26	0.08	0.26
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG12	2	0.26	0.08	0.26
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG13	2	0.26	0.08	0.26
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG21	2	0.26	0.08	0.26
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG22	2	0.26	0.08	0.26
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG23	2	0.26	0.08	0.26
(1,1225)	1:104:A:VAL:HB	1:107:A:ARG:H	2	0.26	0.03	0.26
(1,1655)	1:140:A:LYS:HE3	1:142:A:VAL:H	2	0.26	0.12	0.26
(1,398)	1:27:A:ILE:HA	1:43:A:VAL:HB	2	0.25	0.13	0.25
(1,879)	1:75:A:GLU:HB2	1:88:A:THR:HA	2	0.24	0.13	0.24
(1,224)	1:13:A:ASN:HA	1:16:A:ASP:H	2	0.24	0.11	0.24
(1,1236)	1:104:A:VAL:HG21	1:108:A:MET:HB2	2	0.24	0.04	0.24
(1,1236)	1:104:A:VAL:HG22	1:108:A:MET:HB2	2	0.24	0.04	0.24
(1,1236)	1:104:A:VAL:HG23	1:108:A:MET:HB2	2	0.24	0.04	0.24
(1,1236)	1:104:A:VAL:HG21	1:108:A:MET:HB3	2	0.24	0.04	0.24
(1,1236)	1:104:A:VAL:HG22	1:108:A:MET:HB3	2	0.24	0.04	0.24
(1,1236)	1:104:A:VAL:HG23	1:108:A:MET:HB3	2	0.24	0.04	0.24
(1,1396)	1:115:A:ARG:HA	1:118:A:LYS:H	2	0.22	0.02	0.22
(1,1421)	1:117:A:LEU:HA	1:120:A:SER:H	2	0.22	0.07	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,730)	1:57:A:MET:HA	1:60:A:LEU:H	2	0.21	0.01	0.21
(1,1179)	1:99:A:PRO:HB2	1:132:A:SER:HA	2	0.21	0.11	0.21
(1,753)	1:58:A:LYS:HB3	1:60:A:LEU:H	2	0.21	0.08	0.21
(1,1723)	1:144:A:SER:HB2	1:146:A:LEU:H	2	0.2	0.04	0.2
(2,39)	1:135:A:SER:HA	1:140:A:LYS:HE3	2	0.2	0.07	0.2
(1,1727)	1:144:A:SER:HB3	1:147:A:MET:H	2	0.19	0.02	0.19
(1,131)	1:8:A:ASP:HB2	1:10:A:SER:H	2	0.18	0.01	0.18
(1,131)	1:8:A:ASP:HB3	1:10:A:SER:H	2	0.18	0.01	0.18
(1,1402)	1:115:A:ARG:HB2	1:118:A:LYS:H	2	0.18	0.08	0.18
(1,1402)	1:115:A:ARG:HB3	1:118:A:LYS:H	2	0.18	0.08	0.18
(1,291)	1:17:A:LEU:HA	1:20:A:ASN:H	2	0.18	0.06	0.18
(1,1135)	1:95:A:VAL:HG11	1:131:A:ALA:HA	2	0.18	0.03	0.18
(1,1135)	1:95:A:VAL:HG12	1:131:A:ALA:HA	2	0.18	0.03	0.18
(1,1135)	1:95:A:VAL:HG13	1:131:A:ALA:HA	2	0.18	0.03	0.18
(1,1488)	1:121:A:LEU:HD21	1:122:A:GLY:H	2	0.18	0.03	0.18
(1,1488)	1:121:A:LEU:HD22	1:122:A:GLY:H	2	0.18	0.03	0.18
(1,1488)	1:121:A:LEU:HD23	1:122:A:GLY:H	2	0.18	0.03	0.18
(1,273)	1:16:A:ASP:HA	1:19:A:HIS:H	2	0.17	0.0	0.17
(1,1244)	1:104:A:VAL:HG11	1:108:A:MET:HB2	2	0.17	0.06	0.17
(1,1244)	1:104:A:VAL:HG11	1:108:A:MET:HB3	2	0.17	0.06	0.17
(1,1244)	1:104:A:VAL:HG12	1:108:A:MET:HB2	2	0.17	0.06	0.17
(1,1244)	1:104:A:VAL:HG12	1:108:A:MET:HB3	2	0.17	0.06	0.17
(1,1244)	1:104:A:VAL:HG13	1:108:A:MET:HB2	2	0.17	0.06	0.17
(1,1244)	1:104:A:VAL:HG13	1:108:A:MET:HB3	2	0.17	0.06	0.17
(1,1244)	1:104:A:VAL:HG21	1:108:A:MET:HB2	2	0.17	0.06	0.17
(1,1244)	1:104:A:VAL:HG21	1:108:A:MET:HB3	2	0.17	0.06	0.17
(1,1244)	1:104:A:VAL:HG22	1:108:A:MET:HB2	2	0.17	0.06	0.17
(1,1244)	1:104:A:VAL:HG22	1:108:A:MET:HB3	2	0.17	0.06	0.17
(1,1244)	1:104:A:VAL:HG23	1:108:A:MET:HB2	2	0.17	0.06	0.17
(1,1244)	1:104:A:VAL:HG23	1:108:A:MET:HB3	2	0.17	0.06	0.17
(1,147)	1:10:A:SER:H	1:13:A:ASN:H	2	0.16	0.02	0.16
(1,184)	1:11:A:CYS:HB2	1:13:A:ASN:H	2	0.16	0.04	0.16
(1,184)	1:11:A:CYS:HB3	1:13:A:ASN:H	2	0.16	0.04	0.16
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD11	2	0.16	0.02	0.16
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD12	2	0.16	0.02	0.16
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD13	2	0.16	0.02	0.16
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD21	2	0.16	0.02	0.16
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD22	2	0.16	0.02	0.16
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD23	2	0.16	0.02	0.16
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD11	2	0.16	0.02	0.16
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD12	2	0.16	0.02	0.16
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD13	2	0.16	0.02	0.16

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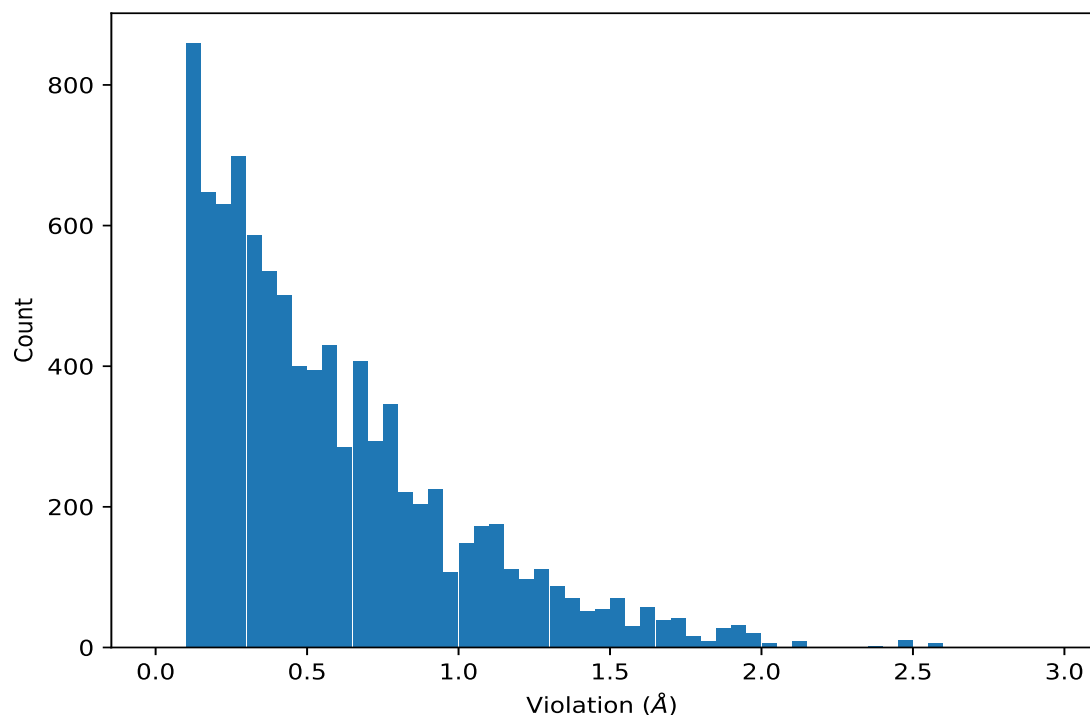
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD21	2	0.16	0.02	0.16
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD22	2	0.16	0.02	0.16
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD23	2	0.16	0.02	0.16
(1,1585)	1:135:A:SER:HA	1:136:A:ASP:HA	2	0.15	0.02	0.15
(1,1119)	1:94:A:PHE:HA	1:128:A:GLN:HG2	2	0.15	0.0	0.15
(1,1119)	1:94:A:PHE:HA	1:128:A:GLN:HG3	2	0.15	0.0	0.15
(1,1147)	1:95:A:VAL:HG11	1:97:A:TYR:HB2	2	0.15	0.02	0.15
(1,1147)	1:95:A:VAL:HG11	1:97:A:TYR:HB3	2	0.15	0.02	0.15
(1,1147)	1:95:A:VAL:HG12	1:97:A:TYR:HB2	2	0.15	0.02	0.15
(1,1147)	1:95:A:VAL:HG12	1:97:A:TYR:HB3	2	0.15	0.02	0.15
(1,1147)	1:95:A:VAL:HG13	1:97:A:TYR:HB2	2	0.15	0.02	0.15
(1,1147)	1:95:A:VAL:HG13	1:97:A:TYR:HB3	2	0.15	0.02	0.15
(1,1147)	1:95:A:VAL:HG21	1:97:A:TYR:HB2	2	0.15	0.02	0.15
(1,1147)	1:95:A:VAL:HG21	1:97:A:TYR:HB3	2	0.15	0.02	0.15
(1,1147)	1:95:A:VAL:HG22	1:97:A:TYR:HB2	2	0.15	0.02	0.15
(1,1147)	1:95:A:VAL:HG22	1:97:A:TYR:HB3	2	0.15	0.02	0.15
(1,1147)	1:95:A:VAL:HG23	1:97:A:TYR:HB2	2	0.15	0.02	0.15
(1,1147)	1:95:A:VAL:HG23	1:97:A:TYR:HB3	2	0.15	0.02	0.15
(1,1469)	1:120:A:SER:HB2	1:122:A:GLY:H	2	0.15	0.03	0.15
(1,1469)	1:120:A:SER:HB3	1:122:A:GLY:H	2	0.15	0.03	0.15
(1,1645)	1:140:A:LYS:HA	1:142:A:VAL:H	2	0.14	0.01	0.14
(1,63)	1:7:A:VAL:H	1:8:A:ASP:H	2	0.14	0.01	0.14
(1,833)	1:71:A:ALA:HB1	1:93:A:ILE:H	2	0.14	0.02	0.14
(1,833)	1:71:A:ALA:HB2	1:93:A:ILE:H	2	0.14	0.02	0.14
(1,833)	1:71:A:ALA:HB3	1:93:A:ILE:H	2	0.14	0.02	0.14
(1,210)	1:12:A:LYS:HG2	1:13:A:ASN:H	2	0.13	0.01	0.13
(1,391)	1:27:A:ILE:H	1:28:A:ILE:H	2	0.13	0.03	0.13
(1,1037)	1:88:A:THR:HB	1:89:A:LEU:H	2	0.13	0.01	0.13
(1,1296)	1:108:A:MET:HA	1:112:A:SER:H	2	0.13	0.02	0.13
(1,709)	1:55:A:GLU:HB2	1:58:A:LYS:H	2	0.12	0.02	0.12
(1,1385)	1:114:A:VAL:HG11	1:116:A:ALA:H	2	0.12	0.0	0.12
(1,1385)	1:114:A:VAL:HG12	1:116:A:ALA:H	2	0.12	0.0	0.12
(1,1385)	1:114:A:VAL:HG13	1:116:A:ALA:H	2	0.12	0.0	0.12
(1,1385)	1:114:A:VAL:HG21	1:116:A:ALA:H	2	0.12	0.0	0.12
(1,1385)	1:114:A:VAL:HG22	1:116:A:ALA:H	2	0.12	0.0	0.12
(1,1385)	1:114:A:VAL:HG23	1:116:A:ALA:H	2	0.12	0.0	0.12
(1,1736)	1:146:A:LEU:H	1:146:A:LEU:HG	2	0.12	0.0	0.12

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)
(1,889)	1:75:A:GLU:HG2	1:88:A:THR:HB	3	2.93
(1,889)	1:75:A:GLU:HG2	1:88:A:THR:HB	10	2.61
(1,1074)	1:92:A:VAL:HG11	1:125:A:SER:HA	7	2.58
(1,1074)	1:92:A:VAL:HG12	1:125:A:SER:HA	7	2.58
(1,1074)	1:92:A:VAL:HG13	1:125:A:SER:HA	7	2.58
(1,1074)	1:92:A:VAL:HG21	1:125:A:SER:HA	7	2.58
(1,1074)	1:92:A:VAL:HG22	1:125:A:SER:HA	7	2.58
(1,1074)	1:92:A:VAL:HG23	1:125:A:SER:HA	7	2.58
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE2	5	2.47
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE3	5	2.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE2	5	2.47
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE3	5	2.47
(1,1074)	1:92:A:VAL:HG11	1:125:A:SER:HA	3	2.46
(1,1074)	1:92:A:VAL:HG12	1:125:A:SER:HA	3	2.46
(1,1074)	1:92:A:VAL:HG13	1:125:A:SER:HA	3	2.46
(1,1074)	1:92:A:VAL:HG21	1:125:A:SER:HA	3	2.46
(1,1074)	1:92:A:VAL:HG22	1:125:A:SER:HA	3	2.46
(1,1074)	1:92:A:VAL:HG23	1:125:A:SER:HA	3	2.46
(1,945)	1:78:A:VAL:H	1:86:A:THR:HB	6	2.38
(1,895)	1:75:A:GLU:HG3	1:88:A:THR:HB	3	2.38
(1,170)	1:11:A:CYS:H	1:40:A:VAL:HB	3	2.33
(1,170)	1:11:A:CYS:H	1:40:A:VAL:HB	2	2.16
(1,170)	1:11:A:CYS:H	1:40:A:VAL:HB	5	2.14
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB2	10	2.12
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB3	10	2.12
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB2	10	2.12
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB3	10	2.12
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB2	3	2.1
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB3	3	2.1
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB2	3	2.1
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB3	3	2.1
(1,170)	1:11:A:CYS:H	1:40:A:VAL:HB	7	2.07
(1,1074)	1:92:A:VAL:HG11	1:125:A:SER:HA	2	2.04
(1,1074)	1:92:A:VAL:HG12	1:125:A:SER:HA	2	2.04
(1,1074)	1:92:A:VAL:HG13	1:125:A:SER:HA	2	2.04
(1,1074)	1:92:A:VAL:HG21	1:125:A:SER:HA	2	2.04
(1,1074)	1:92:A:VAL:HG22	1:125:A:SER:HA	2	2.04
(1,1074)	1:92:A:VAL:HG23	1:125:A:SER:HA	2	2.04
(1,684)	1:54:A:VAL:HG11	1:138:A:ASP:H	10	1.99
(1,684)	1:54:A:VAL:HG12	1:138:A:ASP:H	10	1.99
(1,684)	1:54:A:VAL:HG13	1:138:A:ASP:H	10	1.99
(1,684)	1:54:A:VAL:HG21	1:138:A:ASP:H	10	1.99
(1,684)	1:54:A:VAL:HG22	1:138:A:ASP:H	10	1.99
(1,684)	1:54:A:VAL:HG23	1:138:A:ASP:H	10	1.99
(1,170)	1:11:A:CYS:H	1:40:A:VAL:HB	9	1.99
(1,163)	1:10:A:SER:HB2	1:40:A:VAL:HB	5	1.99
(1,163)	1:10:A:SER:HB3	1:40:A:VAL:HB	5	1.99
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB2	4	1.98
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB3	4	1.98
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB2	4	1.98
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB3	4	1.98
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB2	9	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB3	9	1.98
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD11	3	1.97
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD12	3	1.97
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD13	3	1.97
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB2	7	1.96
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB3	7	1.96
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG2	6	1.95
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG3	6	1.95
(1,592)	1:45:A:GLU:HB3	1:48:A:ALA:HA	4	1.94
(1,889)	1:75:A:GLU:HG2	1:88:A:THR:HB	1	1.93
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB2	6	1.93
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB3	6	1.93
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB2	6	1.93
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB3	6	1.93
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB2	6	1.93
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB3	6	1.93
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB2	6	1.93
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB3	6	1.93
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB2	6	1.93
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB3	6	1.93
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB2	6	1.93
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB3	6	1.93
(1,592)	1:45:A:GLU:HB3	1:48:A:ALA:HA	9	1.93
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB2	10	1.91
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB3	10	1.91
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB2	10	1.91
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB3	10	1.91
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB2	10	1.91
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB3	10	1.91
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB2	10	1.91
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB3	10	1.91
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB2	10	1.91
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB3	10	1.91
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB2	10	1.91
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB3	10	1.91
(1,592)	1:45:A:GLU:HB3	1:48:A:ALA:HA	2	1.91
(1,170)	1:11:A:CYS:H	1:40:A:VAL:HB	6	1.91
(1,170)	1:11:A:CYS:H	1:40:A:VAL:HB	8	1.91
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD11	7	1.88
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD12	7	1.88
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD13	7	1.88
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB2	3	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB3	3	1.88
(1,170)	1:11:A:CYS:H	1:40:A:VAL:HB	1	1.88
(1,1074)	1:92:A:VAL:HG11	1:125:A:SER:HA	4	1.87
(1,1074)	1:92:A:VAL:HG12	1:125:A:SER:HA	4	1.87
(1,1074)	1:92:A:VAL:HG13	1:125:A:SER:HA	4	1.87
(1,1074)	1:92:A:VAL:HG21	1:125:A:SER:HA	4	1.87
(1,1074)	1:92:A:VAL:HG22	1:125:A:SER:HA	4	1.87
(1,1074)	1:92:A:VAL:HG23	1:125:A:SER:HA	4	1.87
(1,1074)	1:92:A:VAL:HG11	1:125:A:SER:HA	8	1.87
(1,1074)	1:92:A:VAL:HG12	1:125:A:SER:HA	8	1.87
(1,1074)	1:92:A:VAL:HG13	1:125:A:SER:HA	8	1.87
(1,1074)	1:92:A:VAL:HG21	1:125:A:SER:HA	8	1.87
(1,1074)	1:92:A:VAL:HG22	1:125:A:SER:HA	8	1.87
(1,1074)	1:92:A:VAL:HG23	1:125:A:SER:HA	8	1.87
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD11	10	1.87
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD12	10	1.87
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD13	10	1.87
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD11	10	1.87
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD12	10	1.87
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD13	10	1.87
(1,1084)	1:93:A:ILE:HA	1:146:A:LEU:HB2	3	1.85
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG21	6	1.85
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG22	6	1.85
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG23	6	1.85
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB2	2	1.83
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB3	2	1.83
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG21	8	1.83
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG22	8	1.83
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG23	8	1.83
(1,592)	1:45:A:GLU:HB3	1:48:A:ALA:HA	3	1.82
(1,379)	1:26:A:TYR:HB2	1:72:A:VAL:HA	8	1.81
(1,736)	1:57:A:MET:HB2	1:60:A:LEU:HG	8	1.8
(1,736)	1:57:A:MET:HB3	1:60:A:LEU:HG	8	1.8
(1,757)	1:58:A:LYS:HD3	1:60:A:LEU:H	6	1.79
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE2	6	1.79
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE3	6	1.79
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE2	6	1.79
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE3	6	1.79
(1,76)	1:7:A:VAL:HB	1:38:A:ILE:HB	9	1.79
(1,1653)	1:140:A:LYS:HE2	1:142:A:VAL:H	3	1.78
(1,491)	1:31:A:ILE:HG12	1:109:A:LEU:HA	4	1.78
(1,1084)	1:93:A:ILE:HA	1:146:A:LEU:HB2	1	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,889)	1:75:A:GLU:HG2	1:88:A:THR:HB	5	1.77
(1,502)	1:31:A:ILE:HD11	1:109:A:LEU:HA	1	1.77
(1,502)	1:31:A:ILE:HD12	1:109:A:LEU:HA	1	1.77
(1,502)	1:31:A:ILE:HD13	1:109:A:LEU:HA	1	1.77
(1,1084)	1:93:A:ILE:HA	1:146:A:LEU:HB2	8	1.76
(1,491)	1:31:A:ILE:HG12	1:109:A:LEU:HA	7	1.75
(1,379)	1:26:A:TYR:HB2	1:72:A:VAL:HA	6	1.75
(1,170)	1:11:A:CYS:H	1:40:A:VAL:HB	10	1.74
(1,76)	1:7:A:VAL:HB	1:38:A:ILE:HB	3	1.74
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD11	2	1.73
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD12	2	1.73
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD13	2	1.73
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD21	2	1.73
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD22	2	1.73
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD23	2	1.73
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD11	2	1.73
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD12	2	1.73
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD13	2	1.73
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD21	2	1.73
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD22	2	1.73
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD23	2	1.73
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD11	5	1.73
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD12	5	1.73
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD13	5	1.73
(1,491)	1:31:A:ILE:HG12	1:109:A:LEU:HA	3	1.73
(1,491)	1:31:A:ILE:HG12	1:109:A:LEU:HA	9	1.73
(1,692)	1:54:A:VAL:HG11	1:58:A:LYS:HE2	5	1.72
(1,692)	1:54:A:VAL:HG11	1:58:A:LYS:HE3	5	1.72
(1,692)	1:54:A:VAL:HG12	1:58:A:LYS:HE2	5	1.72
(1,692)	1:54:A:VAL:HG12	1:58:A:LYS:HE3	5	1.72
(1,692)	1:54:A:VAL:HG13	1:58:A:LYS:HE2	5	1.72
(1,692)	1:54:A:VAL:HG13	1:58:A:LYS:HE3	5	1.72
(1,692)	1:54:A:VAL:HG21	1:58:A:LYS:HE2	5	1.72
(1,692)	1:54:A:VAL:HG21	1:58:A:LYS:HE3	5	1.72
(1,692)	1:54:A:VAL:HG22	1:58:A:LYS:HE2	5	1.72
(1,692)	1:54:A:VAL:HG22	1:58:A:LYS:HE3	5	1.72
(1,692)	1:54:A:VAL:HG23	1:58:A:LYS:HE2	5	1.72
(1,692)	1:54:A:VAL:HG23	1:58:A:LYS:HE3	5	1.72
(1,275)	1:16:A:ASP:HA	1:20:A:ASN:H	9	1.72
(1,897)	1:75:A:GLU:HG3	1:89:A:LEU:H	3	1.71
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD11	4	1.71
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD12	4	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD13	4	1.71
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD21	4	1.71
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD22	4	1.71
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD23	4	1.71
(1,169)	1:11:A:CYS:H	1:40:A:VAL:HA	8	1.71
(1,163)	1:10:A:SER:HB2	1:40:A:VAL:HB	7	1.71
(1,163)	1:10:A:SER:HB3	1:40:A:VAL:HB	7	1.71
(1,895)	1:75:A:GLU:HG3	1:88:A:THR:HB	10	1.7
(1,76)	1:7:A:VAL:HB	1:38:A:ILE:HB	8	1.7
(1,1788)	1:150:A:GLN:HB2	1:152:A:ILE:H	5	1.69
(1,1074)	1:92:A:VAL:HG11	1:125:A:SER:HA	1	1.69
(1,1074)	1:92:A:VAL:HG12	1:125:A:SER:HA	1	1.69
(1,1074)	1:92:A:VAL:HG13	1:125:A:SER:HA	1	1.69
(1,1074)	1:92:A:VAL:HG21	1:125:A:SER:HA	1	1.69
(1,1074)	1:92:A:VAL:HG22	1:125:A:SER:HA	1	1.69
(1,1074)	1:92:A:VAL:HG23	1:125:A:SER:HA	1	1.69
(1,897)	1:75:A:GLU:HG3	1:89:A:LEU:H	4	1.69
(1,736)	1:57:A:MET:HB2	1:60:A:LEU:HG	9	1.69
(1,736)	1:57:A:MET:HB3	1:60:A:LEU:HG	9	1.69
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB1	9	1.69
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB2	9	1.69
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB3	9	1.69
(1,491)	1:31:A:ILE:HG12	1:109:A:LEU:HA	5	1.69
(1,170)	1:11:A:CYS:H	1:40:A:VAL:HB	4	1.69
(1,169)	1:11:A:CYS:H	1:40:A:VAL:HA	5	1.69
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG21	7	1.69
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG22	7	1.69
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG23	7	1.69
(1,1074)	1:92:A:VAL:HG11	1:125:A:SER:HA	5	1.68
(1,1074)	1:92:A:VAL:HG12	1:125:A:SER:HA	5	1.68
(1,1074)	1:92:A:VAL:HG13	1:125:A:SER:HA	5	1.68
(1,1074)	1:92:A:VAL:HG21	1:125:A:SER:HA	5	1.68
(1,1074)	1:92:A:VAL:HG22	1:125:A:SER:HA	5	1.68
(1,1074)	1:92:A:VAL:HG23	1:125:A:SER:HA	5	1.68
(1,897)	1:75:A:GLU:HG3	1:89:A:LEU:H	5	1.68
(1,757)	1:58:A:LYS:HD3	1:60:A:LEU:H	9	1.68
(1,592)	1:45:A:GLU:HB3	1:48:A:ALA:HA	1	1.68
(1,978)	1:79:A:GLN:HG2	1:85:A:GLY:H	4	1.67
(1,897)	1:75:A:GLU:HG3	1:89:A:LEU:H	10	1.67
(1,736)	1:57:A:MET:HB2	1:60:A:LEU:HG	4	1.67
(1,736)	1:57:A:MET:HB3	1:60:A:LEU:HG	4	1.67
(1,169)	1:11:A:CYS:H	1:40:A:VAL:HA	6	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:31:A:ILE:HG21	1:109:A:LEU:HG	4	1.66
(1,511)	1:31:A:ILE:HG22	1:109:A:LEU:HG	4	1.66
(1,511)	1:31:A:ILE:HG23	1:109:A:LEU:HG	4	1.66
(1,169)	1:11:A:CYS:H	1:40:A:VAL:HA	4	1.66
(1,1790)	1:150:A:GLN:HB3	1:152:A:ILE:H	2	1.65
(1,1790)	1:150:A:GLN:HB3	1:152:A:ILE:H	9	1.65
(1,1074)	1:92:A:VAL:HG11	1:125:A:SER:HA	6	1.65
(1,1074)	1:92:A:VAL:HG12	1:125:A:SER:HA	6	1.65
(1,1074)	1:92:A:VAL:HG13	1:125:A:SER:HA	6	1.65
(1,1074)	1:92:A:VAL:HG21	1:125:A:SER:HA	6	1.65
(1,1074)	1:92:A:VAL:HG22	1:125:A:SER:HA	6	1.65
(1,1074)	1:92:A:VAL:HG23	1:125:A:SER:HA	6	1.65
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB1	2	1.65
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB2	2	1.65
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB3	2	1.65
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD11	6	1.65
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD12	6	1.65
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD13	6	1.65
(1,169)	1:11:A:CYS:H	1:40:A:VAL:HA	9	1.65
(1,685)	1:54:A:VAL:HG11	1:138:A:ASP:HA	10	1.64
(1,685)	1:54:A:VAL:HG12	1:138:A:ASP:HA	10	1.64
(1,685)	1:54:A:VAL:HG13	1:138:A:ASP:HA	10	1.64
(1,685)	1:54:A:VAL:HG21	1:138:A:ASP:HA	10	1.64
(1,685)	1:54:A:VAL:HG22	1:138:A:ASP:HA	10	1.64
(1,685)	1:54:A:VAL:HG23	1:138:A:ASP:HA	10	1.64
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB2	5	1.63
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB3	5	1.63
(1,76)	1:7:A:VAL:HB	1:38:A:ILE:HB	2	1.63
(1,31)	1:5:A:VAL:HB	1:36:A:THR:HB	2	1.63
(1,1021)	1:85:A:GLY:H	1:86:A:THR:H	5	1.62
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB2	10	1.62
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB3	10	1.62
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD11	4	1.61
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD12	4	1.61
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD13	4	1.61
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD21	4	1.61
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD22	4	1.61
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD23	4	1.61
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD11	4	1.61
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD12	4	1.61
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD13	4	1.61
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD21	4	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD22	4	1.61
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD23	4	1.61
(1,969)	1:79:A:GLN:HA	1:86:A:THR:HA	5	1.61
(1,685)	1:54:A:VAL:HG11	1:138:A:ASP:HA	6	1.61
(1,685)	1:54:A:VAL:HG12	1:138:A:ASP:HA	6	1.61
(1,685)	1:54:A:VAL:HG13	1:138:A:ASP:HA	6	1.61
(1,685)	1:54:A:VAL:HG21	1:138:A:ASP:HA	6	1.61
(1,685)	1:54:A:VAL:HG22	1:138:A:ASP:HA	6	1.61
(1,685)	1:54:A:VAL:HG23	1:138:A:ASP:HA	6	1.61
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	5	1.6
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	5	1.6
(1,994)	1:80:A:ARG:HG2	1:86:A:THR:HA	9	1.6
(1,994)	1:80:A:ARG:HG3	1:86:A:THR:HA	9	1.6
(1,609)	1:49:A:PRO:HG2	1:51:A:ALA:H	2	1.6
(1,609)	1:49:A:PRO:HG3	1:51:A:ALA:H	2	1.6
(1,169)	1:11:A:CYS:H	1:40:A:VAL:HA	10	1.6
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG21	3	1.6
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG22	3	1.6
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG23	3	1.6
(1,1790)	1:150:A:GLN:HB3	1:152:A:ILE:H	6	1.59
(1,1788)	1:150:A:GLN:HB2	1:152:A:ILE:H	4	1.59
(1,1576)	1:134:A:MET:HA	1:138:A:ASP:H	3	1.59
(1,1084)	1:93:A:ILE:HA	1:146:A:LEU:HB2	5	1.59
(1,945)	1:78:A:VAL:H	1:86:A:THR:HB	9	1.59
(1,169)	1:11:A:CYS:H	1:40:A:VAL:HA	2	1.59
(1,169)	1:11:A:CYS:H	1:40:A:VAL:HA	3	1.59
(1,169)	1:11:A:CYS:H	1:40:A:VAL:HA	7	1.59
(1,1788)	1:150:A:GLN:HB2	1:152:A:ILE:H	6	1.58
(1,907)	1:76:A:VAL:H	1:88:A:THR:HB	1	1.58
(1,907)	1:76:A:VAL:H	1:88:A:THR:HB	10	1.58
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE2	3	1.58
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE3	3	1.58
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE2	3	1.58
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE3	3	1.58
(1,76)	1:7:A:VAL:HB	1:38:A:ILE:HB	1	1.58
(1,1555)	1:132:A:SER:H	1:136:A:ASP:HA	1	1.57
(1,969)	1:79:A:GLN:HA	1:86:A:THR:HA	2	1.57
(1,945)	1:78:A:VAL:H	1:86:A:THR:HB	2	1.57
(1,757)	1:58:A:LYS:HD3	1:60:A:LEU:H	2	1.57
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB2	1	1.57
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB3	1	1.57
(1,969)	1:79:A:GLN:HA	1:86:A:THR:HA	4	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:7:A:VAL:HB	1:38:A:ILE:HB	7	1.56
(1,1788)	1:150:A:GLN:HB2	1:152:A:ILE:H	2	1.55
(1,1074)	1:92:A:VAL:HG11	1:125:A:SER:HA	9	1.55
(1,1074)	1:92:A:VAL:HG12	1:125:A:SER:HA	9	1.55
(1,1074)	1:92:A:VAL:HG13	1:125:A:SER:HA	9	1.55
(1,1074)	1:92:A:VAL:HG21	1:125:A:SER:HA	9	1.55
(1,1074)	1:92:A:VAL:HG22	1:125:A:SER:HA	9	1.55
(1,1074)	1:92:A:VAL:HG23	1:125:A:SER:HA	9	1.55
(1,1653)	1:140:A:LYS:HE2	1:142:A:VAL:H	1	1.54
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD11	5	1.54
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD12	5	1.54
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD13	5	1.54
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD21	5	1.54
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD22	5	1.54
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD23	5	1.54
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD11	5	1.54
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD12	5	1.54
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD13	5	1.54
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD21	5	1.54
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD22	5	1.54
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD23	5	1.54
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD11	4	1.54
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD12	4	1.54
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD13	4	1.54
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD21	4	1.54
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD22	4	1.54
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD23	4	1.54
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD11	4	1.54
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD12	4	1.54
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD13	4	1.54
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD21	4	1.54
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD22	4	1.54
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD23	4	1.54
(1,935)	1:77:A:THR:HB	1:87:A:SER:H	3	1.54
(1,732)	1:57:A:MET:HA	1:60:A:LEU:HG	9	1.54
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB2	6	1.54
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB3	6	1.54
(1,163)	1:10:A:SER:HB2	1:40:A:VAL:HB	3	1.54
(1,163)	1:10:A:SER:HB3	1:40:A:VAL:HB	3	1.54
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG21	8	1.53
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG22	8	1.53
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG23	8	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,889)	1:75:A:GLU:HG2	1:88:A:THR:HB	4	1.53
(1,757)	1:58:A:LYS:HD3	1:60:A:LEU:H	1	1.53
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG21	1	1.53
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG22	1	1.53
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG23	1	1.53
(1,1653)	1:140:A:LYS:HE2	1:142:A:VAL:H	4	1.52
(1,1286)	1:107:A:ARG:HD2	1:111:A:ALA:HA	4	1.52
(1,1286)	1:107:A:ARG:HD3	1:111:A:ALA:HA	4	1.52
(1,994)	1:80:A:ARG:HG2	1:86:A:THR:HA	6	1.52
(1,994)	1:80:A:ARG:HG3	1:86:A:THR:HA	6	1.52
(1,316)	1:18:A:LEU:HD11	1:123:A:LEU:HG	8	1.52
(1,316)	1:18:A:LEU:HD12	1:123:A:LEU:HG	8	1.52
(1,316)	1:18:A:LEU:HD13	1:123:A:LEU:HG	8	1.52
(1,1653)	1:140:A:LYS:HE2	1:142:A:VAL:H	9	1.51
(1,1286)	1:107:A:ARG:HD2	1:111:A:ALA:HA	3	1.51
(1,1286)	1:107:A:ARG:HD3	1:111:A:ALA:HA	3	1.51
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD11	2	1.5
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD12	2	1.5
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD13	2	1.5
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD21	2	1.5
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD22	2	1.5
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD23	2	1.5
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD11	2	1.5
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD12	2	1.5
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD13	2	1.5
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD21	2	1.5
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD22	2	1.5
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD23	2	1.5
(1,978)	1:79:A:GLN:HG2	1:85:A:GLY:H	3	1.5
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE2	2	1.5
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE3	2	1.5
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE2	2	1.5
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE3	2	1.5
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG21	9	1.5
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG22	9	1.5
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG23	9	1.5
(1,76)	1:7:A:VAL:HB	1:38:A:ILE:HB	5	1.5
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE2	8	1.49
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE3	8	1.49
(1,1084)	1:93:A:ILE:HA	1:146:A:LEU:HB2	6	1.49
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD11	8	1.49
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD12	8	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD13	8	1.49
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD21	8	1.49
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD22	8	1.49
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD23	8	1.49
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD11	8	1.49
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD12	8	1.49
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD13	8	1.49
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD21	8	1.49
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD22	8	1.49
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD23	8	1.49
(1,994)	1:80:A:ARG:HG2	1:86:A:THR:HA	1	1.49
(1,994)	1:80:A:ARG:HG3	1:86:A:THR:HA	1	1.49
(1,994)	1:80:A:ARG:HG2	1:86:A:THR:HA	3	1.49
(1,994)	1:80:A:ARG:HG3	1:86:A:THR:HA	3	1.49
(1,429)	1:28:A:ILE:H	1:42:A:LYS:HG2	6	1.49
(1,429)	1:28:A:ILE:H	1:42:A:LYS:HG3	6	1.49
(1,123)	1:8:A:ASP:HB2	1:39:A:VAL:HA	3	1.49
(1,1286)	1:107:A:ARG:HD2	1:111:A:ALA:HA	7	1.48
(1,1286)	1:107:A:ARG:HD3	1:111:A:ALA:HA	7	1.48
(1,755)	1:58:A:LYS:HD2	1:60:A:LEU:H	6	1.48
(1,714)	1:55:A:GLU:HG2	1:58:A:LYS:HB2	4	1.48
(1,714)	1:55:A:GLU:HG2	1:58:A:LYS:HB3	4	1.48
(1,714)	1:55:A:GLU:HG3	1:58:A:LYS:HB2	4	1.48
(1,714)	1:55:A:GLU:HG3	1:58:A:LYS:HB3	4	1.48
(1,163)	1:10:A:SER:HB2	1:40:A:VAL:HB	1	1.48
(1,163)	1:10:A:SER:HB3	1:40:A:VAL:HB	1	1.48
(1,163)	1:10:A:SER:HB2	1:40:A:VAL:HB	9	1.48
(1,163)	1:10:A:SER:HB3	1:40:A:VAL:HB	9	1.48
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG21	2	1.48
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG22	2	1.48
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG23	2	1.48
(1,1802)	1:151:A:ARG:HD2	1:152:A:ILE:H	8	1.47
(1,1802)	1:151:A:ARG:HD3	1:152:A:ILE:H	8	1.47
(1,994)	1:80:A:ARG:HG2	1:86:A:THR:HA	2	1.47
(1,994)	1:80:A:ARG:HG3	1:86:A:THR:HA	2	1.47
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG21	8	1.47
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG22	8	1.47
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG23	8	1.47
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG21	8	1.47
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG22	8	1.47
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG23	8	1.47
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG21	8	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG22	8	1.47
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG23	8	1.47
(1,1653)	1:140:A:LYS:HE2	1:142:A:VAL:H	2	1.46
(1,1653)	1:140:A:LYS:HE2	1:142:A:VAL:H	10	1.46
(1,1084)	1:93:A:ILE:HA	1:146:A:LEU:HB2	7	1.46
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB2	8	1.46
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB3	8	1.46
(1,945)	1:78:A:VAL:H	1:86:A:THR:HB	10	1.45
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	4	1.44
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	4	1.44
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB2	4	1.44
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB3	4	1.44
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB2	4	1.44
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB3	4	1.44
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB2	4	1.44
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB3	4	1.44
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB2	4	1.44
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB3	4	1.44
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB2	4	1.44
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB3	4	1.44
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB2	4	1.44
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB3	4	1.44
(1,580)	1:42:A:LYS:HG2	1:56:A:GLU:HG2	4	1.44
(1,580)	1:42:A:LYS:HG2	1:56:A:GLU:HG3	4	1.44
(1,580)	1:42:A:LYS:HG3	1:56:A:GLU:HG2	4	1.44
(1,580)	1:42:A:LYS:HG3	1:56:A:GLU:HG3	4	1.44
(1,379)	1:26:A:TYR:HB2	1:72:A:VAL:HA	5	1.44
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG21	9	1.43
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG22	9	1.43
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG23	9	1.43
(1,894)	1:75:A:GLU:HG3	1:76:A:VAL:H	4	1.43
(1,894)	1:75:A:GLU:HG3	1:76:A:VAL:H	8	1.43
(1,891)	1:75:A:GLU:HG2	1:89:A:LEU:H	10	1.43
(1,897)	1:75:A:GLU:HG3	1:89:A:LEU:H	1	1.42
(1,894)	1:75:A:GLU:HG3	1:76:A:VAL:H	7	1.42
(1,592)	1:45:A:GLU:HB3	1:48:A:ALA:HA	5	1.42
(1,1344)	1:111:A:ALA:HA	1:115:A:ARG:H	10	1.41
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD11	3	1.41
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD12	3	1.41
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD13	3	1.41
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD21	3	1.41
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD22	3	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD23	3	1.41
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD11	3	1.41
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD12	3	1.41
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD13	3	1.41
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD21	3	1.41
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD22	3	1.41
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD23	3	1.41
(1,969)	1:79:A:GLN:HA	1:86:A:THR:HA	3	1.41
(1,959)	1:78:A:VAL:HG21	1:87:A:SER:HA	4	1.41
(1,959)	1:78:A:VAL:HG22	1:87:A:SER:HA	4	1.41
(1,959)	1:78:A:VAL:HG23	1:87:A:SER:HA	4	1.41
(1,894)	1:75:A:GLU:HG3	1:76:A:VAL:H	1	1.41
(1,755)	1:58:A:LYS:HD2	1:60:A:LEU:H	5	1.41
(1,524)	1:33:A:LYS:HG2	1:36:A:THR:HB	7	1.41
(1,316)	1:18:A:LEU:HD11	1:123:A:LEU:HG	10	1.41
(1,316)	1:18:A:LEU:HD12	1:123:A:LEU:HG	10	1.41
(1,316)	1:18:A:LEU:HD13	1:123:A:LEU:HG	10	1.41
(1,592)	1:45:A:GLU:HB3	1:48:A:ALA:HA	6	1.4
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB1	8	1.4
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB2	8	1.4
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB3	8	1.4
(1,292)	1:17:A:LEU:HA	1:21:A:LYS:H	9	1.4
(1,237)	1:14:A:ALA:HA	1:18:A:LEU:H	9	1.4
(1,94)	1:7:A:VAL:HG21	1:38:A:ILE:HB	8	1.4
(1,94)	1:7:A:VAL:HG22	1:38:A:ILE:HB	8	1.4
(1,94)	1:7:A:VAL:HG23	1:38:A:ILE:HB	8	1.4
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD11	10	1.39
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD12	10	1.39
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD13	10	1.39
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD21	10	1.39
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD22	10	1.39
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD23	10	1.39
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD11	10	1.39
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD12	10	1.39
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD13	10	1.39
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD21	10	1.39
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD22	10	1.39
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD23	10	1.39
(1,609)	1:49:A:PRO:HG2	1:51:A:ALA:H	5	1.39
(1,609)	1:49:A:PRO:HG3	1:51:A:ALA:H	5	1.39
(1,491)	1:31:A:ILE:HG12	1:109:A:LEU:HA	6	1.39
(1,316)	1:18:A:LEU:HD11	1:123:A:LEU:HG	2	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,316)	1:18:A:LEU:HD12	1:123:A:LEU:HG	2	1.39
(1,316)	1:18:A:LEU:HD13	1:123:A:LEU:HG	2	1.39
(1,316)	1:18:A:LEU:HD11	1:123:A:LEU:HG	9	1.39
(1,316)	1:18:A:LEU:HD12	1:123:A:LEU:HG	9	1.39
(1,316)	1:18:A:LEU:HD13	1:123:A:LEU:HG	9	1.39
(1,72)	1:7:A:VAL:HB	1:117:A:LEU:HA	1	1.39
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD11	6	1.39
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD12	6	1.39
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD13	6	1.39
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD11	6	1.39
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD12	6	1.39
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD13	6	1.39
(1,894)	1:75:A:GLU:HG3	1:76:A:VAL:H	9	1.38
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB1	7	1.38
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB2	7	1.38
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB3	7	1.38
(1,316)	1:18:A:LEU:HD11	1:123:A:LEU:HG	1	1.38
(1,316)	1:18:A:LEU:HD12	1:123:A:LEU:HG	1	1.38
(1,316)	1:18:A:LEU:HD13	1:123:A:LEU:HG	1	1.38
(1,1021)	1:85:A:GLY:H	1:86:A:THR:H	8	1.37
(1,891)	1:75:A:GLU:HG2	1:89:A:LEU:H	3	1.37
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB2	2	1.37
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB3	2	1.37
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB2	2	1.37
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB3	2	1.37
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB2	2	1.37
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB3	2	1.37
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB2	2	1.37
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB3	2	1.37
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB2	2	1.37
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB3	2	1.37
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB2	2	1.37
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB3	2	1.37
(1,516)	1:32:A:ASP:HB2	1:37:A:ALA:H	9	1.37
(1,894)	1:75:A:GLU:HG3	1:76:A:VAL:H	10	1.36
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB1	2	1.36
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB2	2	1.36
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB3	2	1.36
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB1	2	1.36
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB2	2	1.36
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB3	2	1.36
(1,491)	1:31:A:ILE:HG12	1:109:A:LEU:HA	10	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:7:A:VAL:HB	1:117:A:LEU:HA	10	1.36
(1,959)	1:78:A:VAL:HG21	1:87:A:SER:HA	2	1.35
(1,959)	1:78:A:VAL:HG22	1:87:A:SER:HA	2	1.35
(1,959)	1:78:A:VAL:HG23	1:87:A:SER:HA	2	1.35
(1,1790)	1:150:A:GLN:HB3	1:152:A:ILE:H	7	1.34
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB1	2	1.34
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB2	2	1.34
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB3	2	1.34
(1,519)	1:32:A:ASP:HB2	1:37:A:ALA:HB1	2	1.34
(1,519)	1:32:A:ASP:HB2	1:37:A:ALA:HB2	2	1.34
(1,519)	1:32:A:ASP:HB2	1:37:A:ALA:HB3	2	1.34
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB1	2	1.34
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB2	2	1.34
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB3	2	1.34
(1,429)	1:28:A:ILE:H	1:42:A:LYS:HG2	4	1.34
(1,429)	1:28:A:ILE:H	1:42:A:LYS:HG3	4	1.34
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	4	1.33
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	4	1.33
(1,755)	1:58:A:LYS:HD2	1:60:A:LEU:H	9	1.33
(1,609)	1:49:A:PRO:HG2	1:51:A:ALA:H	1	1.33
(1,609)	1:49:A:PRO:HG3	1:51:A:ALA:H	1	1.33
(1,1443)	1:118:A:LYS:HE3	1:119:A:ALA:H	2	1.32
(1,891)	1:75:A:GLU:HG2	1:89:A:LEU:H	2	1.32
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG21	10	1.32
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG22	10	1.32
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG23	10	1.32
(1,385)	1:26:A:TYR:HB2	1:72:A:VAL:HA	8	1.31
(1,385)	1:26:A:TYR:HB3	1:72:A:VAL:HA	8	1.31
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG21	7	1.31
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG22	7	1.31
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG23	7	1.31
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG21	7	1.31
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG22	7	1.31
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG23	7	1.31
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG21	7	1.31
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG22	7	1.31
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG23	7	1.31
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	8	1.3
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	8	1.3
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD11	3	1.3
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD12	3	1.3
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD13	3	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD21	3	1.3
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD22	3	1.3
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD23	3	1.3
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD11	3	1.3
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD12	3	1.3
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD13	3	1.3
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD21	3	1.3
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD22	3	1.3
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD23	3	1.3
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD11	3	1.3
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD12	3	1.3
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD13	3	1.3
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD21	3	1.3
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD22	3	1.3
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD23	3	1.3
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD11	3	1.3
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD12	3	1.3
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD13	3	1.3
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD21	3	1.3
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD22	3	1.3
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD23	3	1.3
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD11	3	1.3
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD12	3	1.3
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD13	3	1.3
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD21	3	1.3
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD22	3	1.3
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD23	3	1.3
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD11	3	1.3
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD12	3	1.3
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD13	3	1.3
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD21	3	1.3
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD22	3	1.3
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD23	3	1.3
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD11	5	1.3
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD12	5	1.3
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD13	5	1.3
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD21	5	1.3
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD22	5	1.3
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD23	5	1.3
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD11	5	1.3
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD12	5	1.3
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD13	5	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD21	5	1.3
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD22	5	1.3
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD23	5	1.3
(1,907)	1:76:A:VAL:H	1:88:A:THR:HB	4	1.3
(1,895)	1:75:A:GLU:HG3	1:88:A:THR:HB	5	1.3
(1,609)	1:49:A:PRO:HG2	1:51:A:ALA:H	9	1.3
(1,609)	1:49:A:PRO:HG3	1:51:A:ALA:H	9	1.3
(1,1189)	1:99:A:PRO:HG3	1:102:A:ALA:HA	3	1.29
(1,994)	1:80:A:ARG:HG2	1:86:A:THR:HA	4	1.29
(1,994)	1:80:A:ARG:HG3	1:86:A:THR:HA	4	1.29
(1,518)	1:32:A:ASP:HB3	1:37:A:ALA:H	9	1.29
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	4	1.28
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	4	1.28
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	4	1.28
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	4	1.28
(1,1172)	1:98:A:CYS:HB2	1:107:A:ARG:HA	1	1.28
(1,1172)	1:98:A:CYS:HB3	1:107:A:ARG:HA	1	1.28
(1,1067)	1:92:A:VAL:H	1:127:A:PHE:H	10	1.28
(1,894)	1:75:A:GLU:HG3	1:76:A:VAL:H	6	1.28
(1,732)	1:57:A:MET:HA	1:60:A:LEU:HG	8	1.28
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD11	9	1.28
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD12	9	1.28
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD13	9	1.28
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD21	9	1.28
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD22	9	1.28
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD23	9	1.28
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD11	9	1.28
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD12	9	1.28
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD13	9	1.28
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD21	9	1.28
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD22	9	1.28
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD23	9	1.28
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB2	4	1.28
(1,252)	1:15:A:TYR:HA	1:121:A:LEU:HB3	4	1.28
(1,1653)	1:140:A:LYS:HE2	1:142:A:VAL:H	6	1.27
(1,1589)	1:135:A:SER:HA	1:140:A:LYS:HE2	4	1.27
(1,1241)	1:104:A:VAL:HG11	1:107:A:ARG:HB2	7	1.27
(1,1241)	1:104:A:VAL:HG11	1:107:A:ARG:HB3	7	1.27
(1,1241)	1:104:A:VAL:HG12	1:107:A:ARG:HB2	7	1.27
(1,1241)	1:104:A:VAL:HG12	1:107:A:ARG:HB3	7	1.27
(1,1241)	1:104:A:VAL:HG13	1:107:A:ARG:HB2	7	1.27
(1,1241)	1:104:A:VAL:HG13	1:107:A:ARG:HB3	7	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1241)	1:104:A:VAL:HG21	1:107:A:ARG:HB2	7	1.27
(1,1241)	1:104:A:VAL:HG21	1:107:A:ARG:HB3	7	1.27
(1,1241)	1:104:A:VAL:HG22	1:107:A:ARG:HB2	7	1.27
(1,1241)	1:104:A:VAL:HG22	1:107:A:ARG:HB3	7	1.27
(1,1241)	1:104:A:VAL:HG23	1:107:A:ARG:HB2	7	1.27
(1,1241)	1:104:A:VAL:HG23	1:107:A:ARG:HB3	7	1.27
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD11	10	1.27
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD12	10	1.27
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD13	10	1.27
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD21	10	1.27
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD22	10	1.27
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD23	10	1.27
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD11	10	1.27
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD12	10	1.27
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD13	10	1.27
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD21	10	1.27
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD22	10	1.27
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD23	10	1.27
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD11	10	1.27
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD12	10	1.27
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD13	10	1.27
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD21	10	1.27
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD22	10	1.27
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD23	10	1.27
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD11	10	1.27
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD12	10	1.27
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD13	10	1.27
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD21	10	1.27
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD22	10	1.27
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD23	10	1.27
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD11	10	1.27
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD12	10	1.27
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD13	10	1.27
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD21	10	1.27
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD22	10	1.27
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD23	10	1.27
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD11	10	1.27
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD12	10	1.27
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD13	10	1.27
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD21	10	1.27
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD22	10	1.27
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD23	10	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:92:A:VAL:H	1:127:A:PHE:H	7	1.27
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG21	7	1.27
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG22	7	1.27
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG23	7	1.27
(1,895)	1:75:A:GLU:HG3	1:88:A:THR:HB	1	1.27
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB2	9	1.27
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB3	9	1.27
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB2	9	1.27
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB3	9	1.27
(1,501)	1:31:A:ILE:HD11	1:109:A:LEU:H	8	1.27
(1,501)	1:31:A:ILE:HD12	1:109:A:LEU:H	8	1.27
(1,501)	1:31:A:ILE:HD13	1:109:A:LEU:H	8	1.27
(1,1443)	1:118:A:LYS:HE3	1:119:A:ALA:H	10	1.26
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	3	1.26
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	3	1.26
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	3	1.26
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	3	1.26
(1,1084)	1:93:A:ILE:HA	1:146:A:LEU:HB2	2	1.26
(1,937)	1:77:A:THR:HB	1:88:A:THR:HB	9	1.26
(1,714)	1:55:A:GLU:HG2	1:58:A:LYS:HB2	10	1.26
(1,714)	1:55:A:GLU:HG2	1:58:A:LYS:HB3	10	1.26
(1,714)	1:55:A:GLU:HG3	1:58:A:LYS:HB2	10	1.26
(1,714)	1:55:A:GLU:HG3	1:58:A:LYS:HB3	10	1.26
(1,518)	1:32:A:ASP:HB3	1:37:A:ALA:H	2	1.26
(1,1281)	1:107:A:ARG:HA	1:110:A:TYR:HA	8	1.25
(1,1067)	1:92:A:VAL:H	1:127:A:PHE:H	6	1.25
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE2	1	1.25
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE3	1	1.25
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE2	1	1.25
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE3	1	1.25
(1,528)	1:33:A:LYS:HG3	1:36:A:THR:HB	10	1.25
(1,527)	1:33:A:LYS:HG3	1:36:A:THR:HA	10	1.25
(1,94)	1:7:A:VAL:HG21	1:38:A:ILE:HB	7	1.25
(1,94)	1:7:A:VAL:HG22	1:38:A:ILE:HB	7	1.25
(1,94)	1:7:A:VAL:HG23	1:38:A:ILE:HB	7	1.25
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	1	1.24
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	1	1.24
(1,959)	1:78:A:VAL:HG21	1:87:A:SER:HA	7	1.24
(1,959)	1:78:A:VAL:HG22	1:87:A:SER:HA	7	1.24
(1,959)	1:78:A:VAL:HG23	1:87:A:SER:HA	7	1.24
(1,351)	1:21:A:LYS:HE2	1:22:A:HIS:H	9	1.24
(1,351)	1:21:A:LYS:HE3	1:22:A:HIS:H	9	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:17:A:LEU:HA	1:21:A:LYS:HG2	2	1.24
(1,295)	1:17:A:LEU:HA	1:21:A:LYS:HG3	2	1.24
(1,295)	1:17:A:LEU:HA	1:21:A:LYS:HG2	5	1.24
(1,295)	1:17:A:LEU:HA	1:21:A:LYS:HG3	5	1.24
(1,1773)	1:149:A:ASN:HB3	1:151:A:ARG:HA	1	1.23
(1,1653)	1:140:A:LYS:HE2	1:142:A:VAL:H	7	1.23
(1,1241)	1:104:A:VAL:HG11	1:107:A:ARG:HB2	4	1.23
(1,1241)	1:104:A:VAL:HG11	1:107:A:ARG:HB3	4	1.23
(1,1241)	1:104:A:VAL:HG12	1:107:A:ARG:HB2	4	1.23
(1,1241)	1:104:A:VAL:HG12	1:107:A:ARG:HB3	4	1.23
(1,1241)	1:104:A:VAL:HG13	1:107:A:ARG:HB2	4	1.23
(1,1241)	1:104:A:VAL:HG13	1:107:A:ARG:HB3	4	1.23
(1,1241)	1:104:A:VAL:HG21	1:107:A:ARG:HB2	4	1.23
(1,1241)	1:104:A:VAL:HG21	1:107:A:ARG:HB3	4	1.23
(1,1241)	1:104:A:VAL:HG22	1:107:A:ARG:HB2	4	1.23
(1,1241)	1:104:A:VAL:HG22	1:107:A:ARG:HB3	4	1.23
(1,1241)	1:104:A:VAL:HG23	1:107:A:ARG:HB2	4	1.23
(1,1241)	1:104:A:VAL:HG23	1:107:A:ARG:HB3	4	1.23
(1,1067)	1:92:A:VAL:H	1:127:A:PHE:H	1	1.23
(1,1067)	1:92:A:VAL:H	1:127:A:PHE:H	2	1.23
(1,684)	1:54:A:VAL:HG11	1:138:A:ASP:H	6	1.23
(1,684)	1:54:A:VAL:HG12	1:138:A:ASP:H	6	1.23
(1,684)	1:54:A:VAL:HG13	1:138:A:ASP:H	6	1.23
(1,684)	1:54:A:VAL:HG21	1:138:A:ASP:H	6	1.23
(1,684)	1:54:A:VAL:HG22	1:138:A:ASP:H	6	1.23
(1,684)	1:54:A:VAL:HG23	1:138:A:ASP:H	6	1.23
(1,351)	1:21:A:LYS:HE2	1:22:A:HIS:H	8	1.23
(1,351)	1:21:A:LYS:HE3	1:22:A:HIS:H	8	1.23
(1,1773)	1:149:A:ASN:HB3	1:151:A:ARG:HA	3	1.22
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG11	10	1.22
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG12	10	1.22
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG13	10	1.22
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG21	10	1.22
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG22	10	1.22
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG23	10	1.22
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG11	10	1.22
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG12	10	1.22
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG13	10	1.22
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG21	10	1.22
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG22	10	1.22
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG23	10	1.22
(1,994)	1:80:A:ARG:HG2	1:86:A:THR:HA	5	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:80:A:ARG:HG3	1:86:A:THR:HA	5	1.22
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG21	5	1.22
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG22	5	1.22
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG23	5	1.22
(1,970)	1:79:A:GLN:HA	1:86:A:THR:HB	2	1.22
(1,970)	1:79:A:GLN:HA	1:86:A:THR:HB	5	1.22
(1,969)	1:79:A:GLN:HA	1:86:A:THR:HA	6	1.22
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD11	9	1.22
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD12	9	1.22
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD13	9	1.22
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD21	9	1.22
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD22	9	1.22
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD23	9	1.22
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD11	9	1.22
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD12	9	1.22
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD13	9	1.22
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD21	9	1.22
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD22	9	1.22
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD23	9	1.22
(1,163)	1:10:A:SER:HB2	1:40:A:VAL:HB	6	1.22
(1,163)	1:10:A:SER:HB3	1:40:A:VAL:HB	6	1.22
(1,1808)	1:152:A:ILE:H	1:152:A:ILE:HG12	9	1.21
(1,1808)	1:152:A:ILE:H	1:152:A:ILE:HG13	9	1.21
(1,1589)	1:135:A:SER:HA	1:140:A:LYS:HE2	1	1.21
(1,1443)	1:118:A:LYS:HE3	1:119:A:ALA:H	6	1.21
(1,1084)	1:93:A:ILE:HA	1:146:A:LEU:HB2	4	1.21
(1,897)	1:75:A:GLU:HG3	1:89:A:LEU:H	9	1.21
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB2	8	1.21
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB3	8	1.21
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB2	8	1.21
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB3	8	1.21
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB2	8	1.21
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB3	8	1.21
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB2	8	1.21
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB3	8	1.21
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB2	8	1.21
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB3	8	1.21
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB2	8	1.21
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB3	8	1.21
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB2	5	1.21
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB3	5	1.21
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB2	5	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB3	5	1.21
(1,523)	1:33:A:LYS:HG2	1:36:A:THR:HA	10	1.21
(1,516)	1:32:A:ASP:HB2	1:37:A:ALA:H	2	1.21
(1,275)	1:16:A:ASP:HA	1:20:A:ASN:H	8	1.21
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG21	5	1.21
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG22	5	1.21
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG23	5	1.21
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG11	2	1.2
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG12	2	1.2
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG13	2	1.2
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG21	2	1.2
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG22	2	1.2
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG23	2	1.2
(1,1774)	1:149:A:ASN:HB3	1:152:A:ILE:HD11	10	1.2
(1,1774)	1:149:A:ASN:HB3	1:152:A:ILE:HD12	10	1.2
(1,1774)	1:149:A:ASN:HB3	1:152:A:ILE:HD13	10	1.2
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD11	2	1.2
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD12	2	1.2
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD13	2	1.2
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD21	2	1.2
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD22	2	1.2
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD23	2	1.2
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD11	2	1.2
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD12	2	1.2
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD13	2	1.2
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD21	2	1.2
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD22	2	1.2
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD23	2	1.2
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD11	2	1.2
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD12	2	1.2
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD13	2	1.2
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD21	2	1.2
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD22	2	1.2
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD23	2	1.2
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD11	2	1.2
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD12	2	1.2
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD13	2	1.2
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD21	2	1.2
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD22	2	1.2
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD23	2	1.2
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD11	2	1.2
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD12	2	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD13	2	1.2
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD21	2	1.2
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD22	2	1.2
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD23	2	1.2
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD11	2	1.2
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD12	2	1.2
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD13	2	1.2
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD21	2	1.2
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD22	2	1.2
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD23	2	1.2
(1,959)	1:78:A:VAL:HG21	1:87:A:SER:HA	5	1.2
(1,959)	1:78:A:VAL:HG22	1:87:A:SER:HA	5	1.2
(1,959)	1:78:A:VAL:HG23	1:87:A:SER:HA	5	1.2
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG21	2	1.2
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG22	2	1.2
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG23	2	1.2
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG21	10	1.2
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG22	10	1.2
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG23	10	1.2
(1,237)	1:14:A:ALA:HA	1:18:A:LEU:H	10	1.2
(1,75)	1:7:A:VAL:HB	1:38:A:ILE:H	9	1.2
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD2	6	1.19
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD3	6	1.19
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD2	6	1.19
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD3	6	1.19
(1,1084)	1:93:A:ILE:HA	1:146:A:LEU:HB2	10	1.19
(1,994)	1:80:A:ARG:HG2	1:86:A:THR:HA	10	1.19
(1,994)	1:80:A:ARG:HG3	1:86:A:THR:HA	10	1.19
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG21	4	1.19
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG22	4	1.19
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG23	4	1.19
(1,907)	1:76:A:VAL:H	1:88:A:THR:HB	3	1.19
(1,523)	1:33:A:LYS:HG2	1:36:A:THR:HA	6	1.19
(1,292)	1:17:A:LEU:HA	1:21:A:LYS:H	10	1.19
(1,113)	1:8:A:ASP:H	1:37:A:ALA:HA	4	1.19
(1,94)	1:7:A:VAL:HG21	1:38:A:ILE:HB	3	1.19
(1,94)	1:7:A:VAL:HG22	1:38:A:ILE:HB	3	1.19
(1,94)	1:7:A:VAL:HG23	1:38:A:ILE:HB	3	1.19
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB2	4	1.18
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB3	4	1.18
(1,895)	1:75:A:GLU:HG3	1:88:A:THR:HB	4	1.18
(1,737)	1:57:A:MET:HG2	1:60:A:LEU:HG	4	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,737)	1:57:A:MET:HG3	1:60:A:LEU:HG	4	1.18
(1,524)	1:33:A:LYS:HG2	1:36:A:THR:HB	9	1.18
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD11	7	1.18
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD12	7	1.18
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD13	7	1.18
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD21	7	1.18
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD22	7	1.18
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD23	7	1.18
(1,163)	1:10:A:SER:HB2	1:40:A:VAL:HB	8	1.18
(1,163)	1:10:A:SER:HB3	1:40:A:VAL:HB	8	1.18
(1,1189)	1:99:A:PRO:HG3	1:102:A:ALA:HA	9	1.17
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB2	10	1.17
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB3	10	1.17
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD11	9	1.16
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD12	9	1.16
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD13	9	1.16
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB2	7	1.16
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB3	7	1.16
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB2	7	1.16
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB3	7	1.16
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB2	2	1.16
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB3	2	1.16
(1,959)	1:78:A:VAL:HG21	1:87:A:SER:HA	8	1.16
(1,959)	1:78:A:VAL:HG22	1:87:A:SER:HA	8	1.16
(1,959)	1:78:A:VAL:HG23	1:87:A:SER:HA	8	1.16
(1,891)	1:75:A:GLU:HG2	1:89:A:LEU:H	4	1.16
(1,351)	1:21:A:LYS:HE2	1:22:A:HIS:H	5	1.16
(1,351)	1:21:A:LYS:HE3	1:22:A:HIS:H	5	1.16
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD11	4	1.16
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD12	4	1.16
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD13	4	1.16
(1,207)	1:12:A:LYS:HD3	1:15:A:TYR:HA	7	1.16
(1,169)	1:11:A:CYS:H	1:40:A:VAL:HA	1	1.16
(1,163)	1:10:A:SER:HB2	1:40:A:VAL:HB	2	1.16
(1,163)	1:10:A:SER:HB3	1:40:A:VAL:HB	2	1.16
(1,1773)	1:149:A:ASN:HB3	1:151:A:ARG:HA	5	1.15
(1,1589)	1:135:A:SER:HA	1:140:A:LYS:HE2	10	1.15
(1,1122)	1:94:A:PHE:HB2	1:118:A:LYS:HE2	3	1.15
(1,1122)	1:94:A:PHE:HB2	1:118:A:LYS:HE3	3	1.15
(1,1122)	1:94:A:PHE:HB3	1:118:A:LYS:HE2	3	1.15
(1,1122)	1:94:A:PHE:HB3	1:118:A:LYS:HE3	3	1.15
(1,970)	1:79:A:GLN:HA	1:86:A:THR:HB	4	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,969)	1:79:A:GLN:HA	1:86:A:THR:HA	10	1.15
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG21	3	1.15
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG22	3	1.15
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG23	3	1.15
(1,123)	1:8:A:ASP:HB2	1:39:A:VAL:HA	6	1.15
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	1	1.14
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	1	1.14
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	1	1.14
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	1	1.14
(1,1021)	1:85:A:GLY:H	1:86:A:THR:H	7	1.14
(1,891)	1:75:A:GLU:HG2	1:89:A:LEU:H	1	1.14
(1,757)	1:58:A:LYS:HD3	1:60:A:LEU:H	4	1.14
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB2	3	1.14
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB3	3	1.14
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB2	3	1.14
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB3	3	1.14
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB2	3	1.14
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB3	3	1.14
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB2	3	1.14
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB3	3	1.14
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB2	3	1.14
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB3	3	1.14
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB2	3	1.14
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB3	3	1.14
(1,685)	1:54:A:VAL:HG11	1:138:A:ASP:HA	2	1.14
(1,685)	1:54:A:VAL:HG12	1:138:A:ASP:HA	2	1.14
(1,685)	1:54:A:VAL:HG13	1:138:A:ASP:HA	2	1.14
(1,685)	1:54:A:VAL:HG21	1:138:A:ASP:HA	2	1.14
(1,685)	1:54:A:VAL:HG22	1:138:A:ASP:HA	2	1.14
(1,685)	1:54:A:VAL:HG23	1:138:A:ASP:HA	2	1.14
(1,611)	1:49:A:PRO:HG2	1:52:A:GLU:H	10	1.14
(1,611)	1:49:A:PRO:HG3	1:52:A:GLU:H	10	1.14
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD11	10	1.14
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD12	10	1.14
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD13	10	1.14
(1,385)	1:26:A:TYR:HB2	1:72:A:VAL:HA	6	1.14
(1,385)	1:26:A:TYR:HB3	1:72:A:VAL:HA	6	1.14
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB1	7	1.14
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB2	7	1.14
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB3	7	1.14
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB1	7	1.14
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB2	7	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB3	7	1.14
(1,207)	1:12:A:LYS:HD3	1:15:A:TYR:HA	5	1.14
(1,117)	1:8:A:ASP:H	1:39:A:VAL:HB	5	1.14
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG21	3	1.14
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG22	3	1.14
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG23	3	1.14
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG21	3	1.14
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG22	3	1.14
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG23	3	1.14
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG21	3	1.14
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG22	3	1.14
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG23	3	1.14
(1,94)	1:7:A:VAL:HG21	1:38:A:ILE:HB	2	1.14
(1,94)	1:7:A:VAL:HG22	1:38:A:ILE:HB	2	1.14
(1,94)	1:7:A:VAL:HG23	1:38:A:ILE:HB	2	1.14
(3,19)	1:29:A:PHE:O	1:69:A:TYR:H	8	1.13
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	7	1.13
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	7	1.13
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB2	1	1.13
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB3	1	1.13
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG21	3	1.13
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG22	3	1.13
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG23	3	1.13
(1,757)	1:58:A:LYS:HD3	1:60:A:LEU:H	10	1.13
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG2	4	1.13
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG3	4	1.13
(1,528)	1:33:A:LYS:HG3	1:36:A:THR:HB	6	1.13
(1,524)	1:33:A:LYS:HG2	1:36:A:THR:HB	1	1.13
(1,499)	1:31:A:ILE:HG13	1:38:A:ILE:HB	8	1.13
(1,382)	1:26:A:TYR:HB3	1:72:A:VAL:HA	2	1.13
(1,351)	1:21:A:LYS:HE2	1:22:A:HIS:H	7	1.13
(1,351)	1:21:A:LYS:HE3	1:22:A:HIS:H	7	1.13
(1,225)	1:13:A:ASN:HA	1:17:A:LEU:H	10	1.13
(1,163)	1:10:A:SER:HB2	1:40:A:VAL:HB	4	1.13
(1,163)	1:10:A:SER:HB3	1:40:A:VAL:HB	4	1.13
(1,113)	1:8:A:ASP:H	1:37:A:ALA:HA	5	1.13
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG21	1	1.13
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG22	1	1.13
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG23	1	1.13
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG21	1	1.13
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG22	1	1.13
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG23	1	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG21	1	1.13
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG22	1	1.13
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG23	1	1.13
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG21	6	1.12
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG22	6	1.12
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG23	6	1.12
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD11	10	1.12
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD12	10	1.12
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD13	10	1.12
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD2	10	1.12
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD3	10	1.12
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD2	10	1.12
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD3	10	1.12
(1,1021)	1:85:A:GLY:H	1:86:A:THR:H	9	1.12
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG2	7	1.12
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG3	7	1.12
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG2	9	1.12
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG3	9	1.12
(1,207)	1:12:A:LYS:HD3	1:15:A:TYR:HA	1	1.12
(1,207)	1:12:A:LYS:HD3	1:15:A:TYR:HA	9	1.12
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB1	7	1.11
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB2	7	1.11
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB3	7	1.11
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG21	2	1.11
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG22	2	1.11
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG23	2	1.11
(1,684)	1:54:A:VAL:HG11	1:138:A:ASP:H	3	1.11
(1,684)	1:54:A:VAL:HG12	1:138:A:ASP:H	3	1.11
(1,684)	1:54:A:VAL:HG13	1:138:A:ASP:H	3	1.11
(1,684)	1:54:A:VAL:HG21	1:138:A:ASP:H	3	1.11
(1,684)	1:54:A:VAL:HG22	1:138:A:ASP:H	3	1.11
(1,684)	1:54:A:VAL:HG23	1:138:A:ASP:H	3	1.11
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB2	1	1.11
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB3	1	1.11
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB2	1	1.11
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB3	1	1.11
(1,527)	1:33:A:LYS:HG3	1:36:A:THR:HA	6	1.11
(1,524)	1:33:A:LYS:HG2	1:36:A:THR:HB	6	1.11
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB1	9	1.11
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB2	9	1.11
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB3	9	1.11
(1,519)	1:32:A:ASP:HB2	1:37:A:ALA:HB1	9	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,519)	1:32:A:ASP:HB2	1:37:A:ALA:HB2	9	1.11
(1,519)	1:32:A:ASP:HB2	1:37:A:ALA:HB3	9	1.11
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB1	9	1.11
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB2	9	1.11
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB3	9	1.11
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD11	2	1.11
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD12	2	1.11
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD13	2	1.11
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD21	2	1.11
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD22	2	1.11
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD23	2	1.11
(1,316)	1:18:A:LEU:HD11	1:123:A:LEU:HG	7	1.11
(1,316)	1:18:A:LEU:HD12	1:123:A:LEU:HG	7	1.11
(1,316)	1:18:A:LEU:HD13	1:123:A:LEU:HG	7	1.11
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD2	7	1.11
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD3	7	1.11
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD2	7	1.11
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD3	7	1.11
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD2	7	1.11
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD3	7	1.11
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD2	7	1.11
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD3	7	1.11
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD2	7	1.11
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD3	7	1.11
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD2	7	1.11
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD3	7	1.11
(1,207)	1:12:A:LYS:HD3	1:15:A:TYR:HA	10	1.11
(1,75)	1:7:A:VAL:HB	1:38:A:ILE:H	5	1.11
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG21	10	1.1
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG22	10	1.1
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG23	10	1.1
(1,970)	1:79:A:GLN:HA	1:86:A:THR:HB	6	1.1
(1,700)	1:55:A:GLU:HA	1:58:A:LYS:HE2	5	1.1
(1,700)	1:55:A:GLU:HA	1:58:A:LYS:HE3	5	1.1
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD11	4	1.1
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD12	4	1.1
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD13	4	1.1
(1,94)	1:7:A:VAL:HG21	1:38:A:ILE:HB	1	1.1
(1,94)	1:7:A:VAL:HG22	1:38:A:ILE:HB	1	1.1
(1,94)	1:7:A:VAL:HG23	1:38:A:ILE:HB	1	1.1
(1,94)	1:7:A:VAL:HG21	1:38:A:ILE:HB	9	1.1
(1,94)	1:7:A:VAL:HG22	1:38:A:ILE:HB	9	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:7:A:VAL:HG23	1:38:A:ILE:HB	9	1.1
(1,1773)	1:149:A:ASN:HB3	1:151:A:ARG:HA	8	1.09
(1,1609)	1:137:A:LEU:HG	1:138:A:ASP:H	9	1.09
(1,1443)	1:118:A:LYS:HE3	1:119:A:ALA:H	1	1.09
(1,959)	1:78:A:VAL:HG21	1:87:A:SER:HA	6	1.09
(1,959)	1:78:A:VAL:HG22	1:87:A:SER:HA	6	1.09
(1,959)	1:78:A:VAL:HG23	1:87:A:SER:HA	6	1.09
(1,891)	1:75:A:GLU:HG2	1:89:A:LEU:H	5	1.09
(1,885)	1:75:A:GLU:HB3	1:88:A:THR:HB	3	1.09
(1,207)	1:12:A:LYS:HD3	1:15:A:TYR:HA	3	1.09
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB2	4	1.08
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB3	4	1.08
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB2	4	1.08
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB3	4	1.08
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG21	2	1.08
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG22	2	1.08
(1,908)	1:76:A:VAL:H	1:88:A:THR:HG23	2	1.08
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD11	10	1.08
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD12	10	1.08
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD13	10	1.08
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD21	10	1.08
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD22	10	1.08
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD23	10	1.08
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG2	1	1.08
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG3	1	1.08
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG2	1	1.08
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG3	1	1.08
(1,524)	1:33:A:LYS:HG2	1:36:A:THR:HB	10	1.08
(1,429)	1:28:A:ILE:H	1:42:A:LYS:HG2	7	1.08
(1,429)	1:28:A:ILE:H	1:42:A:LYS:HG3	7	1.08
(1,382)	1:26:A:TYR:HB3	1:72:A:VAL:HA	8	1.08
(1,207)	1:12:A:LYS:HD3	1:15:A:TYR:HA	8	1.08
(1,205)	1:12:A:LYS:HD3	1:14:A:ALA:H	1	1.08
(1,205)	1:12:A:LYS:HD3	1:14:A:ALA:H	10	1.08
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG21	2	1.08
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG22	2	1.08
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG23	2	1.08
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG21	2	1.08
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG22	2	1.08
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG23	2	1.08
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG21	2	1.08
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG22	2	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG23	2	1.08
(1,1788)	1:150:A:GLN:HB2	1:152:A:ILE:H	9	1.07
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG21	2	1.07
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG22	2	1.07
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG23	2	1.07
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	6	1.07
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	6	1.07
(1,1107)	1:93:A:ILE:HG21	1:146:A:LEU:HA	3	1.07
(1,1107)	1:93:A:ILE:HG22	1:146:A:LEU:HA	3	1.07
(1,1107)	1:93:A:ILE:HG23	1:146:A:LEU:HA	3	1.07
(1,970)	1:79:A:GLN:HA	1:86:A:THR:HB	9	1.07
(1,935)	1:77:A:THR:HB	1:87:A:SER:H	8	1.07
(1,889)	1:75:A:GLU:HG2	1:88:A:THR:HB	2	1.07
(1,737)	1:57:A:MET:HG2	1:60:A:LEU:HG	8	1.07
(1,737)	1:57:A:MET:HG3	1:60:A:LEU:HG	8	1.07
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD2	9	1.07
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD3	9	1.07
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB2	8	1.07
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB3	8	1.07
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB2	8	1.07
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB3	8	1.07
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB2	3	1.07
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB3	3	1.07
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG21	9	1.07
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG22	9	1.07
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG23	9	1.07
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD11	3	1.07
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD12	3	1.07
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD13	3	1.07
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD21	3	1.07
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD22	3	1.07
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD23	3	1.07
(1,351)	1:21:A:LYS:HE2	1:22:A:HIS:H	2	1.07
(1,351)	1:21:A:LYS:HE3	1:22:A:HIS:H	2	1.07
(1,205)	1:12:A:LYS:HD3	1:14:A:ALA:H	4	1.07
(1,1721)	1:144:A:SER:HA	1:148:A:SER:H	10	1.06
(1,1441)	1:118:A:LYS:HE2	1:119:A:ALA:H	2	1.06
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD11	9	1.06
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD12	9	1.06
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD13	9	1.06
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD21	9	1.06
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD22	9	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD23	9	1.06
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD11	9	1.06
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD12	9	1.06
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD13	9	1.06
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD21	9	1.06
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD22	9	1.06
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD23	9	1.06
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD11	9	1.06
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD12	9	1.06
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD13	9	1.06
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD21	9	1.06
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD22	9	1.06
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD23	9	1.06
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD11	9	1.06
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD12	9	1.06
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD13	9	1.06
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD21	9	1.06
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD22	9	1.06
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD23	9	1.06
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD11	9	1.06
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD12	9	1.06
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD13	9	1.06
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD21	9	1.06
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD22	9	1.06
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD23	9	1.06
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD11	9	1.06
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD12	9	1.06
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD13	9	1.06
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD21	9	1.06
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD22	9	1.06
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD23	9	1.06
(1,987)	1:80:A:ARG:H	1:85:A:GLY:H	3	1.06
(1,889)	1:75:A:GLU:HG2	1:88:A:THR:HB	6	1.06
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB1	5	1.06
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB2	5	1.06
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB3	5	1.06
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB1	5	1.06
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB2	5	1.06
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB3	5	1.06
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB1	7	1.06
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB2	7	1.06
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB3	7	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,519)	1:32:A:ASP:HB2	1:37:A:ALA:HB1	7	1.06
(1,519)	1:32:A:ASP:HB2	1:37:A:ALA:HB2	7	1.06
(1,519)	1:32:A:ASP:HB2	1:37:A:ALA:HB3	7	1.06
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB1	7	1.06
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB2	7	1.06
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB3	7	1.06
(1,511)	1:31:A:ILE:HG21	1:109:A:LEU:HG	7	1.06
(1,511)	1:31:A:ILE:HG22	1:109:A:LEU:HG	7	1.06
(1,511)	1:31:A:ILE:HG23	1:109:A:LEU:HG	7	1.06
(1,498)	1:31:A:ILE:HG13	1:38:A:ILE:HA	6	1.06
(1,498)	1:31:A:ILE:HG13	1:38:A:ILE:HA	9	1.06
(1,316)	1:18:A:LEU:HD11	1:123:A:LEU:HG	3	1.06
(1,316)	1:18:A:LEU:HD12	1:123:A:LEU:HG	3	1.06
(1,316)	1:18:A:LEU:HD13	1:123:A:LEU:HG	3	1.06
(1,205)	1:12:A:LYS:HD3	1:14:A:ALA:H	6	1.06
(1,75)	1:7:A:VAL:HB	1:38:A:ILE:H	2	1.06
(1,1286)	1:107:A:ARG:HD2	1:111:A:ALA:HA	10	1.05
(1,1286)	1:107:A:ARG:HD3	1:111:A:ALA:HA	10	1.05
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB2	1	1.05
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB3	1	1.05
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD11	8	1.05
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD12	8	1.05
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD13	8	1.05
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD21	8	1.05
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD22	8	1.05
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD23	8	1.05
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD11	8	1.05
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD12	8	1.05
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD13	8	1.05
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD21	8	1.05
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD22	8	1.05
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD23	8	1.05
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG21	10	1.05
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG22	10	1.05
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG23	10	1.05
(1,755)	1:58:A:LYS:HD2	1:60:A:LEU:H	8	1.05
(1,699)	1:55:A:GLU:HA	1:58:A:LYS:HD2	2	1.05
(1,699)	1:55:A:GLU:HA	1:58:A:LYS:HD3	2	1.05
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG21	6	1.05
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG22	6	1.05
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG23	6	1.05
(1,499)	1:31:A:ILE:HG13	1:38:A:ILE:HB	4	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:18:A:LEU:HD21	1:73:A:ASP:HA	6	1.05
(1,327)	1:18:A:LEU:HD22	1:73:A:ASP:HA	6	1.05
(1,327)	1:18:A:LEU:HD23	1:73:A:ASP:HA	6	1.05
(1,205)	1:12:A:LYS:HD3	1:14:A:ALA:H	5	1.05
(1,205)	1:12:A:LYS:HD3	1:14:A:ALA:H	8	1.05
(1,31)	1:5:A:VAL:HB	1:36:A:THR:HB	5	1.05
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG21	7	1.04
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG22	7	1.04
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG23	7	1.04
(1,894)	1:75:A:GLU:HG3	1:76:A:VAL:H	5	1.04
(1,887)	1:75:A:GLU:HB3	1:89:A:LEU:H	5	1.04
(1,692)	1:54:A:VAL:HG11	1:58:A:LYS:HE2	2	1.04
(1,692)	1:54:A:VAL:HG11	1:58:A:LYS:HE3	2	1.04
(1,692)	1:54:A:VAL:HG12	1:58:A:LYS:HE2	2	1.04
(1,692)	1:54:A:VAL:HG12	1:58:A:LYS:HE3	2	1.04
(1,692)	1:54:A:VAL:HG13	1:58:A:LYS:HE2	2	1.04
(1,692)	1:54:A:VAL:HG13	1:58:A:LYS:HE3	2	1.04
(1,692)	1:54:A:VAL:HG21	1:58:A:LYS:HE2	2	1.04
(1,692)	1:54:A:VAL:HG21	1:58:A:LYS:HE3	2	1.04
(1,692)	1:54:A:VAL:HG22	1:58:A:LYS:HE2	2	1.04
(1,692)	1:54:A:VAL:HG22	1:58:A:LYS:HE3	2	1.04
(1,692)	1:54:A:VAL:HG23	1:58:A:LYS:HE2	2	1.04
(1,692)	1:54:A:VAL:HG23	1:58:A:LYS:HE3	2	1.04
(1,684)	1:54:A:VAL:HG11	1:138:A:ASP:H	9	1.04
(1,684)	1:54:A:VAL:HG12	1:138:A:ASP:H	9	1.04
(1,684)	1:54:A:VAL:HG13	1:138:A:ASP:H	9	1.04
(1,684)	1:54:A:VAL:HG21	1:138:A:ASP:H	9	1.04
(1,684)	1:54:A:VAL:HG22	1:138:A:ASP:H	9	1.04
(1,684)	1:54:A:VAL:HG23	1:138:A:ASP:H	9	1.04
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG21	6	1.04
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG22	6	1.04
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG23	6	1.04
(1,511)	1:31:A:ILE:HG21	1:109:A:LEU:HG	6	1.04
(1,511)	1:31:A:ILE:HG22	1:109:A:LEU:HG	6	1.04
(1,511)	1:31:A:ILE:HG23	1:109:A:LEU:HG	6	1.04
(1,452)	1:28:A:ILE:HD11	1:71:A:ALA:H	6	1.04
(1,452)	1:28:A:ILE:HD12	1:71:A:ALA:H	6	1.04
(1,452)	1:28:A:ILE:HD13	1:71:A:ALA:H	6	1.04
(1,205)	1:12:A:LYS:HD3	1:14:A:ALA:H	2	1.04
(1,205)	1:12:A:LYS:HD3	1:14:A:ALA:H	3	1.04
(1,205)	1:12:A:LYS:HD3	1:14:A:ALA:H	7	1.04
(1,163)	1:10:A:SER:HB2	1:40:A:VAL:HB	10	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:10:A:SER:HB3	1:40:A:VAL:HB	10	1.04
(1,94)	1:7:A:VAL:HG21	1:38:A:ILE:HB	5	1.04
(1,94)	1:7:A:VAL:HG22	1:38:A:ILE:HB	5	1.04
(1,94)	1:7:A:VAL:HG23	1:38:A:ILE:HB	5	1.04
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD11	7	1.04
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD12	7	1.04
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD13	7	1.04
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD11	7	1.04
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD12	7	1.04
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD13	7	1.04
(1,1773)	1:149:A:ASN:HB3	1:151:A:ARG:HA	10	1.03
(1,1378)	1:114:A:VAL:HB	1:118:A:LYS:H	10	1.03
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	2	1.03
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	2	1.03
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	2	1.03
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	2	1.03
(1,1084)	1:93:A:ILE:HA	1:146:A:LEU:HB2	9	1.03
(1,894)	1:75:A:GLU:HG3	1:76:A:VAL:H	3	1.03
(1,775)	1:60:A:LEU:HG	1:61:A:VAL:H	4	1.03
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG2	2	1.03
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG3	2	1.03
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG2	2	1.03
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG3	2	1.03
(1,528)	1:33:A:LYS:HG3	1:36:A:THR:HB	7	1.03
(1,511)	1:31:A:ILE:HG21	1:109:A:LEU:HG	9	1.03
(1,511)	1:31:A:ILE:HG22	1:109:A:LEU:HG	9	1.03
(1,511)	1:31:A:ILE:HG23	1:109:A:LEU:HG	9	1.03
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG21	9	1.03
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG22	9	1.03
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG23	9	1.03
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG21	9	1.03
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG22	9	1.03
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG23	9	1.03
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG21	9	1.03
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG22	9	1.03
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG23	9	1.03
(1,1664)	1:141:A:SER:HA	1:143:A:LYS:H	2	1.02
(1,1325)	1:109:A:LEU:HD11	1:112:A:SER:HB2	8	1.02
(1,1325)	1:109:A:LEU:HD11	1:112:A:SER:HB3	8	1.02
(1,1325)	1:109:A:LEU:HD12	1:112:A:SER:HB2	8	1.02
(1,1325)	1:109:A:LEU:HD12	1:112:A:SER:HB3	8	1.02
(1,1325)	1:109:A:LEU:HD13	1:112:A:SER:HB2	8	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1325)	1:109:A:LEU:HD13	1:112:A:SER:HB3	8	1.02
(1,1325)	1:109:A:LEU:HD21	1:112:A:SER:HB2	8	1.02
(1,1325)	1:109:A:LEU:HD21	1:112:A:SER:HB3	8	1.02
(1,1325)	1:109:A:LEU:HD22	1:112:A:SER:HB2	8	1.02
(1,1325)	1:109:A:LEU:HD22	1:112:A:SER:HB3	8	1.02
(1,1325)	1:109:A:LEU:HD23	1:112:A:SER:HB2	8	1.02
(1,1325)	1:109:A:LEU:HD23	1:112:A:SER:HB3	8	1.02
(1,1185)	1:99:A:PRO:HG2	1:102:A:ALA:HA	3	1.02
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG11	4	1.02
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG12	4	1.02
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG13	4	1.02
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG21	4	1.02
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG22	4	1.02
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG23	4	1.02
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG11	4	1.02
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG12	4	1.02
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG13	4	1.02
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG21	4	1.02
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG22	4	1.02
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG23	4	1.02
(1,969)	1:79:A:GLN:HA	1:86:A:THR:HA	7	1.02
(1,968)	1:79:A:GLN:HA	1:85:A:GLY:H	3	1.02
(1,897)	1:75:A:GLU:HG3	1:89:A:LEU:H	8	1.02
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG2	3	1.02
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG3	3	1.02
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG2	3	1.02
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG3	3	1.02
(1,528)	1:33:A:LYS:HG3	1:36:A:THR:HB	4	1.02
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG21	9	1.02
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG22	9	1.02
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG23	9	1.02
(1,466)	1:29:A:PHE:HB3	1:41:A:GLU:H	4	1.02
(1,205)	1:12:A:LYS:HD3	1:14:A:ALA:H	9	1.02
(1,72)	1:7:A:VAL:HB	1:117:A:LEU:HA	9	1.02
(1,1653)	1:140:A:LYS:HE2	1:142:A:VAL:H	8	1.01
(1,1589)	1:135:A:SER:HA	1:140:A:LYS:HE2	2	1.01
(1,1589)	1:135:A:SER:HA	1:140:A:LYS:HE2	6	1.01
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB2	6	1.01
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB3	6	1.01
(1,884)	1:75:A:GLU:HB3	1:88:A:THR:HA	3	1.01
(1,685)	1:54:A:VAL:HG11	1:138:A:ASP:HA	4	1.01
(1,685)	1:54:A:VAL:HG12	1:138:A:ASP:HA	4	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:54:A:VAL:HG13	1:138:A:ASP:HA	4	1.01
(1,685)	1:54:A:VAL:HG21	1:138:A:ASP:HA	4	1.01
(1,685)	1:54:A:VAL:HG22	1:138:A:ASP:HA	4	1.01
(1,685)	1:54:A:VAL:HG23	1:138:A:ASP:HA	4	1.01
(1,609)	1:49:A:PRO:HG2	1:51:A:ALA:H	3	1.01
(1,609)	1:49:A:PRO:HG3	1:51:A:ALA:H	3	1.01
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB2	4	1.01
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB3	4	1.01
(1,440)	1:28:A:ILE:HB	1:70:A:ALA:HB1	6	1.01
(1,440)	1:28:A:ILE:HB	1:70:A:ALA:HB2	6	1.01
(1,440)	1:28:A:ILE:HB	1:70:A:ALA:HB3	6	1.01
(1,113)	1:8:A:ASP:H	1:37:A:ALA:HA	9	1.01
(1,75)	1:7:A:VAL:HB	1:38:A:ILE:H	3	1.01
(1,1763)	1:148:A:SER:HA	1:150:A:GLN:H	4	1.0
(1,1580)	1:134:A:MET:HB2	1:136:A:ASP:H	9	1.0
(1,1580)	1:134:A:MET:HB3	1:136:A:ASP:H	9	1.0
(1,1282)	1:107:A:ARG:HA	1:110:A:TYR:HB2	8	1.0
(1,1282)	1:107:A:ARG:HA	1:110:A:TYR:HB3	8	1.0
(1,705)	1:55:A:GLU:HA	1:59:A:LYS:HB3	9	1.0
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG2	6	1.0
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG3	6	1.0
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG2	6	1.0
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG3	6	1.0
(1,528)	1:33:A:LYS:HG3	1:36:A:THR:HB	3	1.0
(1,367)	1:25:A:SER:HA	1:73:A:ASP:HB2	8	1.0
(1,367)	1:25:A:SER:HA	1:73:A:ASP:HB3	8	1.0
(1,367)	1:25:A:SER:HA	1:73:A:ASP:HB2	8	1.0
(1,367)	1:25:A:SER:HA	1:73:A:ASP:HB3	8	1.0
(1,1285)	1:107:A:ARG:HD2	1:108:A:MET:H	1	0.99
(1,1285)	1:107:A:ARG:HD3	1:108:A:MET:H	1	0.99
(1,1285)	1:107:A:ARG:HD2	1:108:A:MET:H	1	0.99
(1,1285)	1:107:A:ARG:HD3	1:108:A:MET:H	1	0.99
(1,1220)	1:104:A:VAL:HA	1:107:A:ARG:HB2	7	0.99
(1,1220)	1:104:A:VAL:HA	1:107:A:ARG:HB3	7	0.99
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB2	10	0.99
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB3	10	0.99
(1,945)	1:78:A:VAL:H	1:86:A:THR:HB	4	0.99
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG2	8	0.99
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG3	8	0.99
(1,737)	1:57:A:MET:HG2	1:60:A:LEU:HG	10	0.99
(1,737)	1:57:A:MET:HG3	1:60:A:LEU:HG	10	0.99
(1,684)	1:54:A:VAL:HG11	1:138:A:ASP:H	2	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,684)	1:54:A:VAL:HG12	1:138:A:ASP:H	2	0.99
(1,684)	1:54:A:VAL:HG13	1:138:A:ASP:H	2	0.99
(1,684)	1:54:A:VAL:HG21	1:138:A:ASP:H	2	0.99
(1,684)	1:54:A:VAL:HG22	1:138:A:ASP:H	2	0.99
(1,684)	1:54:A:VAL:HG23	1:138:A:ASP:H	2	0.99
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG2	9	0.99
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG3	9	0.99
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG2	9	0.99
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG3	9	0.99
(1,499)	1:31:A:ILE:HG13	1:38:A:ILE:HB	9	0.99
(1,91)	1:7:A:VAL:HG21	1:120:A:SER:HA	5	0.99
(1,91)	1:7:A:VAL:HG22	1:120:A:SER:HA	5	0.99
(1,91)	1:7:A:VAL:HG23	1:120:A:SER:HA	5	0.99
(1,1285)	1:107:A:ARG:HD2	1:108:A:MET:H	10	0.98
(1,1285)	1:107:A:ARG:HD3	1:108:A:MET:H	10	0.98
(1,1285)	1:107:A:ARG:HD2	1:108:A:MET:H	10	0.98
(1,1285)	1:107:A:ARG:HD3	1:108:A:MET:H	10	0.98
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB1	9	0.98
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB2	9	0.98
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB3	9	0.98
(1,756)	1:58:A:LYS:HD3	1:59:A:LYS:H	2	0.98
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB2	5	0.98
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB3	5	0.98
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB2	5	0.98
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB3	5	0.98
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB2	5	0.98
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB3	5	0.98
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB2	5	0.98
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB3	5	0.98
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB2	5	0.98
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB3	5	0.98
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB2	5	0.98
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB3	5	0.98
(1,524)	1:33:A:LYS:HG2	1:36:A:THR:HB	4	0.98
(1,511)	1:31:A:ILE:HG21	1:109:A:LEU:HG	3	0.98
(1,511)	1:31:A:ILE:HG22	1:109:A:LEU:HG	3	0.98
(1,511)	1:31:A:ILE:HG23	1:109:A:LEU:HG	3	0.98
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG2	9	0.98
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG3	9	0.98
(1,91)	1:7:A:VAL:HG21	1:120:A:SER:HA	3	0.98
(1,91)	1:7:A:VAL:HG22	1:120:A:SER:HA	3	0.98
(1,91)	1:7:A:VAL:HG23	1:120:A:SER:HA	3	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1609)	1:137:A:LEU:HG	1:138:A:ASP:H	3	0.97
(1,1443)	1:118:A:LYS:HE3	1:119:A:ALA:H	7	0.97
(1,1021)	1:85:A:GLY:H	1:86:A:THR:H	6	0.97
(1,732)	1:57:A:MET:HA	1:60:A:LEU:HG	4	0.97
(1,692)	1:54:A:VAL:HG11	1:58:A:LYS:HE2	7	0.97
(1,692)	1:54:A:VAL:HG11	1:58:A:LYS:HE3	7	0.97
(1,692)	1:54:A:VAL:HG12	1:58:A:LYS:HE2	7	0.97
(1,692)	1:54:A:VAL:HG12	1:58:A:LYS:HE3	7	0.97
(1,692)	1:54:A:VAL:HG13	1:58:A:LYS:HE2	7	0.97
(1,692)	1:54:A:VAL:HG13	1:58:A:LYS:HE3	7	0.97
(1,692)	1:54:A:VAL:HG21	1:58:A:LYS:HE2	7	0.97
(1,692)	1:54:A:VAL:HG21	1:58:A:LYS:HE3	7	0.97
(1,692)	1:54:A:VAL:HG22	1:58:A:LYS:HE2	7	0.97
(1,692)	1:54:A:VAL:HG22	1:58:A:LYS:HE3	7	0.97
(1,692)	1:54:A:VAL:HG23	1:58:A:LYS:HE2	7	0.97
(1,692)	1:54:A:VAL:HG23	1:58:A:LYS:HE3	7	0.97
(1,237)	1:14:A:ALA:HA	1:18:A:LEU:H	5	0.97
(1,112)	1:8:A:ASP:H	1:11:A:CYS:HB2	1	0.97
(1,112)	1:8:A:ASP:H	1:11:A:CYS:HB3	1	0.97
(1,75)	1:7:A:VAL:HB	1:38:A:ILE:H	1	0.97
(3,3)	1:8:A:ASP:H	1:38:A:ILE:O	5	0.96
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG21	7	0.96
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG22	7	0.96
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG23	7	0.96
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG21	7	0.96
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG22	7	0.96
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG23	7	0.96
(1,1664)	1:141:A:SER:HA	1:143:A:LYS:H	4	0.96
(1,1576)	1:134:A:MET:HA	1:138:A:ASP:H	6	0.96
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB2	2	0.96
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB3	2	0.96
(1,1107)	1:93:A:ILE:HG21	1:146:A:LEU:HA	5	0.96
(1,1107)	1:93:A:ILE:HG22	1:146:A:LEU:HA	5	0.96
(1,1107)	1:93:A:ILE:HG23	1:146:A:LEU:HA	5	0.96
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG21	6	0.96
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG22	6	0.96
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG23	6	0.96
(1,888)	1:75:A:GLU:HG2	1:76:A:VAL:H	2	0.96
(1,480)	1:30:A:LYS:HB2	1:41:A:GLU:HA	10	0.96
(1,480)	1:30:A:LYS:HB3	1:41:A:GLU:HA	10	0.96
(1,335)	1:19:A:HIS:HA	1:21:A:LYS:H	8	0.96
(1,327)	1:18:A:LEU:HD21	1:73:A:ASP:HA	7	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:18:A:LEU:HD22	1:73:A:ASP:HA	7	0.96
(1,327)	1:18:A:LEU:HD23	1:73:A:ASP:HA	7	0.96
(1,255)	1:15:A:TYR:HA	1:19:A:HIS:H	9	0.96
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD11	7	0.96
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD12	7	0.96
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD13	7	0.96
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD21	7	0.96
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD22	7	0.96
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD23	7	0.96
(1,20)	1:4:A:GLY:H	1:5:A:VAL:HB	5	0.96
(1,1788)	1:150:A:GLN:HB2	1:152:A:ILE:H	7	0.95
(1,1778)	1:149:A:ASN:HB2	1:151:A:ARG:HA	1	0.95
(1,1778)	1:149:A:ASN:HB3	1:151:A:ARG:HA	1	0.95
(1,1576)	1:134:A:MET:HA	1:138:A:ASP:H	1	0.95
(1,1576)	1:134:A:MET:HA	1:138:A:ASP:H	10	0.95
(1,1299)	1:108:A:MET:HB2	1:112:A:SER:H	4	0.95
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB2	4	0.95
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB3	4	0.95
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG21	5	0.95
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG22	5	0.95
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG23	5	0.95
(1,902)	1:75:A:GLU:HG2	1:90:A:ASN:HB2	7	0.95
(1,902)	1:75:A:GLU:HG2	1:90:A:ASN:HB3	7	0.95
(1,902)	1:75:A:GLU:HG3	1:90:A:ASN:HB2	7	0.95
(1,902)	1:75:A:GLU:HG3	1:90:A:ASN:HB3	7	0.95
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB1	8	0.95
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB2	8	0.95
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB3	8	0.95
(1,207)	1:12:A:LYS:HD3	1:15:A:TYR:HA	2	0.95
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD11	1	0.95
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD12	1	0.95
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD13	1	0.95
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD11	1	0.95
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD12	1	0.95
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD13	1	0.95
(1,1664)	1:141:A:SER:HA	1:143:A:LYS:H	3	0.94
(1,1299)	1:108:A:MET:HB2	1:112:A:SER:H	10	0.94
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG21	10	0.94
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG22	10	0.94
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG23	10	0.94
(1,969)	1:79:A:GLN:HA	1:86:A:THR:HA	1	0.94
(1,498)	1:31:A:ILE:HG13	1:38:A:ILE:HA	8	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	1:12:A:LYS:HD3	1:15:A:TYR:HA	4	0.94
(1,1802)	1:151:A:ARG:HD2	1:152:A:ILE:H	10	0.93
(1,1802)	1:151:A:ARG:HD3	1:152:A:ILE:H	10	0.93
(1,1773)	1:149:A:ASN:HB3	1:151:A:ARG:HA	9	0.93
(1,1718)	1:144:A:SER:H	1:146:A:LEU:H	6	0.93
(1,1576)	1:134:A:MET:HA	1:138:A:ASP:H	4	0.93
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	6	0.93
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	6	0.93
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	6	0.93
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	6	0.93
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG11	8	0.93
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG12	8	0.93
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG13	8	0.93
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG21	8	0.93
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG22	8	0.93
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG23	8	0.93
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG11	8	0.93
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG12	8	0.93
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG13	8	0.93
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG21	8	0.93
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG22	8	0.93
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG23	8	0.93
(1,1145)	1:95:A:VAL:HG11	1:131:A:ALA:HA	5	0.93
(1,1145)	1:95:A:VAL:HG12	1:131:A:ALA:HA	5	0.93
(1,1145)	1:95:A:VAL:HG13	1:131:A:ALA:HA	5	0.93
(1,1145)	1:95:A:VAL:HG21	1:131:A:ALA:HA	5	0.93
(1,1145)	1:95:A:VAL:HG22	1:131:A:ALA:HA	5	0.93
(1,1145)	1:95:A:VAL:HG23	1:131:A:ALA:HA	5	0.93
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB2	3	0.93
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB3	3	0.93
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB2	1	0.93
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB3	1	0.93
(1,945)	1:78:A:VAL:H	1:86:A:THR:HB	5	0.93
(1,887)	1:75:A:GLU:HB3	1:89:A:LEU:H	4	0.93
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG2	2	0.93
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG3	2	0.93
(1,327)	1:18:A:LEU:HD21	1:73:A:ASP:HA	3	0.93
(1,327)	1:18:A:LEU:HD22	1:73:A:ASP:HA	3	0.93
(1,327)	1:18:A:LEU:HD23	1:73:A:ASP:HA	3	0.93
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD2	3	0.93
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD3	3	0.93
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD2	3	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD3	3	0.93
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD2	3	0.93
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD3	3	0.93
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD2	3	0.93
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD3	3	0.93
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD2	3	0.93
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD3	3	0.93
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD2	3	0.93
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD3	3	0.93
(1,295)	1:17:A:LEU:HA	1:21:A:LYS:HG2	3	0.93
(1,295)	1:17:A:LEU:HA	1:21:A:LYS:HG3	3	0.93
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD11	2	0.93
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD12	2	0.93
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD13	2	0.93
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD21	2	0.93
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD22	2	0.93
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD23	2	0.93
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD11	2	0.93
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD12	2	0.93
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD13	2	0.93
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD21	2	0.93
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD22	2	0.93
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD23	2	0.93
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG21	5	0.93
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG22	5	0.93
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG23	5	0.93
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG21	5	0.93
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG22	5	0.93
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG23	5	0.93
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG21	5	0.93
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG22	5	0.93
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG23	5	0.93
(1,72)	1:7:A:VAL:HB	1:117:A:LEU:HA	2	0.93
(1,72)	1:7:A:VAL:HB	1:117:A:LEU:HA	6	0.93
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG11	7	0.93
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG12	7	0.93
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG13	7	0.93
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG21	7	0.93
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG22	7	0.93
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG23	7	0.93
(1,1744)	1:146:A:LEU:HA	1:150:A:GLN:HA	9	0.92
(1,1316)	1:109:A:LEU:HA	1:113:A:SER:H	6	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB2	6	0.92
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB3	6	0.92
(1,978)	1:79:A:GLN:HG2	1:85:A:GLY:H	6	0.92
(1,970)	1:79:A:GLN:HA	1:86:A:THR:HB	3	0.92
(1,969)	1:79:A:GLN:HA	1:86:A:THR:HA	9	0.92
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG21	4	0.92
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG22	4	0.92
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG23	4	0.92
(1,699)	1:55:A:GLU:HA	1:58:A:LYS:HD2	1	0.92
(1,699)	1:55:A:GLU:HA	1:58:A:LYS:HD3	1	0.92
(1,684)	1:54:A:VAL:HG11	1:138:A:ASP:H	4	0.92
(1,684)	1:54:A:VAL:HG12	1:138:A:ASP:H	4	0.92
(1,684)	1:54:A:VAL:HG13	1:138:A:ASP:H	4	0.92
(1,684)	1:54:A:VAL:HG21	1:138:A:ASP:H	4	0.92
(1,684)	1:54:A:VAL:HG22	1:138:A:ASP:H	4	0.92
(1,684)	1:54:A:VAL:HG23	1:138:A:ASP:H	4	0.92
(1,611)	1:49:A:PRO:HG2	1:52:A:GLU:H	6	0.92
(1,611)	1:49:A:PRO:HG3	1:52:A:GLU:H	6	0.92
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD11	6	0.92
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD12	6	0.92
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD13	6	0.92
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD21	6	0.92
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD22	6	0.92
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD23	6	0.92
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG2	6	0.92
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG3	6	0.92
(1,102)	1:7:A:VAL:HG11	1:120:A:SER:HA	3	0.92
(1,102)	1:7:A:VAL:HG12	1:120:A:SER:HA	3	0.92
(1,102)	1:7:A:VAL:HG13	1:120:A:SER:HA	3	0.92
(1,102)	1:7:A:VAL:HG21	1:120:A:SER:HA	3	0.92
(1,102)	1:7:A:VAL:HG22	1:120:A:SER:HA	3	0.92
(1,102)	1:7:A:VAL:HG23	1:120:A:SER:HA	3	0.92
(1,14)	1:3:A:SER:H	1:113:A:SER:HA	7	0.92
(1,1285)	1:107:A:ARG:HD2	1:108:A:MET:H	6	0.91
(1,1285)	1:107:A:ARG:HD3	1:108:A:MET:H	6	0.91
(1,1285)	1:107:A:ARG:HD2	1:108:A:MET:H	6	0.91
(1,1285)	1:107:A:ARG:HD3	1:108:A:MET:H	6	0.91
(1,1220)	1:104:A:VAL:HA	1:107:A:ARG:HB2	4	0.91
(1,1220)	1:104:A:VAL:HA	1:107:A:ARG:HB3	4	0.91
(1,968)	1:79:A:GLN:HA	1:85:A:GLY:H	6	0.91
(1,880)	1:75:A:GLU:HB2	1:88:A:THR:HB	3	0.91
(1,705)	1:55:A:GLU:HA	1:59:A:LYS:HB3	1	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,609)	1:49:A:PRO:HG2	1:51:A:ALA:H	7	0.91
(1,609)	1:49:A:PRO:HG3	1:51:A:ALA:H	7	0.91
(1,510)	1:31:A:ILE:HG21	1:109:A:LEU:HA	4	0.91
(1,510)	1:31:A:ILE:HG22	1:109:A:LEU:HA	4	0.91
(1,510)	1:31:A:ILE:HG23	1:109:A:LEU:HA	4	0.91
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD11	4	0.91
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD12	4	0.91
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD13	4	0.91
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD21	4	0.91
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD22	4	0.91
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD23	4	0.91
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB2	5	0.91
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB3	5	0.91
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB2	5	0.91
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB3	5	0.91
(1,102)	1:7:A:VAL:HG11	1:120:A:SER:HA	5	0.91
(1,102)	1:7:A:VAL:HG12	1:120:A:SER:HA	5	0.91
(1,102)	1:7:A:VAL:HG13	1:120:A:SER:HA	5	0.91
(1,102)	1:7:A:VAL:HG21	1:120:A:SER:HA	5	0.91
(1,102)	1:7:A:VAL:HG22	1:120:A:SER:HA	5	0.91
(1,102)	1:7:A:VAL:HG23	1:120:A:SER:HA	5	0.91
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD11	9	0.91
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD12	9	0.91
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD13	9	0.91
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD11	9	0.91
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD12	9	0.91
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD13	9	0.91
(1,1778)	1:149:A:ASN:HB2	1:151:A:ARG:HA	3	0.9
(1,1778)	1:149:A:ASN:HB3	1:151:A:ARG:HA	3	0.9
(1,1378)	1:114:A:VAL:HB	1:118:A:LYS:H	6	0.9
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG2	1	0.9
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG3	1	0.9
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG2	1	0.9
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG3	1	0.9
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG2	1	0.9
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG3	1	0.9
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG2	1	0.9
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG3	1	0.9
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG2	1	0.9
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG3	1	0.9
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG2	1	0.9
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG3	1	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG21	1	0.9
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG22	1	0.9
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG23	1	0.9
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG21	2	0.9
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG22	2	0.9
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG23	2	0.9
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG21	4	0.9
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG22	4	0.9
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG23	4	0.9
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG21	5	0.9
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG22	5	0.9
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG23	5	0.9
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG21	6	0.9
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG22	6	0.9
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG23	6	0.9
(1,897)	1:75:A:GLU:HG3	1:89:A:LEU:H	6	0.9
(1,893)	1:75:A:GLU:HG2	1:90:A:ASN:HB2	7	0.9
(1,893)	1:75:A:GLU:HG2	1:90:A:ASN:HB3	7	0.9
(1,528)	1:33:A:LYS:HG3	1:36:A:THR:HB	9	0.9
(1,316)	1:18:A:LEU:HD11	1:123:A:LEU:HG	6	0.9
(1,316)	1:18:A:LEU:HD12	1:123:A:LEU:HG	6	0.9
(1,316)	1:18:A:LEU:HD13	1:123:A:LEU:HG	6	0.9
(1,238)	1:14:A:ALA:HA	1:27:A:ILE:HD11	5	0.9
(1,238)	1:14:A:ALA:HA	1:27:A:ILE:HD12	5	0.9
(1,238)	1:14:A:ALA:HA	1:27:A:ILE:HD13	5	0.9
(1,1788)	1:150:A:GLN:HB2	1:152:A:ILE:H	3	0.89
(1,1670)	1:141:A:SER:HB3	1:145:A:ASP:HA	5	0.89
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD2	4	0.89
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD3	4	0.89
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD2	4	0.89
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD3	4	0.89
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB2	5	0.89
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB3	5	0.89
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB2	5	0.89
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB3	5	0.89
(1,1196)	1:100:A:ASP:HA	1:132:A:SER:HB3	2	0.89
(1,1145)	1:95:A:VAL:HG11	1:131:A:ALA:HA	7	0.89
(1,1145)	1:95:A:VAL:HG12	1:131:A:ALA:HA	7	0.89
(1,1145)	1:95:A:VAL:HG13	1:131:A:ALA:HA	7	0.89
(1,1145)	1:95:A:VAL:HG21	1:131:A:ALA:HA	7	0.89
(1,1145)	1:95:A:VAL:HG22	1:131:A:ALA:HA	7	0.89
(1,1145)	1:95:A:VAL:HG23	1:131:A:ALA:HA	7	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB2	5	0.89
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB3	5	0.89
(1,935)	1:77:A:THR:HB	1:87:A:SER:H	10	0.89
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD11	9	0.89
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD12	9	0.89
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD13	9	0.89
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD21	9	0.89
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD22	9	0.89
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD23	9	0.89
(1,685)	1:54:A:VAL:HG11	1:138:A:ASP:HA	3	0.89
(1,685)	1:54:A:VAL:HG12	1:138:A:ASP:HA	3	0.89
(1,685)	1:54:A:VAL:HG13	1:138:A:ASP:HA	3	0.89
(1,685)	1:54:A:VAL:HG21	1:138:A:ASP:HA	3	0.89
(1,685)	1:54:A:VAL:HG22	1:138:A:ASP:HA	3	0.89
(1,685)	1:54:A:VAL:HG23	1:138:A:ASP:HA	3	0.89
(1,684)	1:54:A:VAL:HG11	1:138:A:ASP:H	8	0.89
(1,684)	1:54:A:VAL:HG12	1:138:A:ASP:H	8	0.89
(1,684)	1:54:A:VAL:HG13	1:138:A:ASP:H	8	0.89
(1,684)	1:54:A:VAL:HG21	1:138:A:ASP:H	8	0.89
(1,684)	1:54:A:VAL:HG22	1:138:A:ASP:H	8	0.89
(1,684)	1:54:A:VAL:HG23	1:138:A:ASP:H	8	0.89
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG21	7	0.89
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG22	7	0.89
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG23	7	0.89
(1,516)	1:32:A:ASP:HB2	1:37:A:ALA:H	8	0.89
(1,327)	1:18:A:LEU:HD21	1:73:A:ASP:HA	4	0.89
(1,327)	1:18:A:LEU:HD22	1:73:A:ASP:HA	4	0.89
(1,327)	1:18:A:LEU:HD23	1:73:A:ASP:HA	4	0.89
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD11	2	0.89
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD12	2	0.89
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD13	2	0.89
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD11	2	0.89
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD12	2	0.89
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD13	2	0.89
(1,14)	1:3:A:SER:H	1:113:A:SER:HA	3	0.89
(1,1779)	1:149:A:ASN:HB2	1:152:A:ILE:H	9	0.88
(1,1779)	1:149:A:ASN:HB3	1:152:A:ILE:H	9	0.88
(1,1775)	1:149:A:ASN:HB3	1:152:A:ILE:HG21	7	0.88
(1,1775)	1:149:A:ASN:HB3	1:152:A:ILE:HG22	7	0.88
(1,1775)	1:149:A:ASN:HB3	1:152:A:ILE:HG23	7	0.88
(1,1726)	1:144:A:SER:HB3	1:146:A:LEU:H	6	0.88
(1,1196)	1:100:A:ASP:HA	1:132:A:SER:HB3	4	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1196)	1:100:A:ASP:HA	1:132:A:SER:HB3	6	0.88
(1,1173)	1:98:A:CYS:HB2	1:107:A:ARG:HD2	8	0.88
(1,1173)	1:98:A:CYS:HB2	1:107:A:ARG:HD3	8	0.88
(1,1173)	1:98:A:CYS:HB3	1:107:A:ARG:HD2	8	0.88
(1,1173)	1:98:A:CYS:HB3	1:107:A:ARG:HD3	8	0.88
(1,962)	1:78:A:VAL:HG11	1:87:A:SER:HB2	8	0.88
(1,962)	1:78:A:VAL:HG11	1:87:A:SER:HB3	8	0.88
(1,962)	1:78:A:VAL:HG12	1:87:A:SER:HB2	8	0.88
(1,962)	1:78:A:VAL:HG12	1:87:A:SER:HB3	8	0.88
(1,962)	1:78:A:VAL:HG13	1:87:A:SER:HB2	8	0.88
(1,962)	1:78:A:VAL:HG13	1:87:A:SER:HB3	8	0.88
(1,962)	1:78:A:VAL:HG21	1:87:A:SER:HB2	8	0.88
(1,962)	1:78:A:VAL:HG21	1:87:A:SER:HB3	8	0.88
(1,962)	1:78:A:VAL:HG22	1:87:A:SER:HB2	8	0.88
(1,962)	1:78:A:VAL:HG22	1:87:A:SER:HB3	8	0.88
(1,962)	1:78:A:VAL:HG23	1:87:A:SER:HB2	8	0.88
(1,962)	1:78:A:VAL:HG23	1:87:A:SER:HB3	8	0.88
(1,907)	1:76:A:VAL:H	1:88:A:THR:HB	6	0.88
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG2	5	0.88
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG3	5	0.88
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG2	5	0.88
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG3	5	0.88
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG2	8	0.88
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG3	8	0.88
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG2	8	0.88
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG3	8	0.88
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB2	2	0.88
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB3	2	0.88
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB2	2	0.88
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB3	2	0.88
(1,523)	1:33:A:LYS:HG2	1:36:A:THR:HA	4	0.88
(1,502)	1:31:A:ILE:HD11	1:109:A:LEU:HA	2	0.88
(1,502)	1:31:A:ILE:HD12	1:109:A:LEU:HA	2	0.88
(1,502)	1:31:A:ILE:HD13	1:109:A:LEU:HA	2	0.88
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG2	2	0.88
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG3	2	0.88
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG2	2	0.88
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG3	2	0.88
(1,434)	1:28:A:ILE:HB	1:41:A:GLU:HA	8	0.88
(1,237)	1:14:A:ALA:HA	1:18:A:LEU:H	2	0.88
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG11	5	0.88
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG12	5	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG13	5	0.88
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG21	5	0.88
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG22	5	0.88
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG23	5	0.88
(1,1785)	1:150:A:GLN:H	1:151:A:ARG:H	4	0.87
(1,1780)	1:149:A:ASN:HB2	1:152:A:ILE:HD11	10	0.87
(1,1780)	1:149:A:ASN:HB2	1:152:A:ILE:HD12	10	0.87
(1,1780)	1:149:A:ASN:HB2	1:152:A:ILE:HD13	10	0.87
(1,1780)	1:149:A:ASN:HB3	1:152:A:ILE:HD11	10	0.87
(1,1780)	1:149:A:ASN:HB3	1:152:A:ILE:HD12	10	0.87
(1,1780)	1:149:A:ASN:HB3	1:152:A:ILE:HD13	10	0.87
(1,1555)	1:132:A:SER:H	1:136:A:ASP:HA	5	0.87
(1,1550)	1:131:A:ALA:HA	1:136:A:ASP:HA	1	0.87
(1,1443)	1:118:A:LYS:HE3	1:119:A:ALA:H	4	0.87
(1,962)	1:78:A:VAL:HG11	1:87:A:SER:HB2	7	0.87
(1,962)	1:78:A:VAL:HG11	1:87:A:SER:HB3	7	0.87
(1,962)	1:78:A:VAL:HG12	1:87:A:SER:HB2	7	0.87
(1,962)	1:78:A:VAL:HG12	1:87:A:SER:HB3	7	0.87
(1,962)	1:78:A:VAL:HG13	1:87:A:SER:HB2	7	0.87
(1,962)	1:78:A:VAL:HG13	1:87:A:SER:HB3	7	0.87
(1,962)	1:78:A:VAL:HG21	1:87:A:SER:HB2	7	0.87
(1,962)	1:78:A:VAL:HG21	1:87:A:SER:HB3	7	0.87
(1,962)	1:78:A:VAL:HG22	1:87:A:SER:HB2	7	0.87
(1,962)	1:78:A:VAL:HG22	1:87:A:SER:HB3	7	0.87
(1,962)	1:78:A:VAL:HG23	1:87:A:SER:HB2	7	0.87
(1,962)	1:78:A:VAL:HG23	1:87:A:SER:HB3	7	0.87
(1,897)	1:75:A:GLU:HG3	1:89:A:LEU:H	7	0.87
(1,891)	1:75:A:GLU:HG2	1:89:A:LEU:H	9	0.87
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD11	6	0.87
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD12	6	0.87
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD13	6	0.87
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD21	6	0.87
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD22	6	0.87
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD23	6	0.87
(1,527)	1:33:A:LYS:HG3	1:36:A:THR:HA	4	0.87
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD11	4	0.87
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD12	4	0.87
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD13	4	0.87
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD21	4	0.87
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD22	4	0.87
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD23	4	0.87
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD11	4	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD12	4	0.87
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD13	4	0.87
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD21	4	0.87
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD22	4	0.87
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD23	4	0.87
(1,112)	1:8:A:ASP:H	1:11:A:CYS:HB2	3	0.87
(1,112)	1:8:A:ASP:H	1:11:A:CYS:HB3	3	0.87
(1,14)	1:3:A:SER:H	1:113:A:SER:HA	10	0.87
(3,9)	1:26:A:TYR:H	1:44:A:GLY:O	8	0.86
(1,1576)	1:134:A:MET:HA	1:138:A:ASP:H	5	0.86
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB2	10	0.86
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB3	10	0.86
(1,1065)	1:91:A:LYS:HE3	1:150:A:GLN:H	3	0.86
(1,962)	1:78:A:VAL:HG11	1:87:A:SER:HB2	4	0.86
(1,962)	1:78:A:VAL:HG11	1:87:A:SER:HB3	4	0.86
(1,962)	1:78:A:VAL:HG12	1:87:A:SER:HB2	4	0.86
(1,962)	1:78:A:VAL:HG12	1:87:A:SER:HB3	4	0.86
(1,962)	1:78:A:VAL:HG13	1:87:A:SER:HB2	4	0.86
(1,962)	1:78:A:VAL:HG13	1:87:A:SER:HB3	4	0.86
(1,962)	1:78:A:VAL:HG21	1:87:A:SER:HB2	4	0.86
(1,962)	1:78:A:VAL:HG21	1:87:A:SER:HB3	4	0.86
(1,962)	1:78:A:VAL:HG22	1:87:A:SER:HB2	4	0.86
(1,962)	1:78:A:VAL:HG22	1:87:A:SER:HB3	4	0.86
(1,962)	1:78:A:VAL:HG23	1:87:A:SER:HB2	4	0.86
(1,962)	1:78:A:VAL:HG23	1:87:A:SER:HB3	4	0.86
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG21	7	0.86
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG22	7	0.86
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG23	7	0.86
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG21	4	0.86
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG22	4	0.86
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG23	4	0.86
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB1	4	0.86
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB2	4	0.86
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB3	4	0.86
(1,498)	1:31:A:ILE:HG13	1:38:A:ILE:HA	3	0.86
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD11	9	0.86
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD12	9	0.86
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD13	9	0.86
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD21	9	0.86
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD22	9	0.86
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD23	9	0.86
(1,454)	1:28:A:ILE:HG12	1:41:A:GLU:HG2	8	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,454)	1:28:A:ILE:HG12	1:41:A:GLU:HG3	8	0.86
(1,454)	1:28:A:ILE:HG13	1:41:A:GLU:HG2	8	0.86
(1,454)	1:28:A:ILE:HG13	1:41:A:GLU:HG3	8	0.86
(1,351)	1:21:A:LYS:HE2	1:22:A:HIS:H	6	0.86
(1,351)	1:21:A:LYS:HE3	1:22:A:HIS:H	6	0.86
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB1	2	0.86
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB2	2	0.86
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB3	2	0.86
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB1	2	0.86
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB2	2	0.86
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB3	2	0.86
(1,57)	1:6:A:LYS:HB2	1:37:A:ALA:HA	10	0.86
(1,57)	1:6:A:LYS:HB3	1:37:A:ALA:HA	10	0.86
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG11	8	0.86
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG12	8	0.86
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG13	8	0.86
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG21	8	0.86
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG22	8	0.86
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG23	8	0.86
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG21	10	0.85
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG22	10	0.85
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG23	10	0.85
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG21	10	0.85
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG22	10	0.85
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG23	10	0.85
(1,1670)	1:141:A:SER:HB3	1:145:A:ASP:HA	2	0.85
(1,1670)	1:141:A:SER:HB3	1:145:A:ASP:HA	3	0.85
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD2	1	0.85
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD3	1	0.85
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD2	1	0.85
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD3	1	0.85
(1,1576)	1:134:A:MET:HA	1:138:A:ASP:H	2	0.85
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB1	7	0.85
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB2	7	0.85
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB3	7	0.85
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB1	7	0.85
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB2	7	0.85
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB3	7	0.85
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD2	5	0.85
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD3	5	0.85
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD11	1	0.85
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD12	1	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD13	1	0.85
(1,434)	1:28:A:ILE:HB	1:41:A:GLU:HA	9	0.85
(1,382)	1:26:A:TYR:HB3	1:72:A:VAL:HA	6	0.85
(1,245)	1:14:A:ALA:HB1	1:40:A:VAL:HB	1	0.85
(1,245)	1:14:A:ALA:HB2	1:40:A:VAL:HB	1	0.85
(1,245)	1:14:A:ALA:HB3	1:40:A:VAL:HB	1	0.85
(1,1778)	1:149:A:ASN:HB2	1:151:A:ARG:HA	5	0.84
(1,1778)	1:149:A:ASN:HB3	1:151:A:ARG:HA	5	0.84
(1,1726)	1:144:A:SER:HB3	1:146:A:LEU:H	2	0.84
(1,1670)	1:141:A:SER:HB3	1:145:A:ASP:HA	10	0.84
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	6	0.84
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	6	0.84
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB2	4	0.84
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB3	4	0.84
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG21	10	0.84
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG22	10	0.84
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG23	10	0.84
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB2	8	0.84
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB3	8	0.84
(1,498)	1:31:A:ILE:HG13	1:38:A:ILE:HA	7	0.84
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD11	1	0.84
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD12	1	0.84
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD13	1	0.84
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD21	1	0.84
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD22	1	0.84
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD23	1	0.84
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD11	7	0.84
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD12	7	0.84
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD13	7	0.84
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD21	7	0.84
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD22	7	0.84
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD23	7	0.84
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD11	7	0.84
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD12	7	0.84
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD13	7	0.84
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD21	7	0.84
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD22	7	0.84
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD23	7	0.84
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD11	10	0.84
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD12	10	0.84
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD13	10	0.84
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG21	8	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG22	8	0.83
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG23	8	0.83
(1,1670)	1:141:A:SER:HB3	1:145:A:ASP:HA	1	0.83
(1,1670)	1:141:A:SER:HB3	1:145:A:ASP:HA	6	0.83
(1,1670)	1:141:A:SER:HB3	1:145:A:ASP:HA	8	0.83
(1,1664)	1:141:A:SER:HA	1:143:A:LYS:H	6	0.83
(1,1442)	1:118:A:LYS:HE2	1:121:A:LEU:H	8	0.83
(1,1240)	1:104:A:VAL:HG11	1:107:A:ARG:HA	4	0.83
(1,1240)	1:104:A:VAL:HG12	1:107:A:ARG:HA	4	0.83
(1,1240)	1:104:A:VAL:HG13	1:107:A:ARG:HA	4	0.83
(1,1240)	1:104:A:VAL:HG21	1:107:A:ARG:HA	4	0.83
(1,1240)	1:104:A:VAL:HG22	1:107:A:ARG:HA	4	0.83
(1,1240)	1:104:A:VAL:HG23	1:107:A:ARG:HA	4	0.83
(1,1187)	1:99:A:PRO:HG2	1:132:A:SER:HB3	9	0.83
(1,1107)	1:93:A:ILE:HG21	1:146:A:LEU:HA	4	0.83
(1,1107)	1:93:A:ILE:HG22	1:146:A:LEU:HA	4	0.83
(1,1107)	1:93:A:ILE:HG23	1:146:A:LEU:HA	4	0.83
(1,935)	1:77:A:THR:HB	1:87:A:SER:H	5	0.83
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD2	1	0.83
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD3	1	0.83
(1,606)	1:49:A:PRO:HB3	1:52:A:GLU:H	10	0.83
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG21	4	0.83
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG22	4	0.83
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG23	4	0.83
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG21	1	0.83
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG22	1	0.83
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG23	1	0.83
(1,511)	1:31:A:ILE:HG21	1:109:A:LEU:HG	1	0.83
(1,511)	1:31:A:ILE:HG22	1:109:A:LEU:HG	1	0.83
(1,511)	1:31:A:ILE:HG23	1:109:A:LEU:HG	1	0.83
(1,509)	1:31:A:ILE:HG21	1:109:A:LEU:H	9	0.83
(1,509)	1:31:A:ILE:HG22	1:109:A:LEU:H	9	0.83
(1,509)	1:31:A:ILE:HG23	1:109:A:LEU:H	9	0.83
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG2	9	0.83
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG3	9	0.83
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG2	9	0.83
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG3	9	0.83
(1,429)	1:28:A:ILE:H	1:42:A:LYS:HG2	8	0.83
(1,429)	1:28:A:ILE:H	1:42:A:LYS:HG3	8	0.83
(1,1778)	1:149:A:ASN:HB2	1:151:A:ARG:HA	8	0.82
(1,1778)	1:149:A:ASN:HB3	1:151:A:ARG:HA	8	0.82
(1,1721)	1:144:A:SER:HA	1:148:A:SER:H	9	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1670)	1:141:A:SER:HB3	1:145:A:ASP:HA	9	0.82
(1,1664)	1:141:A:SER:HA	1:143:A:LYS:H	5	0.82
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB2	5	0.82
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB3	5	0.82
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB2	5	0.82
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB3	5	0.82
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB2	5	0.82
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB3	5	0.82
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB2	5	0.82
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB3	5	0.82
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB2	5	0.82
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB3	5	0.82
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB2	5	0.82
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB3	5	0.82
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD11	2	0.82
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD12	2	0.82
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD13	2	0.82
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD21	2	0.82
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD22	2	0.82
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD23	2	0.82
(1,1333)	1:110:A:TYR:HA	1:114:A:VAL:H	10	0.82
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB2	8	0.82
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB3	8	0.82
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB2	2	0.82
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB3	2	0.82
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG21	6	0.82
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG22	6	0.82
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG23	6	0.82
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG2	9	0.82
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG3	9	0.82
(1,890)	1:75:A:GLU:HG2	1:88:A:THR:HG21	2	0.82
(1,890)	1:75:A:GLU:HG2	1:88:A:THR:HG22	2	0.82
(1,890)	1:75:A:GLU:HG2	1:88:A:THR:HG23	2	0.82
(1,884)	1:75:A:GLU:HB3	1:88:A:THR:HA	1	0.82
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB2	9	0.82
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB3	9	0.82
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB2	9	0.82
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB3	9	0.82
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB2	9	0.82
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB3	9	0.82
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB2	9	0.82
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB3	9	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB2	9	0.82
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB3	9	0.82
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB2	9	0.82
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB3	9	0.82
(1,429)	1:28:A:ILE:H	1:42:A:LYS:HG2	9	0.82
(1,429)	1:28:A:ILE:H	1:42:A:LYS:HG3	9	0.82
(1,123)	1:8:A:ASP:HB2	1:39:A:VAL:HA	8	0.82
(1,97)	1:7:A:VAL:HG11	1:116:A:ALA:H	10	0.82
(1,97)	1:7:A:VAL:HG12	1:116:A:ALA:H	10	0.82
(1,97)	1:7:A:VAL:HG13	1:116:A:ALA:H	10	0.82
(1,97)	1:7:A:VAL:HG21	1:116:A:ALA:H	10	0.82
(1,97)	1:7:A:VAL:HG22	1:116:A:ALA:H	10	0.82
(1,97)	1:7:A:VAL:HG23	1:116:A:ALA:H	10	0.82
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG21	8	0.82
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG22	8	0.82
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG23	8	0.82
(1,1744)	1:146:A:LEU:HA	1:150:A:GLN:HA	10	0.81
(1,1651)	1:140:A:LYS:HD3	1:142:A:VAL:H	6	0.81
(1,1442)	1:118:A:LYS:HE2	1:121:A:LEU:H	2	0.81
(1,1442)	1:118:A:LYS:HE2	1:121:A:LEU:H	5	0.81
(1,1344)	1:111:A:ALA:HA	1:115:A:ARG:H	9	0.81
(1,1316)	1:109:A:LEU:HA	1:113:A:SER:H	9	0.81
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	6	0.81
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	6	0.81
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	6	0.81
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	6	0.81
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB1	9	0.81
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB2	9	0.81
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB3	9	0.81
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB1	9	0.81
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB2	9	0.81
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB3	9	0.81
(1,527)	1:33:A:LYS:HG3	1:36:A:THR:HA	3	0.81
(1,498)	1:31:A:ILE:HG13	1:38:A:ILE:HA	4	0.81
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG2	2	0.81
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG3	2	0.81
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG2	3	0.81
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG3	3	0.81
(1,351)	1:21:A:LYS:HE2	1:22:A:HIS:H	1	0.81
(1,351)	1:21:A:LYS:HE3	1:22:A:HIS:H	1	0.81
(1,316)	1:18:A:LEU:HD11	1:123:A:LEU:HG	5	0.81
(1,316)	1:18:A:LEU:HD12	1:123:A:LEU:HG	5	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,316)	1:18:A:LEU:HD13	1:123:A:LEU:HG	5	0.81
(1,158)	1:10:A:SER:HB3	1:12:A:LYS:H	10	0.81
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB2	1	0.81
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB3	1	0.81
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB2	1	0.81
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB3	1	0.81
(1,124)	1:8:A:ASP:HB2	1:39:A:VAL:HB	3	0.81
(1,1773)	1:149:A:ASN:HB3	1:151:A:ARG:HA	2	0.8
(1,1744)	1:146:A:LEU:HA	1:150:A:GLN:HA	1	0.8
(1,1664)	1:141:A:SER:HA	1:143:A:LYS:H	10	0.8
(1,1443)	1:118:A:LYS:HE3	1:119:A:ALA:H	9	0.8
(1,1442)	1:118:A:LYS:HE2	1:121:A:LEU:H	1	0.8
(1,1442)	1:118:A:LYS:HE2	1:121:A:LEU:H	3	0.8
(1,1442)	1:118:A:LYS:HE2	1:121:A:LEU:H	7	0.8
(1,1303)	1:108:A:MET:HG3	1:112:A:SER:H	7	0.8
(1,1187)	1:99:A:PRO:HG2	1:132:A:SER:HB3	5	0.8
(1,1117)	1:94:A:PHE:HA	1:128:A:GLN:HA	10	0.8
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB2	6	0.8
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB3	6	0.8
(1,936)	1:77:A:THR:HB	1:88:A:THR:HA	9	0.8
(1,884)	1:75:A:GLU:HB3	1:88:A:THR:HA	4	0.8
(1,884)	1:75:A:GLU:HB3	1:88:A:THR:HA	5	0.8
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG2	7	0.8
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG3	7	0.8
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG2	7	0.8
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG3	7	0.8
(1,576)	1:42:A:LYS:HD2	1:43:A:VAL:H	4	0.8
(1,576)	1:42:A:LYS:HD3	1:43:A:VAL:H	4	0.8
(1,527)	1:33:A:LYS:HG3	1:36:A:THR:HA	7	0.8
(1,499)	1:31:A:ILE:HG13	1:38:A:ILE:HB	7	0.8
(1,1774)	1:149:A:ASN:HB3	1:152:A:ILE:HD11	9	0.79
(1,1774)	1:149:A:ASN:HB3	1:152:A:ILE:HD12	9	0.79
(1,1774)	1:149:A:ASN:HB3	1:152:A:ILE:HD13	9	0.79
(1,1594)	1:135:A:SER:HB2	1:140:A:LYS:HG2	6	0.79
(1,1594)	1:135:A:SER:HB2	1:140:A:LYS:HG3	6	0.79
(1,1594)	1:135:A:SER:HB3	1:140:A:LYS:HG2	6	0.79
(1,1594)	1:135:A:SER:HB3	1:140:A:LYS:HG3	6	0.79
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	5	0.79
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	5	0.79
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	5	0.79
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	5	0.79
(1,1333)	1:110:A:TYR:HA	1:114:A:VAL:H	7	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1189)	1:99:A:PRO:HG3	1:102:A:ALA:HA	6	0.79
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD11	10	0.79
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD12	10	0.79
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD13	10	0.79
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD21	10	0.79
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD22	10	0.79
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD23	10	0.79
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD11	10	0.79
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD12	10	0.79
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD13	10	0.79
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD21	10	0.79
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD22	10	0.79
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD23	10	0.79
(1,968)	1:79:A:GLN:HA	1:85:A:GLY:H	5	0.79
(1,935)	1:77:A:THR:HB	1:87:A:SER:H	6	0.79
(1,692)	1:54:A:VAL:HG11	1:58:A:LYS:HE2	3	0.79
(1,692)	1:54:A:VAL:HG11	1:58:A:LYS:HE3	3	0.79
(1,692)	1:54:A:VAL:HG12	1:58:A:LYS:HE2	3	0.79
(1,692)	1:54:A:VAL:HG12	1:58:A:LYS:HE3	3	0.79
(1,692)	1:54:A:VAL:HG13	1:58:A:LYS:HE2	3	0.79
(1,692)	1:54:A:VAL:HG13	1:58:A:LYS:HE3	3	0.79
(1,692)	1:54:A:VAL:HG21	1:58:A:LYS:HE2	3	0.79
(1,692)	1:54:A:VAL:HG21	1:58:A:LYS:HE3	3	0.79
(1,692)	1:54:A:VAL:HG22	1:58:A:LYS:HE2	3	0.79
(1,692)	1:54:A:VAL:HG22	1:58:A:LYS:HE3	3	0.79
(1,692)	1:54:A:VAL:HG23	1:58:A:LYS:HE2	3	0.79
(1,692)	1:54:A:VAL:HG23	1:58:A:LYS:HE3	3	0.79
(1,607)	1:49:A:PRO:HG2	1:51:A:ALA:HB1	2	0.79
(1,607)	1:49:A:PRO:HG2	1:51:A:ALA:HB2	2	0.79
(1,607)	1:49:A:PRO:HG2	1:51:A:ALA:HB3	2	0.79
(1,607)	1:49:A:PRO:HG3	1:51:A:ALA:HB1	2	0.79
(1,607)	1:49:A:PRO:HG3	1:51:A:ALA:HB2	2	0.79
(1,607)	1:49:A:PRO:HG3	1:51:A:ALA:HB3	2	0.79
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD11	3	0.79
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD12	3	0.79
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD13	3	0.79
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD21	3	0.79
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD22	3	0.79
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD23	3	0.79
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD11	8	0.79
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD12	8	0.79
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD13	8	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD2	9	0.79
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD3	9	0.79
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD2	9	0.79
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD3	9	0.79
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD2	9	0.79
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD3	9	0.79
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD2	9	0.79
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD3	9	0.79
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD2	9	0.79
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD3	9	0.79
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD2	9	0.79
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD3	9	0.79
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB2	7	0.79
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB3	7	0.79
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB2	7	0.79
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB3	7	0.79
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB2	9	0.79
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB3	9	0.79
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB2	9	0.79
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB3	9	0.79
(1,114)	1:8:A:ASP:H	1:37:A:ALA:HB1	5	0.79
(1,114)	1:8:A:ASP:H	1:37:A:ALA:HB2	5	0.79
(1,114)	1:8:A:ASP:H	1:37:A:ALA:HB3	5	0.79
(1,91)	1:7:A:VAL:HG21	1:120:A:SER:HA	1	0.79
(1,91)	1:7:A:VAL:HG22	1:120:A:SER:HA	1	0.79
(1,91)	1:7:A:VAL:HG23	1:120:A:SER:HA	1	0.79
(1,91)	1:7:A:VAL:HG21	1:120:A:SER:HA	9	0.79
(1,91)	1:7:A:VAL:HG22	1:120:A:SER:HA	9	0.79
(1,91)	1:7:A:VAL:HG23	1:120:A:SER:HA	9	0.79
(3,26)	1:68:A:ARG:N	1:97:A:TYR:O	9	0.78
(1,1670)	1:141:A:SER:HB3	1:145:A:ASP:HA	4	0.78
(1,1594)	1:135:A:SER:HB2	1:140:A:LYS:HG2	5	0.78
(1,1594)	1:135:A:SER:HB2	1:140:A:LYS:HG3	5	0.78
(1,1594)	1:135:A:SER:HB3	1:140:A:LYS:HG2	5	0.78
(1,1594)	1:135:A:SER:HB3	1:140:A:LYS:HG3	5	0.78
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD11	7	0.78
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD12	7	0.78
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD13	7	0.78
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD21	7	0.78
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD22	7	0.78
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD23	7	0.78
(1,1333)	1:110:A:TYR:HA	1:114:A:VAL:H	4	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1083)	1:93:A:ILE:HA	1:127:A:PHE:HB2	10	0.78
(1,1083)	1:93:A:ILE:HA	1:127:A:PHE:HB3	10	0.78
(1,1083)	1:93:A:ILE:HA	1:127:A:PHE:HB2	10	0.78
(1,1083)	1:93:A:ILE:HA	1:127:A:PHE:HB3	10	0.78
(1,1027)	1:86:A:THR:HB	1:87:A:SER:H	9	0.78
(1,755)	1:58:A:LYS:HD2	1:60:A:LEU:H	7	0.78
(1,736)	1:57:A:MET:HB2	1:60:A:LEU:HG	3	0.78
(1,736)	1:57:A:MET:HB3	1:60:A:LEU:HG	3	0.78
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG2	3	0.78
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG3	3	0.78
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG2	3	0.78
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG3	3	0.78
(1,387)	1:26:A:TYR:HB2	1:73:A:ASP:H	8	0.78
(1,387)	1:26:A:TYR:HB3	1:73:A:ASP:H	8	0.78
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD11	7	0.78
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD12	7	0.78
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD13	7	0.78
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD21	7	0.78
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD22	7	0.78
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD23	7	0.78
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD11	7	0.78
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD12	7	0.78
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD13	7	0.78
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD21	7	0.78
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD22	7	0.78
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD23	7	0.78
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD11	1	0.78
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD12	1	0.78
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD13	1	0.78
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD21	1	0.78
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD22	1	0.78
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD23	1	0.78
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD11	1	0.78
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD12	1	0.78
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD13	1	0.78
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD21	1	0.78
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD22	1	0.78
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD23	1	0.78
(1,207)	1:12:A:LYS:HD3	1:15:A:TYR:HA	6	0.78
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB2	6	0.78
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB3	6	0.78
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB2	6	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB3	6	0.78
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB2	8	0.78
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB3	8	0.78
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB2	8	0.78
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB3	8	0.78
(1,1651)	1:140:A:LYS:HD3	1:142:A:VAL:H	1	0.77
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	10	0.77
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	10	0.77
(1,1442)	1:118:A:LYS:HE2	1:121:A:LEU:H	6	0.77
(1,1442)	1:118:A:LYS:HE2	1:121:A:LEU:H	9	0.77
(1,1410)	1:116:A:ALA:HA	1:120:A:SER:H	2	0.77
(1,1240)	1:104:A:VAL:HG11	1:107:A:ARG:HA	7	0.77
(1,1240)	1:104:A:VAL:HG12	1:107:A:ARG:HA	7	0.77
(1,1240)	1:104:A:VAL:HG13	1:107:A:ARG:HA	7	0.77
(1,1240)	1:104:A:VAL:HG21	1:107:A:ARG:HA	7	0.77
(1,1240)	1:104:A:VAL:HG22	1:107:A:ARG:HA	7	0.77
(1,1240)	1:104:A:VAL:HG23	1:107:A:ARG:HA	7	0.77
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB1	10	0.77
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB2	10	0.77
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB3	10	0.77
(1,912)	1:76:A:VAL:HA	1:88:A:THR:HG21	6	0.77
(1,912)	1:76:A:VAL:HA	1:88:A:THR:HG22	6	0.77
(1,912)	1:76:A:VAL:HA	1:88:A:THR:HG23	6	0.77
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG2	6	0.77
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG3	6	0.77
(1,909)	1:76:A:VAL:H	1:89:A:LEU:H	2	0.77
(1,898)	1:75:A:GLU:HG3	1:90:A:ASN:HA	9	0.77
(1,891)	1:75:A:GLU:HG2	1:89:A:LEU:H	6	0.77
(1,887)	1:75:A:GLU:HB3	1:89:A:LEU:H	10	0.77
(1,755)	1:58:A:LYS:HD2	1:60:A:LEU:H	3	0.77
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB2	1	0.77
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB3	1	0.77
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB2	1	0.77
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB3	1	0.77
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB2	1	0.77
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB3	1	0.77
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB2	1	0.77
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB3	1	0.77
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB2	1	0.77
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB3	1	0.77
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB2	1	0.77
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB3	1	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB1	1	0.77
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB2	1	0.77
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB3	1	0.77
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB1	1	0.77
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB2	1	0.77
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB3	1	0.77
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD11	3	0.77
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD12	3	0.77
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD13	3	0.77
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD21	3	0.77
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD22	3	0.77
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD23	3	0.77
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD11	3	0.77
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD12	3	0.77
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD13	3	0.77
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD21	3	0.77
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD22	3	0.77
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD23	3	0.77
(1,454)	1:28:A:ILE:HG12	1:41:A:GLU:HG2	10	0.77
(1,454)	1:28:A:ILE:HG12	1:41:A:GLU:HG3	10	0.77
(1,454)	1:28:A:ILE:HG13	1:41:A:GLU:HG2	10	0.77
(1,454)	1:28:A:ILE:HG13	1:41:A:GLU:HG3	10	0.77
(1,385)	1:26:A:TYR:HB2	1:72:A:VAL:HA	5	0.77
(1,385)	1:26:A:TYR:HB3	1:72:A:VAL:HA	5	0.77
(1,350)	1:21:A:LYS:HD3	1:22:A:HIS:H	10	0.77
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB2	2	0.77
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB3	2	0.77
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB2	2	0.77
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB3	2	0.77
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB2	4	0.77
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB3	4	0.77
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB2	4	0.77
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB3	4	0.77
(1,55)	1:6:A:LYS:HE2	1:7:A:VAL:H	2	0.77
(1,55)	1:6:A:LYS:HE3	1:7:A:VAL:H	2	0.77
(3,7)	1:13:A:ASN:O	1:17:A:LEU:H	10	0.76
(1,1574)	1:134:A:MET:HA	1:136:A:ASP:H	9	0.76
(1,1550)	1:131:A:ALA:HA	1:136:A:ASP:HA	9	0.76
(1,1466)	1:120:A:SER:HB3	1:122:A:GLY:H	10	0.76
(1,1443)	1:118:A:LYS:HE3	1:119:A:ALA:H	8	0.76
(1,1378)	1:114:A:VAL:HB	1:118:A:LYS:H	4	0.76
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD11	3	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD12	3	0.76
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD13	3	0.76
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD21	3	0.76
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD22	3	0.76
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD23	3	0.76
(1,1344)	1:111:A:ALA:HA	1:115:A:ARG:H	8	0.76
(1,1299)	1:108:A:MET:HB2	1:112:A:SER:H	5	0.76
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG2	10	0.76
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG3	10	0.76
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG2	10	0.76
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG3	10	0.76
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG2	10	0.76
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG3	10	0.76
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG2	10	0.76
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG3	10	0.76
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG2	10	0.76
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG3	10	0.76
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG2	10	0.76
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG3	10	0.76
(1,1145)	1:95:A:VAL:HG11	1:131:A:ALA:HA	10	0.76
(1,1145)	1:95:A:VAL:HG12	1:131:A:ALA:HA	10	0.76
(1,1145)	1:95:A:VAL:HG13	1:131:A:ALA:HA	10	0.76
(1,1145)	1:95:A:VAL:HG21	1:131:A:ALA:HA	10	0.76
(1,1145)	1:95:A:VAL:HG22	1:131:A:ALA:HA	10	0.76
(1,1145)	1:95:A:VAL:HG23	1:131:A:ALA:HA	10	0.76
(1,978)	1:79:A:GLN:HG2	1:85:A:GLY:H	7	0.76
(1,970)	1:79:A:GLN:HA	1:86:A:THR:HB	10	0.76
(1,945)	1:78:A:VAL:H	1:86:A:THR:HB	1	0.76
(1,907)	1:76:A:VAL:H	1:88:A:THR:HB	5	0.76
(1,890)	1:75:A:GLU:HG2	1:88:A:THR:HG21	6	0.76
(1,890)	1:75:A:GLU:HG2	1:88:A:THR:HG22	6	0.76
(1,890)	1:75:A:GLU:HG2	1:88:A:THR:HG23	6	0.76
(1,783)	1:61:A:VAL:HG11	1:66:A:GLU:HB2	10	0.76
(1,783)	1:61:A:VAL:HG12	1:66:A:GLU:HB2	10	0.76
(1,783)	1:61:A:VAL:HG13	1:66:A:GLU:HB2	10	0.76
(1,783)	1:61:A:VAL:HG11	1:66:A:GLU:HB3	10	0.76
(1,783)	1:61:A:VAL:HG12	1:66:A:GLU:HB3	10	0.76
(1,783)	1:61:A:VAL:HG13	1:66:A:GLU:HB3	10	0.76
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG2	10	0.76
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG3	10	0.76
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG2	10	0.76
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG3	10	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG21	2	0.76
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG22	2	0.76
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG23	2	0.76
(1,516)	1:32:A:ASP:HB2	1:37:A:ALA:H	7	0.76
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG2	10	0.76
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG3	10	0.76
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG2	10	0.76
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG3	10	0.76
(1,439)	1:28:A:ILE:HB	1:42:A:LYS:HD2	5	0.76
(1,439)	1:28:A:ILE:HB	1:42:A:LYS:HD3	5	0.76
(1,335)	1:19:A:HIS:HA	1:21:A:LYS:H	2	0.76
(1,102)	1:7:A:VAL:HG11	1:120:A:SER:HA	2	0.76
(1,102)	1:7:A:VAL:HG12	1:120:A:SER:HA	2	0.76
(1,102)	1:7:A:VAL:HG13	1:120:A:SER:HA	2	0.76
(1,102)	1:7:A:VAL:HG21	1:120:A:SER:HA	2	0.76
(1,102)	1:7:A:VAL:HG22	1:120:A:SER:HA	2	0.76
(1,102)	1:7:A:VAL:HG23	1:120:A:SER:HA	2	0.76
(1,102)	1:7:A:VAL:HG11	1:120:A:SER:HA	9	0.76
(1,102)	1:7:A:VAL:HG12	1:120:A:SER:HA	9	0.76
(1,102)	1:7:A:VAL:HG13	1:120:A:SER:HA	9	0.76
(1,102)	1:7:A:VAL:HG21	1:120:A:SER:HA	9	0.76
(1,102)	1:7:A:VAL:HG22	1:120:A:SER:HA	9	0.76
(1,102)	1:7:A:VAL:HG23	1:120:A:SER:HA	9	0.76
(1,31)	1:5:A:VAL:HB	1:36:A:THR:HB	1	0.76
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG11	10	0.75
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG12	10	0.75
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG13	10	0.75
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG21	10	0.75
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG22	10	0.75
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG23	10	0.75
(1,1797)	1:151:A:ARG:H	1:151:A:ARG:HG2	5	0.75
(1,1797)	1:151:A:ARG:H	1:151:A:ARG:HG3	5	0.75
(1,1670)	1:141:A:SER:HB3	1:145:A:ASP:HA	7	0.75
(1,1664)	1:141:A:SER:HA	1:143:A:LYS:H	9	0.75
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD2	9	0.75
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD3	9	0.75
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD2	9	0.75
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD3	9	0.75
(1,1442)	1:118:A:LYS:HE2	1:121:A:LEU:H	10	0.75
(1,1344)	1:111:A:ALA:HA	1:115:A:ARG:H	1	0.75
(1,1286)	1:107:A:ARG:HD2	1:111:A:ALA:HA	6	0.75
(1,1286)	1:107:A:ARG:HD3	1:111:A:ALA:HA	6	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1185)	1:99:A:PRO:HG2	1:102:A:ALA:HA	9	0.75
(1,1178)	1:99:A:PRO:HB2	1:102:A:ALA:HA	6	0.75
(1,1172)	1:98:A:CYS:HB2	1:107:A:ARG:HA	6	0.75
(1,1172)	1:98:A:CYS:HB3	1:107:A:ARG:HA	6	0.75
(1,887)	1:75:A:GLU:HB3	1:89:A:LEU:H	3	0.75
(1,790)	1:61:A:VAL:HG11	1:66:A:GLU:HG2	7	0.75
(1,790)	1:61:A:VAL:HG11	1:66:A:GLU:HG3	7	0.75
(1,790)	1:61:A:VAL:HG12	1:66:A:GLU:HG2	7	0.75
(1,790)	1:61:A:VAL:HG12	1:66:A:GLU:HG3	7	0.75
(1,790)	1:61:A:VAL:HG13	1:66:A:GLU:HG2	7	0.75
(1,790)	1:61:A:VAL:HG13	1:66:A:GLU:HG3	7	0.75
(1,790)	1:61:A:VAL:HG21	1:66:A:GLU:HG2	7	0.75
(1,790)	1:61:A:VAL:HG21	1:66:A:GLU:HG3	7	0.75
(1,790)	1:61:A:VAL:HG22	1:66:A:GLU:HG2	7	0.75
(1,790)	1:61:A:VAL:HG22	1:66:A:GLU:HG3	7	0.75
(1,790)	1:61:A:VAL:HG23	1:66:A:GLU:HG2	7	0.75
(1,790)	1:61:A:VAL:HG23	1:66:A:GLU:HG3	7	0.75
(1,659)	1:53:A:PHE:HB2	1:56:A:GLU:H	6	0.75
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB2	6	0.75
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB3	6	0.75
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB2	6	0.75
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB3	6	0.75
(1,524)	1:33:A:LYS:HG2	1:36:A:THR:HB	8	0.75
(1,439)	1:28:A:ILE:HB	1:42:A:LYS:HD2	3	0.75
(1,439)	1:28:A:ILE:HB	1:42:A:LYS:HD3	3	0.75
(1,277)	1:16:A:ASP:HB2	1:18:A:LEU:H	5	0.75
(1,116)	1:8:A:ASP:H	1:39:A:VAL:HA	5	0.75
(1,113)	1:8:A:ASP:H	1:37:A:ALA:HA	1	0.75
(1,91)	1:7:A:VAL:HG21	1:120:A:SER:HA	2	0.75
(1,91)	1:7:A:VAL:HG22	1:120:A:SER:HA	2	0.75
(1,91)	1:7:A:VAL:HG23	1:120:A:SER:HA	2	0.75
(1,83)	1:7:A:VAL:HG11	1:120:A:SER:HA	6	0.75
(1,83)	1:7:A:VAL:HG12	1:120:A:SER:HA	6	0.75
(1,83)	1:7:A:VAL:HG13	1:120:A:SER:HA	6	0.75
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG11	9	0.75
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG12	9	0.75
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG13	9	0.75
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG21	9	0.75
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG22	9	0.75
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG23	9	0.75
(1,1726)	1:144:A:SER:HB3	1:146:A:LEU:H	9	0.74
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	1	0.74
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	1	0.74
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	1	0.74
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	3	0.74
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	3	0.74
(1,1358)	1:113:A:SER:H	1:115:A:ARG:H	10	0.74
(1,1285)	1:107:A:ARG:HD2	1:108:A:MET:H	3	0.74
(1,1285)	1:107:A:ARG:HD3	1:108:A:MET:H	3	0.74
(1,1285)	1:107:A:ARG:HD2	1:108:A:MET:H	3	0.74
(1,1285)	1:107:A:ARG:HD3	1:108:A:MET:H	3	0.74
(1,1172)	1:98:A:CYS:HB2	1:107:A:ARG:HA	8	0.74
(1,1172)	1:98:A:CYS:HB3	1:107:A:ARG:HA	8	0.74
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG11	1	0.74
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG12	1	0.74
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG13	1	0.74
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG21	1	0.74
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG22	1	0.74
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG23	1	0.74
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG11	1	0.74
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG12	1	0.74
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG13	1	0.74
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG21	1	0.74
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG22	1	0.74
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG23	1	0.74
(1,1122)	1:94:A:PHE:HB2	1:118:A:LYS:HE2	8	0.74
(1,1122)	1:94:A:PHE:HB2	1:118:A:LYS:HE3	8	0.74
(1,1122)	1:94:A:PHE:HB3	1:118:A:LYS:HE2	8	0.74
(1,1122)	1:94:A:PHE:HB3	1:118:A:LYS:HE3	8	0.74
(1,1067)	1:92:A:VAL:H	1:127:A:PHE:H	9	0.74
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE2	4	0.74
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE3	4	0.74
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE2	4	0.74
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE3	4	0.74
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD2	2	0.74
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD3	2	0.74
(1,523)	1:33:A:LYS:HG2	1:36:A:THR:HA	7	0.74
(1,480)	1:30:A:LYS:HB2	1:41:A:GLU:HA	6	0.74
(1,480)	1:30:A:LYS:HB3	1:41:A:GLU:HA	6	0.74
(1,480)	1:30:A:LYS:HB2	1:41:A:GLU:HA	9	0.74
(1,480)	1:30:A:LYS:HB3	1:41:A:GLU:HA	9	0.74
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG2	10	0.74
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG3	10	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:28:A:ILE:HD11	1:71:A:ALA:H	10	0.74
(1,452)	1:28:A:ILE:HD12	1:71:A:ALA:H	10	0.74
(1,452)	1:28:A:ILE:HD13	1:71:A:ALA:H	10	0.74
(1,321)	1:18:A:LEU:HD11	1:73:A:ASP:HA	4	0.74
(1,321)	1:18:A:LEU:HD12	1:73:A:ASP:HA	4	0.74
(1,321)	1:18:A:LEU:HD13	1:73:A:ASP:HA	4	0.74
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB1	3	0.74
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB2	3	0.74
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB3	3	0.74
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB1	3	0.74
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB2	3	0.74
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB3	3	0.74
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB2	3	0.74
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB3	3	0.74
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB2	3	0.74
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB3	3	0.74
(3,37)	1:74:A:VAL:H	1:91:A:LYS:O	1	0.73
(1,1718)	1:144:A:SER:H	1:146:A:LEU:H	5	0.73
(1,1709)	1:143:A:LYS:HB2	1:147:A:MET:H	3	0.73
(1,1709)	1:143:A:LYS:HB2	1:147:A:MET:H	7	0.73
(1,1709)	1:143:A:LYS:HB2	1:147:A:MET:H	10	0.73
(1,1651)	1:140:A:LYS:HD3	1:142:A:VAL:H	3	0.73
(1,1398)	1:115:A:ARG:HA	1:119:A:ALA:H	6	0.73
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	8	0.73
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	8	0.73
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	8	0.73
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	8	0.73
(1,1173)	1:98:A:CYS:HB2	1:107:A:ARG:HD2	5	0.73
(1,1173)	1:98:A:CYS:HB2	1:107:A:ARG:HD3	5	0.73
(1,1173)	1:98:A:CYS:HB3	1:107:A:ARG:HD2	5	0.73
(1,1173)	1:98:A:CYS:HB3	1:107:A:ARG:HD3	5	0.73
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD11	6	0.73
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD12	6	0.73
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD13	6	0.73
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD21	6	0.73
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD22	6	0.73
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD23	6	0.73
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD11	6	0.73
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD12	6	0.73
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD13	6	0.73
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD21	6	0.73
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD22	6	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD23	6	0.73
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD11	6	0.73
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD12	6	0.73
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD13	6	0.73
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD21	6	0.73
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD22	6	0.73
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD23	6	0.73
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD11	6	0.73
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD12	6	0.73
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD13	6	0.73
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD21	6	0.73
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD22	6	0.73
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD23	6	0.73
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD11	6	0.73
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD12	6	0.73
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD13	6	0.73
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD21	6	0.73
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD22	6	0.73
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD23	6	0.73
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD11	6	0.73
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD12	6	0.73
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD13	6	0.73
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD21	6	0.73
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD22	6	0.73
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD23	6	0.73
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG21	4	0.73
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG22	4	0.73
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG23	4	0.73
(1,909)	1:76:A:VAL:H	1:89:A:LEU:H	1	0.73
(1,685)	1:54:A:VAL:HG11	1:138:A:ASP:HA	9	0.73
(1,685)	1:54:A:VAL:HG12	1:138:A:ASP:HA	9	0.73
(1,685)	1:54:A:VAL:HG13	1:138:A:ASP:HA	9	0.73
(1,685)	1:54:A:VAL:HG21	1:138:A:ASP:HA	9	0.73
(1,685)	1:54:A:VAL:HG22	1:138:A:ASP:HA	9	0.73
(1,685)	1:54:A:VAL:HG23	1:138:A:ASP:HA	9	0.73
(1,609)	1:49:A:PRO:HG2	1:51:A:ALA:H	10	0.73
(1,609)	1:49:A:PRO:HG3	1:51:A:ALA:H	10	0.73
(1,516)	1:32:A:ASP:HB2	1:37:A:ALA:H	4	0.73
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD11	2	0.73
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD12	2	0.73
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD13	2	0.73
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD21	2	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD22	2	0.73
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD23	2	0.73
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD11	2	0.73
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD12	2	0.73
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD13	2	0.73
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD21	2	0.73
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD22	2	0.73
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD23	2	0.73
(1,499)	1:31:A:ILE:HG13	1:38:A:ILE:HB	3	0.73
(1,499)	1:31:A:ILE:HG13	1:38:A:ILE:HB	6	0.73
(1,439)	1:28:A:ILE:HB	1:42:A:LYS:HD2	2	0.73
(1,439)	1:28:A:ILE:HB	1:42:A:LYS:HD3	2	0.73
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD11	2	0.73
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD12	2	0.73
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD13	2	0.73
(1,102)	1:7:A:VAL:HG11	1:120:A:SER:HA	1	0.73
(1,102)	1:7:A:VAL:HG12	1:120:A:SER:HA	1	0.73
(1,102)	1:7:A:VAL:HG13	1:120:A:SER:HA	1	0.73
(1,102)	1:7:A:VAL:HG21	1:120:A:SER:HA	1	0.73
(1,102)	1:7:A:VAL:HG22	1:120:A:SER:HA	1	0.73
(1,102)	1:7:A:VAL:HG23	1:120:A:SER:HA	1	0.73
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD11	3	0.73
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD12	3	0.73
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD13	3	0.73
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD11	3	0.73
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD12	3	0.73
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD13	3	0.73
(1,33)	1:5:A:VAL:HB	1:7:A:VAL:HA	10	0.73
(3,10)	1:26:A:TYR:N	1:44:A:GLY:O	8	0.72
(1,1790)	1:150:A:GLN:HB3	1:152:A:ILE:H	5	0.72
(1,1726)	1:144:A:SER:HB3	1:146:A:LEU:H	5	0.72
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE2	7	0.72
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE3	7	0.72
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	7	0.72
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	7	0.72
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	7	0.72
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	7	0.72
(1,1333)	1:110:A:TYR:HA	1:114:A:VAL:H	6	0.72
(1,1299)	1:108:A:MET:HB2	1:112:A:SER:H	9	0.72
(1,985)	1:80:A:ARG:H	1:80:A:ARG:HG2	1	0.72
(1,985)	1:80:A:ARG:H	1:80:A:ARG:HG3	1	0.72
(1,907)	1:76:A:VAL:H	1:88:A:THR:HB	2	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,737)	1:57:A:MET:HG2	1:60:A:LEU:HG	7	0.72
(1,737)	1:57:A:MET:HG3	1:60:A:LEU:HG	7	0.72
(1,577)	1:42:A:LYS:HB2	1:53:A:PHE:HA	10	0.72
(1,577)	1:42:A:LYS:HB3	1:53:A:PHE:HA	10	0.72
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB2	2	0.72
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB3	2	0.72
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB1	10	0.72
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB2	10	0.72
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB3	10	0.72
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD11	7	0.72
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD12	7	0.72
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD13	7	0.72
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD21	7	0.72
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD22	7	0.72
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD23	7	0.72
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD11	9	0.72
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD12	9	0.72
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD13	9	0.72
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD21	9	0.72
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD22	9	0.72
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD23	9	0.72
(1,176)	1:11:A:CYS:HB2	1:121:A:LEU:HD11	9	0.72
(1,176)	1:11:A:CYS:HB2	1:121:A:LEU:HD12	9	0.72
(1,176)	1:11:A:CYS:HB2	1:121:A:LEU:HD13	9	0.72
(1,176)	1:11:A:CYS:HB2	1:121:A:LEU:HD21	9	0.72
(1,176)	1:11:A:CYS:HB2	1:121:A:LEU:HD22	9	0.72
(1,176)	1:11:A:CYS:HB2	1:121:A:LEU:HD23	9	0.72
(1,159)	1:10:A:SER:HB3	1:13:A:ASN:H	3	0.72
(1,159)	1:10:A:SER:HB3	1:13:A:ASN:H	10	0.72
(1,137)	1:8:A:ASP:HB2	1:9:A:PRO:HA	4	0.72
(1,137)	1:8:A:ASP:HB3	1:9:A:PRO:HA	4	0.72
(1,124)	1:8:A:ASP:HB2	1:39:A:VAL:HB	4	0.72
(1,83)	1:7:A:VAL:HG11	1:120:A:SER:HA	3	0.72
(1,83)	1:7:A:VAL:HG12	1:120:A:SER:HA	3	0.72
(1,83)	1:7:A:VAL:HG13	1:120:A:SER:HA	3	0.72
(1,14)	1:3:A:SER:H	1:113:A:SER:HA	6	0.72
(3,20)	1:29:A:PHE:O	1:69:A:TYR:N	8	0.71
(1,1719)	1:144:A:SER:HA	1:146:A:LEU:H	6	0.71
(1,1709)	1:143:A:LYS:HB2	1:147:A:MET:H	6	0.71
(1,1325)	1:109:A:LEU:HD11	1:112:A:SER:HB2	9	0.71
(1,1325)	1:109:A:LEU:HD11	1:112:A:SER:HB3	9	0.71
(1,1325)	1:109:A:LEU:HD12	1:112:A:SER:HB2	9	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1325)	1:109:A:LEU:HD12	1:112:A:SER:HB3	9	0.71
(1,1325)	1:109:A:LEU:HD13	1:112:A:SER:HB2	9	0.71
(1,1325)	1:109:A:LEU:HD13	1:112:A:SER:HB3	9	0.71
(1,1325)	1:109:A:LEU:HD21	1:112:A:SER:HB2	9	0.71
(1,1325)	1:109:A:LEU:HD21	1:112:A:SER:HB3	9	0.71
(1,1325)	1:109:A:LEU:HD22	1:112:A:SER:HB2	9	0.71
(1,1325)	1:109:A:LEU:HD22	1:112:A:SER:HB3	9	0.71
(1,1325)	1:109:A:LEU:HD23	1:112:A:SER:HB2	9	0.71
(1,1325)	1:109:A:LEU:HD23	1:112:A:SER:HB3	9	0.71
(1,1299)	1:108:A:MET:HB2	1:112:A:SER:H	3	0.71
(1,1285)	1:107:A:ARG:HD2	1:108:A:MET:H	2	0.71
(1,1285)	1:107:A:ARG:HD3	1:108:A:MET:H	2	0.71
(1,1285)	1:107:A:ARG:HD2	1:108:A:MET:H	2	0.71
(1,1285)	1:107:A:ARG:HD3	1:108:A:MET:H	2	0.71
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	10	0.71
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	10	0.71
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	10	0.71
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	10	0.71
(1,1184)	1:99:A:PRO:HG2	1:100:A:ASP:H	7	0.71
(1,1172)	1:98:A:CYS:HB2	1:107:A:ARG:HA	9	0.71
(1,1172)	1:98:A:CYS:HB3	1:107:A:ARG:HA	9	0.71
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG11	10	0.71
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG12	10	0.71
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG13	10	0.71
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG21	10	0.71
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG22	10	0.71
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG23	10	0.71
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG11	10	0.71
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG12	10	0.71
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG13	10	0.71
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG21	10	0.71
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG22	10	0.71
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG23	10	0.71
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD11	1	0.71
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD12	1	0.71
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD13	1	0.71
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD21	1	0.71
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD22	1	0.71
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD23	1	0.71
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD11	1	0.71
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD12	1	0.71
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD13	1	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD21	1	0.71
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD22	1	0.71
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD23	1	0.71
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG21	1	0.71
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG22	1	0.71
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG23	1	0.71
(1,935)	1:77:A:THR:HB	1:87:A:SER:H	7	0.71
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB1	1	0.71
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB2	1	0.71
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB3	1	0.71
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB1	1	0.71
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB2	1	0.71
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB3	1	0.71
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB1	1	0.71
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB2	1	0.71
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB3	1	0.71
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB1	1	0.71
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB2	1	0.71
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB3	1	0.71
(1,507)	1:31:A:ILE:HG12	1:109:A:LEU:HB2	9	0.71
(1,507)	1:31:A:ILE:HG12	1:109:A:LEU:HB3	9	0.71
(1,507)	1:31:A:ILE:HG13	1:109:A:LEU:HB2	9	0.71
(1,507)	1:31:A:ILE:HG13	1:109:A:LEU:HB3	9	0.71
(1,501)	1:31:A:ILE:HD11	1:109:A:LEU:H	1	0.71
(1,501)	1:31:A:ILE:HD12	1:109:A:LEU:H	1	0.71
(1,501)	1:31:A:ILE:HD13	1:109:A:LEU:H	1	0.71
(1,370)	1:25:A:SER:HB2	1:73:A:ASP:HB2	9	0.71
(1,370)	1:25:A:SER:HB2	1:73:A:ASP:HB3	9	0.71
(1,370)	1:25:A:SER:HB3	1:73:A:ASP:HB2	9	0.71
(1,370)	1:25:A:SER:HB3	1:73:A:ASP:HB3	9	0.71
(1,237)	1:14:A:ALA:HA	1:18:A:LEU:H	7	0.71
(1,135)	1:8:A:ASP:HB2	1:39:A:VAL:HB	5	0.71
(1,135)	1:8:A:ASP:HB3	1:39:A:VAL:HB	5	0.71
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG21	6	0.71
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG22	6	0.71
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG23	6	0.71
(1,55)	1:6:A:LYS:HE2	1:7:A:VAL:H	3	0.71
(1,55)	1:6:A:LYS:HE3	1:7:A:VAL:H	3	0.71
(1,20)	1:4:A:GLY:H	1:5:A:VAL:HB	1	0.71
(1,1726)	1:144:A:SER:HB3	1:146:A:LEU:H	4	0.7
(1,1589)	1:135:A:SER:HA	1:140:A:LYS:HE2	3	0.7
(1,1224)	1:104:A:VAL:HB	1:106:A:ARG:H	1	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1218)	1:104:A:VAL:HA	1:106:A:ARG:H	6	0.7
(1,1173)	1:98:A:CYS:HB2	1:107:A:ARG:HD2	4	0.7
(1,1173)	1:98:A:CYS:HB2	1:107:A:ARG:HD3	4	0.7
(1,1173)	1:98:A:CYS:HB3	1:107:A:ARG:HD2	4	0.7
(1,1173)	1:98:A:CYS:HB3	1:107:A:ARG:HD3	4	0.7
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB1	8	0.7
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB2	8	0.7
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB3	8	0.7
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD11	4	0.7
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD12	4	0.7
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD13	4	0.7
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD21	4	0.7
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD22	4	0.7
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD23	4	0.7
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD11	4	0.7
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD12	4	0.7
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD13	4	0.7
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD21	4	0.7
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD22	4	0.7
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD23	4	0.7
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD11	4	0.7
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD12	4	0.7
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD13	4	0.7
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD21	4	0.7
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD22	4	0.7
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD23	4	0.7
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD11	4	0.7
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD12	4	0.7
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD13	4	0.7
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD21	4	0.7
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD22	4	0.7
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD23	4	0.7
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD11	4	0.7
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD12	4	0.7
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD13	4	0.7
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD21	4	0.7
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD22	4	0.7
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD23	4	0.7
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD11	4	0.7
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD12	4	0.7
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD13	4	0.7
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD21	4	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD22	4	0.7
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD23	4	0.7
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG21	3	0.7
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG22	3	0.7
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG23	3	0.7
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG21	7	0.7
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG22	7	0.7
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG23	7	0.7
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG21	7	0.7
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG22	7	0.7
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG23	7	0.7
(1,884)	1:75:A:GLU:HB3	1:88:A:THR:HA	10	0.7
(1,721)	1:56:A:GLU:HA	1:59:A:LYS:HE2	5	0.7
(1,721)	1:56:A:GLU:HA	1:59:A:LYS:HE3	5	0.7
(1,577)	1:42:A:LYS:HB2	1:53:A:PHE:HA	5	0.7
(1,577)	1:42:A:LYS:HB3	1:53:A:PHE:HA	5	0.7
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB1	2	0.7
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB2	2	0.7
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB3	2	0.7
(1,524)	1:33:A:LYS:HG2	1:36:A:THR:HB	3	0.7
(1,384)	1:26:A:TYR:HB2	1:71:A:ALA:H	8	0.7
(1,384)	1:26:A:TYR:HB3	1:71:A:ALA:H	8	0.7
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB1	1	0.7
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB2	1	0.7
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB3	1	0.7
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB1	1	0.7
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB2	1	0.7
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB3	1	0.7
(1,137)	1:8:A:ASP:HB2	1:9:A:PRO:HA	6	0.7
(1,137)	1:8:A:ASP:HB3	1:9:A:PRO:HA	6	0.7
(1,48)	1:6:A:LYS:H	1:6:A:LYS:HE2	5	0.7
(1,48)	1:6:A:LYS:H	1:6:A:LYS:HE3	5	0.7
(3,20)	1:29:A:PHE:O	1:69:A:TYR:N	5	0.69
(3,3)	1:8:A:ASP:H	1:38:A:ILE:O	4	0.69
(1,1780)	1:149:A:ASN:HB2	1:152:A:ILE:HD11	9	0.69
(1,1780)	1:149:A:ASN:HB2	1:152:A:ILE:HD12	9	0.69
(1,1780)	1:149:A:ASN:HB2	1:152:A:ILE:HD13	9	0.69
(1,1780)	1:149:A:ASN:HB3	1:152:A:ILE:HD11	9	0.69
(1,1780)	1:149:A:ASN:HB3	1:152:A:ILE:HD12	9	0.69
(1,1780)	1:149:A:ASN:HB3	1:152:A:ILE:HD13	9	0.69
(1,1765)	1:148:A:SER:HB2	1:150:A:GLN:H	4	0.69
(1,1709)	1:143:A:LYS:HB2	1:147:A:MET:H	2	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1664)	1:141:A:SER:HA	1:143:A:LYS:H	1	0.69
(1,1651)	1:140:A:LYS:HD3	1:142:A:VAL:H	9	0.69
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB2	8	0.69
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB3	8	0.69
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB2	8	0.69
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB3	8	0.69
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB2	8	0.69
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB3	8	0.69
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB2	8	0.69
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB3	8	0.69
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB2	8	0.69
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB3	8	0.69
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB2	8	0.69
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB3	8	0.69
(1,1316)	1:109:A:LEU:HA	1:113:A:SER:H	4	0.69
(1,1298)	1:108:A:MET:HB2	1:110:A:TYR:H	8	0.69
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD11	5	0.69
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD12	5	0.69
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD13	5	0.69
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD21	5	0.69
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD22	5	0.69
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD23	5	0.69
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD11	5	0.69
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD12	5	0.69
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD13	5	0.69
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD21	5	0.69
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD22	5	0.69
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD23	5	0.69
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD11	5	0.69
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD12	5	0.69
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD13	5	0.69
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD21	5	0.69
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD22	5	0.69
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD23	5	0.69
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD11	5	0.69
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD12	5	0.69
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD13	5	0.69
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD21	5	0.69
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD22	5	0.69
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD23	5	0.69
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD11	5	0.69
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD12	5	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD13	5	0.69
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD21	5	0.69
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD22	5	0.69
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD23	5	0.69
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD11	5	0.69
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD12	5	0.69
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD13	5	0.69
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD21	5	0.69
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD22	5	0.69
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD23	5	0.69
(1,1067)	1:92:A:VAL:H	1:127:A:PHE:H	3	0.69
(1,978)	1:79:A:GLN:HG2	1:85:A:GLY:H	5	0.69
(1,978)	1:79:A:GLN:HG2	1:85:A:GLY:H	8	0.69
(1,962)	1:78:A:VAL:HG11	1:87:A:SER:HB2	5	0.69
(1,962)	1:78:A:VAL:HG11	1:87:A:SER:HB3	5	0.69
(1,962)	1:78:A:VAL:HG12	1:87:A:SER:HB2	5	0.69
(1,962)	1:78:A:VAL:HG12	1:87:A:SER:HB3	5	0.69
(1,962)	1:78:A:VAL:HG13	1:87:A:SER:HB2	5	0.69
(1,962)	1:78:A:VAL:HG13	1:87:A:SER:HB3	5	0.69
(1,962)	1:78:A:VAL:HG21	1:87:A:SER:HB2	5	0.69
(1,962)	1:78:A:VAL:HG21	1:87:A:SER:HB3	5	0.69
(1,962)	1:78:A:VAL:HG22	1:87:A:SER:HB2	5	0.69
(1,962)	1:78:A:VAL:HG22	1:87:A:SER:HB3	5	0.69
(1,962)	1:78:A:VAL:HG23	1:87:A:SER:HB2	5	0.69
(1,962)	1:78:A:VAL:HG23	1:87:A:SER:HB3	5	0.69
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG21	3	0.69
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG22	3	0.69
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG23	3	0.69
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG21	5	0.69
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG22	5	0.69
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG23	5	0.69
(1,886)	1:75:A:GLU:HB3	1:88:A:THR:HG21	6	0.69
(1,886)	1:75:A:GLU:HB3	1:88:A:THR:HG22	6	0.69
(1,886)	1:75:A:GLU:HB3	1:88:A:THR:HG23	6	0.69
(1,737)	1:57:A:MET:HG2	1:60:A:LEU:HG	3	0.69
(1,737)	1:57:A:MET:HG3	1:60:A:LEU:HG	3	0.69
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD11	7	0.69
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD12	7	0.69
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD13	7	0.69
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG2	6	0.69
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG3	6	0.69
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG2	6	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG3	6	0.69
(1,135)	1:8:A:ASP:HB2	1:39:A:VAL:HB	4	0.69
(1,135)	1:8:A:ASP:HB3	1:39:A:VAL:HB	4	0.69
(1,113)	1:8:A:ASP:H	1:37:A:ALA:HA	7	0.69
(1,113)	1:8:A:ASP:H	1:37:A:ALA:HA	8	0.69
(3,38)	1:74:A:VAL:N	1:91:A:LYS:O	1	0.68
(1,1778)	1:149:A:ASN:HB2	1:151:A:ARG:HA	10	0.68
(1,1778)	1:149:A:ASN:HB3	1:151:A:ARG:HA	10	0.68
(1,1718)	1:144:A:SER:H	1:146:A:LEU:H	2	0.68
(1,1665)	1:141:A:SER:HA	1:144:A:SER:H	2	0.68
(1,1555)	1:132:A:SER:H	1:136:A:ASP:HA	9	0.68
(1,970)	1:79:A:GLN:HA	1:86:A:THR:HB	7	0.68
(1,959)	1:78:A:VAL:HG21	1:87:A:SER:HA	9	0.68
(1,959)	1:78:A:VAL:HG22	1:87:A:SER:HA	9	0.68
(1,959)	1:78:A:VAL:HG23	1:87:A:SER:HA	9	0.68
(1,921)	1:76:A:VAL:HG11	1:143:A:LYS:HG2	10	0.68
(1,921)	1:76:A:VAL:HG11	1:143:A:LYS:HG3	10	0.68
(1,921)	1:76:A:VAL:HG12	1:143:A:LYS:HG2	10	0.68
(1,921)	1:76:A:VAL:HG12	1:143:A:LYS:HG3	10	0.68
(1,921)	1:76:A:VAL:HG13	1:143:A:LYS:HG2	10	0.68
(1,921)	1:76:A:VAL:HG13	1:143:A:LYS:HG3	10	0.68
(1,921)	1:76:A:VAL:HG21	1:143:A:LYS:HG2	10	0.68
(1,921)	1:76:A:VAL:HG21	1:143:A:LYS:HG3	10	0.68
(1,921)	1:76:A:VAL:HG22	1:143:A:LYS:HG2	10	0.68
(1,921)	1:76:A:VAL:HG22	1:143:A:LYS:HG3	10	0.68
(1,921)	1:76:A:VAL:HG23	1:143:A:LYS:HG2	10	0.68
(1,921)	1:76:A:VAL:HG23	1:143:A:LYS:HG3	10	0.68
(1,577)	1:42:A:LYS:HB2	1:53:A:PHE:HA	1	0.68
(1,577)	1:42:A:LYS:HB3	1:53:A:PHE:HA	1	0.68
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG21	9	0.68
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG22	9	0.68
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG23	9	0.68
(1,521)	1:33:A:LYS:HE2	1:35:A:ASP:H	9	0.68
(1,521)	1:33:A:LYS:HE3	1:35:A:ASP:H	9	0.68
(1,331)	1:18:A:LEU:HD11	1:92:A:VAL:HA	7	0.68
(1,331)	1:18:A:LEU:HD12	1:92:A:VAL:HA	7	0.68
(1,331)	1:18:A:LEU:HD13	1:92:A:VAL:HA	7	0.68
(1,331)	1:18:A:LEU:HD21	1:92:A:VAL:HA	7	0.68
(1,331)	1:18:A:LEU:HD22	1:92:A:VAL:HA	7	0.68
(1,331)	1:18:A:LEU:HD23	1:92:A:VAL:HA	7	0.68
(1,277)	1:16:A:ASP:HB2	1:18:A:LEU:H	9	0.68
(1,135)	1:8:A:ASP:HB2	1:39:A:VAL:HB	2	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,135)	1:8:A:ASP:HB3	1:39:A:VAL:HB	2	0.68
(1,123)	1:8:A:ASP:HB2	1:39:A:VAL:HA	10	0.68
(1,117)	1:8:A:ASP:H	1:39:A:VAL:HB	4	0.68
(1,97)	1:7:A:VAL:HG11	1:116:A:ALA:H	1	0.68
(1,97)	1:7:A:VAL:HG12	1:116:A:ALA:H	1	0.68
(1,97)	1:7:A:VAL:HG13	1:116:A:ALA:H	1	0.68
(1,97)	1:7:A:VAL:HG21	1:116:A:ALA:H	1	0.68
(1,97)	1:7:A:VAL:HG22	1:116:A:ALA:H	1	0.68
(1,97)	1:7:A:VAL:HG23	1:116:A:ALA:H	1	0.68
(1,97)	1:7:A:VAL:HG11	1:116:A:ALA:H	2	0.68
(1,97)	1:7:A:VAL:HG12	1:116:A:ALA:H	2	0.68
(1,97)	1:7:A:VAL:HG13	1:116:A:ALA:H	2	0.68
(1,97)	1:7:A:VAL:HG21	1:116:A:ALA:H	2	0.68
(1,97)	1:7:A:VAL:HG22	1:116:A:ALA:H	2	0.68
(1,97)	1:7:A:VAL:HG23	1:116:A:ALA:H	2	0.68
(1,93)	1:7:A:VAL:HG21	1:38:A:ILE:H	5	0.68
(1,93)	1:7:A:VAL:HG22	1:38:A:ILE:H	5	0.68
(1,93)	1:7:A:VAL:HG23	1:38:A:ILE:H	5	0.68
(1,83)	1:7:A:VAL:HG11	1:120:A:SER:HA	5	0.68
(1,83)	1:7:A:VAL:HG12	1:120:A:SER:HA	5	0.68
(1,83)	1:7:A:VAL:HG13	1:120:A:SER:HA	5	0.68
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG11	3	0.68
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG12	3	0.68
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG13	3	0.68
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG21	3	0.68
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG22	3	0.68
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG23	3	0.68
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD2	2	0.67
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD3	2	0.67
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD2	2	0.67
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD3	2	0.67
(1,1443)	1:118:A:LYS:HE3	1:119:A:ALA:H	3	0.67
(1,1344)	1:111:A:ALA:HA	1:115:A:ARG:H	7	0.67
(1,1315)	1:109:A:LEU:HA	1:112:A:SER:HB2	8	0.67
(1,1315)	1:109:A:LEU:HA	1:112:A:SER:HB3	8	0.67
(1,1186)	1:99:A:PRO:HG2	1:132:A:SER:HA	4	0.67
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD11	7	0.67
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD12	7	0.67
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD13	7	0.67
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD21	7	0.67
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD22	7	0.67
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD23	7	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD11	7	0.67
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD12	7	0.67
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD13	7	0.67
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD21	7	0.67
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD22	7	0.67
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD23	7	0.67
(1,968)	1:79:A:GLN:HA	1:85:A:GLY:H	4	0.67
(1,962)	1:78:A:VAL:HG11	1:87:A:SER:HB2	2	0.67
(1,962)	1:78:A:VAL:HG11	1:87:A:SER:HB3	2	0.67
(1,962)	1:78:A:VAL:HG12	1:87:A:SER:HB2	2	0.67
(1,962)	1:78:A:VAL:HG12	1:87:A:SER:HB3	2	0.67
(1,962)	1:78:A:VAL:HG13	1:87:A:SER:HB2	2	0.67
(1,962)	1:78:A:VAL:HG13	1:87:A:SER:HB3	2	0.67
(1,962)	1:78:A:VAL:HG21	1:87:A:SER:HB2	2	0.67
(1,962)	1:78:A:VAL:HG21	1:87:A:SER:HB3	2	0.67
(1,962)	1:78:A:VAL:HG22	1:87:A:SER:HB2	2	0.67
(1,962)	1:78:A:VAL:HG22	1:87:A:SER:HB3	2	0.67
(1,962)	1:78:A:VAL:HG23	1:87:A:SER:HB2	2	0.67
(1,962)	1:78:A:VAL:HG23	1:87:A:SER:HB3	2	0.67
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG21	4	0.67
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG22	4	0.67
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG23	4	0.67
(1,579)	1:42:A:LYS:HG2	1:56:A:GLU:HB2	4	0.67
(1,579)	1:42:A:LYS:HG2	1:56:A:GLU:HB3	4	0.67
(1,579)	1:42:A:LYS:HG3	1:56:A:GLU:HB2	4	0.67
(1,579)	1:42:A:LYS:HG3	1:56:A:GLU:HB3	4	0.67
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB1	5	0.67
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB2	5	0.67
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB3	5	0.67
(1,523)	1:33:A:LYS:HG2	1:36:A:THR:HA	9	0.67
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD11	7	0.67
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD12	7	0.67
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD13	7	0.67
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD21	7	0.67
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD22	7	0.67
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD23	7	0.67
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD11	7	0.67
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD12	7	0.67
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD13	7	0.67
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD21	7	0.67
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD22	7	0.67
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD23	7	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,507)	1:31:A:ILE:HG12	1:109:A:LEU:HB2	3	0.67
(1,507)	1:31:A:ILE:HG12	1:109:A:LEU:HB3	3	0.67
(1,507)	1:31:A:ILE:HG13	1:109:A:LEU:HB2	3	0.67
(1,507)	1:31:A:ILE:HG13	1:109:A:LEU:HB3	3	0.67
(1,439)	1:28:A:ILE:HB	1:42:A:LYS:HD2	1	0.67
(1,439)	1:28:A:ILE:HB	1:42:A:LYS:HD3	1	0.67
(1,335)	1:19:A:HIS:HA	1:21:A:LYS:H	3	0.67
(1,137)	1:8:A:ASP:HB2	1:9:A:PRO:HA	1	0.67
(1,137)	1:8:A:ASP:HB3	1:9:A:PRO:HA	1	0.67
(1,72)	1:7:A:VAL:HB	1:117:A:LEU:HA	3	0.67
(3,25)	1:68:A:ARG:H	1:97:A:TYR:O	9	0.66
(1,1651)	1:140:A:LYS:HD3	1:142:A:VAL:H	7	0.66
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE2	9	0.66
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE3	9	0.66
(1,1234)	1:104:A:VAL:HG21	1:107:A:ARG:H	7	0.66
(1,1234)	1:104:A:VAL:HG22	1:107:A:ARG:H	7	0.66
(1,1234)	1:104:A:VAL:HG23	1:107:A:ARG:H	7	0.66
(1,1162)	1:96:A:GLN:HG2	1:130:A:GLN:HA	10	0.66
(1,1162)	1:96:A:GLN:HG3	1:130:A:GLN:HA	10	0.66
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB2	3	0.66
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB3	3	0.66
(1,987)	1:80:A:ARG:H	1:85:A:GLY:H	4	0.66
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG21	1	0.66
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG22	1	0.66
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG23	1	0.66
(1,945)	1:78:A:VAL:H	1:86:A:THR:HB	7	0.66
(1,897)	1:75:A:GLU:HG3	1:89:A:LEU:H	2	0.66
(1,786)	1:61:A:VAL:HG21	1:66:A:GLU:HB2	10	0.66
(1,786)	1:61:A:VAL:HG22	1:66:A:GLU:HB2	10	0.66
(1,786)	1:61:A:VAL:HG23	1:66:A:GLU:HB2	10	0.66
(1,786)	1:61:A:VAL:HG21	1:66:A:GLU:HB3	10	0.66
(1,786)	1:61:A:VAL:HG22	1:66:A:GLU:HB3	10	0.66
(1,786)	1:61:A:VAL:HG23	1:66:A:GLU:HB3	10	0.66
(1,702)	1:55:A:GLU:HA	1:58:A:LYS:HB2	4	0.66
(1,702)	1:55:A:GLU:HA	1:58:A:LYS:HB3	4	0.66
(1,1777)	1:149:A:ASN:HB2	1:151:A:ARG:H	9	0.65
(1,1777)	1:149:A:ASN:HB3	1:151:A:ARG:H	9	0.65
(1,1744)	1:146:A:LEU:HA	1:150:A:GLN:HA	7	0.65
(1,1726)	1:144:A:SER:HB3	1:146:A:LEU:H	7	0.65
(1,1726)	1:144:A:SER:HB3	1:146:A:LEU:H	10	0.65
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG11	5	0.65
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG12	5	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG13	5	0.65
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG21	5	0.65
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG22	5	0.65
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG23	5	0.65
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG11	5	0.65
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG12	5	0.65
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG13	5	0.65
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG21	5	0.65
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG22	5	0.65
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG23	5	0.65
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	10	0.65
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	10	0.65
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	10	0.65
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	10	0.65
(1,1224)	1:104:A:VAL:HB	1:106:A:ARG:H	6	0.65
(1,1122)	1:94:A:PHE:HB2	1:118:A:LYS:HE2	5	0.65
(1,1122)	1:94:A:PHE:HB2	1:118:A:LYS:HE3	5	0.65
(1,1122)	1:94:A:PHE:HB3	1:118:A:LYS:HE2	5	0.65
(1,1122)	1:94:A:PHE:HB3	1:118:A:LYS:HE3	5	0.65
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG21	10	0.65
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG22	10	0.65
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG23	10	0.65
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG2	1	0.65
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG3	1	0.65
(1,892)	1:75:A:GLU:HG2	1:90:A:ASN:HA	3	0.65
(1,820)	1:69:A:TYR:HA	1:96:A:GLN:HG2	6	0.65
(1,820)	1:69:A:TYR:HA	1:96:A:GLN:HG3	6	0.65
(1,790)	1:61:A:VAL:HG11	1:66:A:GLU:HG2	8	0.65
(1,790)	1:61:A:VAL:HG11	1:66:A:GLU:HG3	8	0.65
(1,790)	1:61:A:VAL:HG12	1:66:A:GLU:HG2	8	0.65
(1,790)	1:61:A:VAL:HG12	1:66:A:GLU:HG3	8	0.65
(1,790)	1:61:A:VAL:HG13	1:66:A:GLU:HG2	8	0.65
(1,790)	1:61:A:VAL:HG13	1:66:A:GLU:HG3	8	0.65
(1,790)	1:61:A:VAL:HG21	1:66:A:GLU:HG2	8	0.65
(1,790)	1:61:A:VAL:HG21	1:66:A:GLU:HG3	8	0.65
(1,790)	1:61:A:VAL:HG22	1:66:A:GLU:HG2	8	0.65
(1,790)	1:61:A:VAL:HG22	1:66:A:GLU:HG3	8	0.65
(1,790)	1:61:A:VAL:HG23	1:66:A:GLU:HG2	8	0.65
(1,790)	1:61:A:VAL:HG23	1:66:A:GLU:HG3	8	0.65
(1,756)	1:58:A:LYS:HD3	1:59:A:LYS:H	6	0.65
(1,609)	1:49:A:PRO:HG2	1:51:A:ALA:H	6	0.65
(1,609)	1:49:A:PRO:HG3	1:51:A:ALA:H	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,507)	1:31:A:ILE:HG12	1:109:A:LEU:HB2	5	0.65
(1,507)	1:31:A:ILE:HG12	1:109:A:LEU:HB3	5	0.65
(1,507)	1:31:A:ILE:HG13	1:109:A:LEU:HB2	5	0.65
(1,507)	1:31:A:ILE:HG13	1:109:A:LEU:HB3	5	0.65
(1,498)	1:31:A:ILE:HG13	1:38:A:ILE:HA	5	0.65
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG2	7	0.65
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG3	7	0.65
(1,454)	1:28:A:ILE:HG12	1:41:A:GLU:HG2	6	0.65
(1,454)	1:28:A:ILE:HG12	1:41:A:GLU:HG3	6	0.65
(1,454)	1:28:A:ILE:HG13	1:41:A:GLU:HG2	6	0.65
(1,454)	1:28:A:ILE:HG13	1:41:A:GLU:HG3	6	0.65
(1,366)	1:25:A:SER:H	1:73:A:ASP:H	8	0.65
(1,345)	1:21:A:LYS:H	1:21:A:LYS:HE2	5	0.65
(1,345)	1:21:A:LYS:H	1:21:A:LYS:HE3	5	0.65
(1,117)	1:8:A:ASP:H	1:39:A:VAL:HB	9	0.65
(1,113)	1:8:A:ASP:H	1:37:A:ALA:HA	2	0.65
(1,55)	1:6:A:LYS:HE2	1:7:A:VAL:H	9	0.65
(1,55)	1:6:A:LYS:HE3	1:7:A:VAL:H	9	0.65
(1,48)	1:6:A:LYS:H	1:6:A:LYS:HE2	4	0.65
(1,48)	1:6:A:LYS:H	1:6:A:LYS:HE3	4	0.65
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG11	10	0.65
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG12	10	0.65
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG13	10	0.65
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG21	10	0.65
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG22	10	0.65
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG23	10	0.65
(1,1718)	1:144:A:SER:H	1:146:A:LEU:H	4	0.64
(1,1664)	1:141:A:SER:HA	1:143:A:LYS:H	7	0.64
(1,1651)	1:140:A:LYS:HD3	1:142:A:VAL:H	4	0.64
(1,1443)	1:118:A:LYS:HE3	1:119:A:ALA:H	5	0.64
(1,1241)	1:104:A:VAL:HG11	1:107:A:ARG:HB2	9	0.64
(1,1241)	1:104:A:VAL:HG11	1:107:A:ARG:HB3	9	0.64
(1,1241)	1:104:A:VAL:HG12	1:107:A:ARG:HB2	9	0.64
(1,1241)	1:104:A:VAL:HG12	1:107:A:ARG:HB3	9	0.64
(1,1241)	1:104:A:VAL:HG13	1:107:A:ARG:HB2	9	0.64
(1,1241)	1:104:A:VAL:HG13	1:107:A:ARG:HB3	9	0.64
(1,1241)	1:104:A:VAL:HG21	1:107:A:ARG:HB2	9	0.64
(1,1241)	1:104:A:VAL:HG21	1:107:A:ARG:HB3	9	0.64
(1,1241)	1:104:A:VAL:HG22	1:107:A:ARG:HB2	9	0.64
(1,1241)	1:104:A:VAL:HG22	1:107:A:ARG:HB3	9	0.64
(1,1241)	1:104:A:VAL:HG23	1:107:A:ARG:HB2	9	0.64
(1,1241)	1:104:A:VAL:HG23	1:107:A:ARG:HB3	9	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD11	7	0.64
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD12	7	0.64
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD13	7	0.64
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD21	7	0.64
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD22	7	0.64
(1,1075)	1:92:A:VAL:HG11	1:146:A:LEU:HD23	7	0.64
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD11	7	0.64
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD12	7	0.64
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD13	7	0.64
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD21	7	0.64
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD22	7	0.64
(1,1075)	1:92:A:VAL:HG12	1:146:A:LEU:HD23	7	0.64
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD11	7	0.64
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD12	7	0.64
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD13	7	0.64
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD21	7	0.64
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD22	7	0.64
(1,1075)	1:92:A:VAL:HG13	1:146:A:LEU:HD23	7	0.64
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD11	7	0.64
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD12	7	0.64
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD13	7	0.64
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD21	7	0.64
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD22	7	0.64
(1,1075)	1:92:A:VAL:HG21	1:146:A:LEU:HD23	7	0.64
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD11	7	0.64
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD12	7	0.64
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD13	7	0.64
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD21	7	0.64
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD22	7	0.64
(1,1075)	1:92:A:VAL:HG22	1:146:A:LEU:HD23	7	0.64
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD11	7	0.64
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD12	7	0.64
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD13	7	0.64
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD21	7	0.64
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD22	7	0.64
(1,1075)	1:92:A:VAL:HG23	1:146:A:LEU:HD23	7	0.64
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD11	6	0.64
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD12	6	0.64
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD13	6	0.64
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD21	6	0.64
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD22	6	0.64
(1,1002)	1:81:A:GLN:HG2	1:89:A:LEU:HD23	6	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD11	6	0.64
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD12	6	0.64
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD13	6	0.64
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD21	6	0.64
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD22	6	0.64
(1,1002)	1:81:A:GLN:HG3	1:89:A:LEU:HD23	6	0.64
(1,994)	1:80:A:ARG:HG2	1:86:A:THR:HA	7	0.64
(1,994)	1:80:A:ARG:HG3	1:86:A:THR:HA	7	0.64
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG21	10	0.64
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG22	10	0.64
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG23	10	0.64
(1,889)	1:75:A:GLU:HG2	1:88:A:THR:HB	9	0.64
(1,820)	1:69:A:TYR:HA	1:96:A:GLN:HG2	2	0.64
(1,820)	1:69:A:TYR:HA	1:96:A:GLN:HG3	2	0.64
(1,784)	1:61:A:VAL:HG11	1:66:A:GLU:HG2	9	0.64
(1,784)	1:61:A:VAL:HG12	1:66:A:GLU:HG2	9	0.64
(1,784)	1:61:A:VAL:HG13	1:66:A:GLU:HG2	9	0.64
(1,784)	1:61:A:VAL:HG11	1:66:A:GLU:HG3	9	0.64
(1,784)	1:61:A:VAL:HG12	1:66:A:GLU:HG3	9	0.64
(1,784)	1:61:A:VAL:HG13	1:66:A:GLU:HG3	9	0.64
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE2	10	0.64
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE3	10	0.64
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE2	10	0.64
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE3	10	0.64
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB2	10	0.64
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB3	10	0.64
(1,498)	1:31:A:ILE:HG13	1:38:A:ILE:HA	10	0.64
(1,453)	1:28:A:ILE:HG12	1:41:A:GLU:HB2	9	0.64
(1,453)	1:28:A:ILE:HG12	1:41:A:GLU:HB3	9	0.64
(1,453)	1:28:A:ILE:HG13	1:41:A:GLU:HB2	9	0.64
(1,453)	1:28:A:ILE:HG13	1:41:A:GLU:HB3	9	0.64
(1,345)	1:21:A:LYS:H	1:21:A:LYS:HE2	2	0.64
(1,345)	1:21:A:LYS:H	1:21:A:LYS:HE3	2	0.64
(1,310)	1:18:A:LEU:HA	1:20:A:ASN:H	6	0.64
(1,302)	1:17:A:LEU:HD21	1:19:A:HIS:H	1	0.64
(1,302)	1:17:A:LEU:HD22	1:19:A:HIS:H	1	0.64
(1,302)	1:17:A:LEU:HD23	1:19:A:HIS:H	1	0.64
(1,275)	1:16:A:ASP:HA	1:20:A:ASN:H	10	0.64
(1,137)	1:8:A:ASP:HB2	1:9:A:PRO:HA	10	0.64
(1,137)	1:8:A:ASP:HB3	1:9:A:PRO:HA	10	0.64
(1,64)	1:7:A:VAL:HA	1:117:A:LEU:HA	6	0.64
(1,45)	1:6:A:LYS:H	1:37:A:ALA:HB1	5	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:6:A:LYS:H	1:37:A:ALA:HB2	5	0.64
(1,45)	1:6:A:LYS:H	1:37:A:ALA:HB3	5	0.64
(1,20)	1:4:A:GLY:H	1:5:A:VAL:HB	10	0.64
(3,8)	1:13:A:ASN:O	1:17:A:LEU:N	10	0.63
(1,1775)	1:149:A:ASN:HB3	1:152:A:ILE:HG21	10	0.63
(1,1775)	1:149:A:ASN:HB3	1:152:A:ILE:HG22	10	0.63
(1,1775)	1:149:A:ASN:HB3	1:152:A:ILE:HG23	10	0.63
(1,1566)	1:133:A:GLU:HG2	1:135:A:SER:H	8	0.63
(1,1566)	1:133:A:GLU:HG3	1:135:A:SER:H	8	0.63
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	9	0.63
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	9	0.63
(1,1333)	1:110:A:TYR:HA	1:114:A:VAL:H	1	0.63
(1,1305)	1:108:A:MET:HG2	1:112:A:SER:H	7	0.63
(1,1305)	1:108:A:MET:HG3	1:112:A:SER:H	7	0.63
(1,1293)	1:108:A:MET:HA	1:110:A:TYR:H	8	0.63
(1,1234)	1:104:A:VAL:HG21	1:107:A:ARG:H	4	0.63
(1,1234)	1:104:A:VAL:HG22	1:107:A:ARG:H	4	0.63
(1,1234)	1:104:A:VAL:HG23	1:107:A:ARG:H	4	0.63
(1,1027)	1:86:A:THR:HB	1:87:A:SER:H	6	0.63
(1,987)	1:80:A:ARG:H	1:85:A:GLY:H	9	0.63
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG21	5	0.63
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG22	5	0.63
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG23	5	0.63
(1,947)	1:78:A:VAL:H	1:87:A:SER:H	3	0.63
(1,947)	1:78:A:VAL:H	1:87:A:SER:H	9	0.63
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG2	4	0.63
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG3	4	0.63
(1,892)	1:75:A:GLU:HG2	1:90:A:ASN:HA	9	0.63
(1,790)	1:61:A:VAL:HG11	1:66:A:GLU:HG2	9	0.63
(1,790)	1:61:A:VAL:HG11	1:66:A:GLU:HG3	9	0.63
(1,790)	1:61:A:VAL:HG12	1:66:A:GLU:HG2	9	0.63
(1,790)	1:61:A:VAL:HG12	1:66:A:GLU:HG3	9	0.63
(1,790)	1:61:A:VAL:HG13	1:66:A:GLU:HG2	9	0.63
(1,790)	1:61:A:VAL:HG13	1:66:A:GLU:HG3	9	0.63
(1,790)	1:61:A:VAL:HG21	1:66:A:GLU:HG2	9	0.63
(1,790)	1:61:A:VAL:HG21	1:66:A:GLU:HG3	9	0.63
(1,790)	1:61:A:VAL:HG22	1:66:A:GLU:HG2	9	0.63
(1,790)	1:61:A:VAL:HG22	1:66:A:GLU:HG3	9	0.63
(1,790)	1:61:A:VAL:HG23	1:66:A:GLU:HG2	9	0.63
(1,790)	1:61:A:VAL:HG23	1:66:A:GLU:HG3	9	0.63
(1,705)	1:55:A:GLU:HA	1:59:A:LYS:HB3	4	0.63
(1,237)	1:14:A:ALA:HA	1:18:A:LEU:H	3	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG11	8	0.63
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG12	8	0.63
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG13	8	0.63
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG21	8	0.63
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG22	8	0.63
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG23	8	0.63
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD11	9	0.63
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD12	9	0.63
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD13	9	0.63
(1,14)	1:3:A:SER:H	1:113:A:SER:HA	2	0.63
(1,4)	1:1:A:MET:HA	1:114:A:VAL:HB	10	0.63
(3,10)	1:26:A:TYR:N	1:44:A:GLY:O	4	0.62
(1,1777)	1:149:A:ASN:HB2	1:151:A:ARG:H	6	0.62
(1,1777)	1:149:A:ASN:HB3	1:151:A:ARG:H	6	0.62
(1,1777)	1:149:A:ASN:HB2	1:151:A:ARG:H	7	0.62
(1,1777)	1:149:A:ASN:HB3	1:151:A:ARG:H	7	0.62
(1,1774)	1:149:A:ASN:HB3	1:152:A:ILE:HD11	7	0.62
(1,1774)	1:149:A:ASN:HB3	1:152:A:ILE:HD12	7	0.62
(1,1774)	1:149:A:ASN:HB3	1:152:A:ILE:HD13	7	0.62
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD11	4	0.62
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD12	4	0.62
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD13	4	0.62
(1,1725)	1:144:A:SER:HB3	1:145:A:ASP:H	2	0.62
(1,1189)	1:99:A:PRO:HG3	1:102:A:ALA:HA	7	0.62
(1,1174)	1:99:A:PRO:HA	1:102:A:ALA:H	6	0.62
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD11	3	0.62
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD12	3	0.62
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD13	3	0.62
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD21	3	0.62
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD22	3	0.62
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD23	3	0.62
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD11	3	0.62
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD12	3	0.62
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD13	3	0.62
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD21	3	0.62
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD22	3	0.62
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD23	3	0.62
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG21	2	0.62
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG22	2	0.62
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG23	2	0.62
(1,970)	1:79:A:GLN:HA	1:86:A:THR:HB	1	0.62
(1,874)	1:75:A:GLU:HA	1:88:A:THR:HG21	6	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,874)	1:75:A:GLU:HA	1:88:A:THR:HG22	6	0.62
(1,874)	1:75:A:GLU:HA	1:88:A:THR:HG23	6	0.62
(1,819)	1:69:A:TYR:HA	1:96:A:GLN:HB3	7	0.62
(1,749)	1:58:A:LYS:HA	1:62:A:GLU:H	1	0.62
(1,737)	1:57:A:MET:HG2	1:60:A:LEU:HG	6	0.62
(1,737)	1:57:A:MET:HG3	1:60:A:LEU:HG	6	0.62
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG2	8	0.62
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG3	8	0.62
(1,509)	1:31:A:ILE:HG21	1:109:A:LEU:H	1	0.62
(1,509)	1:31:A:ILE:HG22	1:109:A:LEU:H	1	0.62
(1,509)	1:31:A:ILE:HG23	1:109:A:LEU:H	1	0.62
(1,428)	1:28:A:ILE:H	1:42:A:LYS:HD2	3	0.62
(1,428)	1:28:A:ILE:H	1:42:A:LYS:HD3	3	0.62
(1,402)	1:27:A:ILE:HB	1:43:A:VAL:HA	5	0.62
(1,387)	1:26:A:TYR:HB2	1:73:A:ASP:H	6	0.62
(1,387)	1:26:A:TYR:HB3	1:73:A:ASP:H	6	0.62
(1,158)	1:10:A:SER:HB3	1:12:A:LYS:H	5	0.62
(1,1799)	1:151:A:ARG:H	1:152:A:ILE:H	6	0.61
(1,1726)	1:144:A:SER:HB3	1:146:A:LEU:H	8	0.61
(1,1704)	1:143:A:LYS:HA	1:146:A:LEU:HB2	6	0.61
(1,1704)	1:143:A:LYS:HA	1:146:A:LEU:HB3	6	0.61
(1,1703)	1:143:A:LYS:HA	1:146:A:LEU:HA	6	0.61
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG11	6	0.61
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG12	6	0.61
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG13	6	0.61
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG21	6	0.61
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG22	6	0.61
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG23	6	0.61
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG11	6	0.61
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG12	6	0.61
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG13	6	0.61
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG21	6	0.61
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG22	6	0.61
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG23	6	0.61
(1,1344)	1:111:A:ALA:HA	1:115:A:ARG:H	6	0.61
(1,1172)	1:98:A:CYS:HB2	1:107:A:ARG:HA	10	0.61
(1,1172)	1:98:A:CYS:HB3	1:107:A:ARG:HA	10	0.61
(1,1064)	1:91:A:LYS:HD2	1:92:A:VAL:H	7	0.61
(1,1064)	1:91:A:LYS:HD3	1:92:A:VAL:H	7	0.61
(1,1015)	1:84:A:GLU:H	1:85:A:GLY:H	9	0.61
(1,968)	1:79:A:GLN:HA	1:85:A:GLY:H	9	0.61
(1,960)	1:78:A:VAL:HG21	1:87:A:SER:HB2	4	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,960)	1:78:A:VAL:HG22	1:87:A:SER:HB2	4	0.61
(1,960)	1:78:A:VAL:HG23	1:87:A:SER:HB2	4	0.61
(1,960)	1:78:A:VAL:HG21	1:87:A:SER:HB3	4	0.61
(1,960)	1:78:A:VAL:HG22	1:87:A:SER:HB3	4	0.61
(1,960)	1:78:A:VAL:HG23	1:87:A:SER:HB3	4	0.61
(1,692)	1:54:A:VAL:HG11	1:58:A:LYS:HE2	8	0.61
(1,692)	1:54:A:VAL:HG11	1:58:A:LYS:HE3	8	0.61
(1,692)	1:54:A:VAL:HG12	1:58:A:LYS:HE2	8	0.61
(1,692)	1:54:A:VAL:HG12	1:58:A:LYS:HE3	8	0.61
(1,692)	1:54:A:VAL:HG13	1:58:A:LYS:HE2	8	0.61
(1,692)	1:54:A:VAL:HG13	1:58:A:LYS:HE3	8	0.61
(1,692)	1:54:A:VAL:HG21	1:58:A:LYS:HE2	8	0.61
(1,692)	1:54:A:VAL:HG21	1:58:A:LYS:HE3	8	0.61
(1,692)	1:54:A:VAL:HG22	1:58:A:LYS:HE2	8	0.61
(1,692)	1:54:A:VAL:HG22	1:58:A:LYS:HE3	8	0.61
(1,692)	1:54:A:VAL:HG23	1:58:A:LYS:HE2	8	0.61
(1,692)	1:54:A:VAL:HG23	1:58:A:LYS:HE3	8	0.61
(1,685)	1:54:A:VAL:HG11	1:138:A:ASP:HA	8	0.61
(1,685)	1:54:A:VAL:HG12	1:138:A:ASP:HA	8	0.61
(1,685)	1:54:A:VAL:HG13	1:138:A:ASP:HA	8	0.61
(1,685)	1:54:A:VAL:HG21	1:138:A:ASP:HA	8	0.61
(1,685)	1:54:A:VAL:HG22	1:138:A:ASP:HA	8	0.61
(1,685)	1:54:A:VAL:HG23	1:138:A:ASP:HA	8	0.61
(1,611)	1:49:A:PRO:HG2	1:52:A:GLU:H	2	0.61
(1,611)	1:49:A:PRO:HG3	1:52:A:GLU:H	2	0.61
(1,611)	1:49:A:PRO:HG2	1:52:A:GLU:H	9	0.61
(1,611)	1:49:A:PRO:HG3	1:52:A:GLU:H	9	0.61
(1,605)	1:49:A:PRO:HB3	1:51:A:ALA:HB1	4	0.61
(1,605)	1:49:A:PRO:HB3	1:51:A:ALA:HB2	4	0.61
(1,605)	1:49:A:PRO:HB3	1:51:A:ALA:HB3	4	0.61
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB1	7	0.61
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB2	7	0.61
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB3	7	0.61
(1,523)	1:33:A:LYS:HG2	1:36:A:THR:HA	1	0.61
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD11	3	0.61
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD12	3	0.61
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD13	3	0.61
(1,440)	1:28:A:ILE:HB	1:70:A:ALA:HB1	4	0.61
(1,440)	1:28:A:ILE:HB	1:70:A:ALA:HB2	4	0.61
(1,440)	1:28:A:ILE:HB	1:70:A:ALA:HB3	4	0.61
(1,434)	1:28:A:ILE:HB	1:41:A:GLU:HA	10	0.61
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD2	4	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD3	4	0.61
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD2	4	0.61
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD3	4	0.61
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD2	4	0.61
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD3	4	0.61
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD2	4	0.61
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD3	4	0.61
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD2	4	0.61
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD3	4	0.61
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD2	4	0.61
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD3	4	0.61
(1,137)	1:8:A:ASP:HB2	1:9:A:PRO:HA	5	0.61
(1,137)	1:8:A:ASP:HB3	1:9:A:PRO:HA	5	0.61
(1,117)	1:8:A:ASP:H	1:39:A:VAL:HB	7	0.61
(1,116)	1:8:A:ASP:H	1:39:A:VAL:HA	3	0.61
(1,65)	1:7:A:VAL:HA	1:37:A:ALA:HA	9	0.61
(1,27)	1:5:A:VAL:HA	1:36:A:THR:HA	4	0.61
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD11	8	0.6
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD12	8	0.6
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD13	8	0.6
(1,1664)	1:141:A:SER:HA	1:143:A:LYS:H	8	0.6
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB2	2	0.6
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB2	2	0.6
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB2	2	0.6
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB3	2	0.6
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB3	2	0.6
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB3	2	0.6
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB2	2	0.6
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB3	2	0.6
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB2	2	0.6
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB3	2	0.6
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB2	2	0.6
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB3	2	0.6
(1,1316)	1:109:A:LEU:HA	1:113:A:SER:H	1	0.6
(1,1260)	1:105:A:ARG:HD2	1:106:A:ARG:H	3	0.6
(1,1260)	1:105:A:ARG:HD3	1:106:A:ARG:H	3	0.6
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG11	1	0.6
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG12	1	0.6
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG13	1	0.6
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG21	1	0.6
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG22	1	0.6
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG23	1	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG11	1	0.6
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG12	1	0.6
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG13	1	0.6
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG21	1	0.6
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG22	1	0.6
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG23	1	0.6
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB2	9	0.6
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB3	9	0.6
(1,1104)	1:93:A:ILE:HG12	1:127:A:PHE:HB2	10	0.6
(1,1104)	1:93:A:ILE:HG12	1:127:A:PHE:HB3	10	0.6
(1,1104)	1:93:A:ILE:HG13	1:127:A:PHE:HB2	10	0.6
(1,1104)	1:93:A:ILE:HG13	1:127:A:PHE:HB3	10	0.6
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG21	1	0.6
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG22	1	0.6
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG23	1	0.6
(1,894)	1:75:A:GLU:HG3	1:76:A:VAL:H	2	0.6
(1,887)	1:75:A:GLU:HB3	1:89:A:LEU:H	1	0.6
(1,705)	1:55:A:GLU:HA	1:59:A:LYS:HB3	5	0.6
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB2	7	0.6
(1,578)	1:42:A:LYS:HD2	1:56:A:GLU:HB3	7	0.6
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB2	7	0.6
(1,578)	1:42:A:LYS:HD3	1:56:A:GLU:HB3	7	0.6
(1,489)	1:31:A:ILE:HA	1:38:A:ILE:HD11	2	0.6
(1,489)	1:31:A:ILE:HA	1:38:A:ILE:HD12	2	0.6
(1,489)	1:31:A:ILE:HA	1:38:A:ILE:HD13	2	0.6
(1,453)	1:28:A:ILE:HG12	1:41:A:GLU:HB2	8	0.6
(1,453)	1:28:A:ILE:HG12	1:41:A:GLU:HB3	8	0.6
(1,453)	1:28:A:ILE:HG13	1:41:A:GLU:HB2	8	0.6
(1,453)	1:28:A:ILE:HG13	1:41:A:GLU:HB3	8	0.6
(1,402)	1:27:A:ILE:HB	1:43:A:VAL:HA	6	0.6
(1,331)	1:18:A:LEU:HD11	1:92:A:VAL:HA	6	0.6
(1,331)	1:18:A:LEU:HD12	1:92:A:VAL:HA	6	0.6
(1,331)	1:18:A:LEU:HD13	1:92:A:VAL:HA	6	0.6
(1,331)	1:18:A:LEU:HD21	1:92:A:VAL:HA	6	0.6
(1,331)	1:18:A:LEU:HD22	1:92:A:VAL:HA	6	0.6
(1,331)	1:18:A:LEU:HD23	1:92:A:VAL:HA	6	0.6
(1,323)	1:18:A:LEU:HD21	1:71:A:ALA:HA	7	0.6
(1,323)	1:18:A:LEU:HD22	1:71:A:ALA:HA	7	0.6
(1,323)	1:18:A:LEU:HD23	1:71:A:ALA:HA	7	0.6
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD11	10	0.6
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD12	10	0.6
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD13	10	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD21	10	0.6
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD22	10	0.6
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD23	10	0.6
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD11	10	0.6
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD12	10	0.6
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD13	10	0.6
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD21	10	0.6
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD22	10	0.6
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD23	10	0.6
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD11	10	0.6
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD12	10	0.6
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD13	10	0.6
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG11	9	0.59
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG12	9	0.59
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG13	9	0.59
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG21	9	0.59
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG22	9	0.59
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG23	9	0.59
(1,1441)	1:118:A:LYS:HE2	1:119:A:ALA:H	7	0.59
(1,1316)	1:109:A:LEU:HA	1:113:A:SER:H	7	0.59
(1,1165)	1:97:A:TYR:HA	1:131:A:ALA:HA	9	0.59
(1,752)	1:58:A:LYS:HB3	1:59:A:LYS:H	4	0.59
(1,654)	1:53:A:PHE:HA	1:55:A:GLU:H	6	0.59
(1,524)	1:33:A:LYS:HG2	1:36:A:THR:HB	5	0.59
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB1	5	0.59
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB2	5	0.59
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB3	5	0.59
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB1	5	0.59
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB2	5	0.59
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB3	5	0.59
(1,256)	1:15:A:TYR:HB2	1:121:A:LEU:HG	9	0.59
(1,225)	1:13:A:ASN:HA	1:17:A:LEU:H	2	0.59
(1,206)	1:12:A:LYS:HD3	1:15:A:TYR:H	10	0.59
(1,93)	1:7:A:VAL:HG21	1:38:A:ILE:H	2	0.59
(1,93)	1:7:A:VAL:HG22	1:38:A:ILE:H	2	0.59
(1,93)	1:7:A:VAL:HG23	1:38:A:ILE:H	2	0.59
(1,1799)	1:151:A:ARG:H	1:152:A:ILE:H	4	0.58
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG21	6	0.58
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG22	6	0.58
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG23	6	0.58
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG21	6	0.58
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG22	6	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG23	6	0.58
(1,1777)	1:149:A:ASN:HB2	1:151:A:ARG:H	4	0.58
(1,1777)	1:149:A:ASN:HB3	1:151:A:ARG:H	4	0.58
(1,1709)	1:143:A:LYS:HB2	1:147:A:MET:H	4	0.58
(1,1709)	1:143:A:LYS:HB2	1:147:A:MET:H	9	0.58
(1,1580)	1:134:A:MET:HB2	1:136:A:ASP:H	10	0.58
(1,1580)	1:134:A:MET:HB3	1:136:A:ASP:H	10	0.58
(1,1558)	1:133:A:GLU:H	1:133:A:GLU:HG2	3	0.58
(1,1558)	1:133:A:GLU:H	1:133:A:GLU:HG3	3	0.58
(1,1441)	1:118:A:LYS:HE2	1:119:A:ALA:H	1	0.58
(1,1316)	1:109:A:LEU:HA	1:113:A:SER:H	8	0.58
(1,1299)	1:108:A:MET:HB2	1:112:A:SER:H	1	0.58
(1,1299)	1:108:A:MET:HB2	1:112:A:SER:H	8	0.58
(1,1285)	1:107:A:ARG:HD2	1:108:A:MET:H	8	0.58
(1,1285)	1:107:A:ARG:HD3	1:108:A:MET:H	8	0.58
(1,1285)	1:107:A:ARG:HD2	1:108:A:MET:H	8	0.58
(1,1285)	1:107:A:ARG:HD3	1:108:A:MET:H	8	0.58
(1,1218)	1:104:A:VAL:HA	1:106:A:ARG:H	1	0.58
(1,1174)	1:99:A:PRO:HA	1:102:A:ALA:H	10	0.58
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB1	5	0.58
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB2	5	0.58
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB3	5	0.58
(1,1145)	1:95:A:VAL:HG11	1:131:A:ALA:HA	1	0.58
(1,1145)	1:95:A:VAL:HG12	1:131:A:ALA:HA	1	0.58
(1,1145)	1:95:A:VAL:HG13	1:131:A:ALA:HA	1	0.58
(1,1145)	1:95:A:VAL:HG21	1:131:A:ALA:HA	1	0.58
(1,1145)	1:95:A:VAL:HG22	1:131:A:ALA:HA	1	0.58
(1,1145)	1:95:A:VAL:HG23	1:131:A:ALA:HA	1	0.58
(1,968)	1:79:A:GLN:HA	1:85:A:GLY:H	7	0.58
(1,968)	1:79:A:GLN:HA	1:85:A:GLY:H	8	0.58
(1,891)	1:75:A:GLU:HG2	1:89:A:LEU:H	8	0.58
(1,741)	1:58:A:LYS:H	1:58:A:LYS:HD2	2	0.58
(1,741)	1:58:A:LYS:H	1:58:A:LYS:HD3	2	0.58
(1,705)	1:55:A:GLU:HA	1:59:A:LYS:HB3	10	0.58
(1,702)	1:55:A:GLU:HA	1:58:A:LYS:HB2	10	0.58
(1,702)	1:55:A:GLU:HA	1:58:A:LYS:HB3	10	0.58
(1,655)	1:53:A:PHE:HA	1:56:A:GLU:H	6	0.58
(1,608)	1:49:A:PRO:HG2	1:50:A:TYR:H	2	0.58
(1,608)	1:49:A:PRO:HG3	1:50:A:TYR:H	2	0.58
(1,590)	1:45:A:GLU:HB2	1:48:A:ALA:HA	4	0.58
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB2	5	0.58
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB3	5	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB2	7	0.58
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB3	7	0.58
(1,518)	1:32:A:ASP:HB3	1:37:A:ALA:H	7	0.58
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG2	7	0.58
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG3	7	0.58
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG2	7	0.58
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG3	7	0.58
(1,439)	1:28:A:ILE:HB	1:42:A:LYS:HD2	10	0.58
(1,439)	1:28:A:ILE:HB	1:42:A:LYS:HD3	10	0.58
(1,316)	1:18:A:LEU:HD11	1:123:A:LEU:HG	4	0.58
(1,316)	1:18:A:LEU:HD12	1:123:A:LEU:HG	4	0.58
(1,316)	1:18:A:LEU:HD13	1:123:A:LEU:HG	4	0.58
(1,162)	1:10:A:SER:HB2	1:13:A:ASN:H	10	0.58
(1,162)	1:10:A:SER:HB3	1:13:A:ASN:H	10	0.58
(1,137)	1:8:A:ASP:HB2	1:9:A:PRO:HA	8	0.58
(1,137)	1:8:A:ASP:HB3	1:9:A:PRO:HA	8	0.58
(1,83)	1:7:A:VAL:HG11	1:120:A:SER:HA	2	0.58
(1,83)	1:7:A:VAL:HG12	1:120:A:SER:HA	2	0.58
(1,83)	1:7:A:VAL:HG13	1:120:A:SER:HA	2	0.58
(1,73)	1:7:A:VAL:HB	1:120:A:SER:HA	8	0.58
(1,66)	1:7:A:VAL:HA	1:37:A:ALA:HB1	5	0.58
(1,66)	1:7:A:VAL:HA	1:37:A:ALA:HB2	5	0.58
(1,66)	1:7:A:VAL:HA	1:37:A:ALA:HB3	5	0.58
(1,1778)	1:149:A:ASN:HB2	1:151:A:ARG:HA	9	0.57
(1,1778)	1:149:A:ASN:HB3	1:151:A:ARG:HA	9	0.57
(1,1756)	1:147:A:MET:HA	1:149:A:ASN:H	4	0.57
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG11	3	0.57
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG12	3	0.57
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG13	3	0.57
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG21	3	0.57
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG22	3	0.57
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG23	3	0.57
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG11	3	0.57
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG12	3	0.57
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG13	3	0.57
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG21	3	0.57
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG22	3	0.57
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG23	3	0.57
(1,1442)	1:118:A:LYS:HE2	1:121:A:LEU:H	4	0.57
(1,1299)	1:108:A:MET:HB2	1:112:A:SER:H	2	0.57
(1,1241)	1:104:A:VAL:HG11	1:107:A:ARG:HB2	5	0.57
(1,1241)	1:104:A:VAL:HG11	1:107:A:ARG:HB3	5	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1241)	1:104:A:VAL:HG12	1:107:A:ARG:HB2	5	0.57
(1,1241)	1:104:A:VAL:HG12	1:107:A:ARG:HB3	5	0.57
(1,1241)	1:104:A:VAL:HG13	1:107:A:ARG:HB2	5	0.57
(1,1241)	1:104:A:VAL:HG13	1:107:A:ARG:HB3	5	0.57
(1,1241)	1:104:A:VAL:HG21	1:107:A:ARG:HB2	5	0.57
(1,1241)	1:104:A:VAL:HG21	1:107:A:ARG:HB3	5	0.57
(1,1241)	1:104:A:VAL:HG22	1:107:A:ARG:HB2	5	0.57
(1,1241)	1:104:A:VAL:HG22	1:107:A:ARG:HB3	5	0.57
(1,1241)	1:104:A:VAL:HG23	1:107:A:ARG:HB2	5	0.57
(1,1241)	1:104:A:VAL:HG23	1:107:A:ARG:HB3	5	0.57
(1,1208)	1:103:A:PRO:HA	1:107:A:ARG:H	7	0.57
(1,1082)	1:93:A:ILE:HA	1:127:A:PHE:HA	7	0.57
(1,1067)	1:92:A:VAL:H	1:127:A:PHE:H	4	0.57
(1,1064)	1:91:A:LYS:HD2	1:92:A:VAL:H	5	0.57
(1,1064)	1:91:A:LYS:HD3	1:92:A:VAL:H	5	0.57
(1,973)	1:79:A:GLN:HB2	1:85:A:GLY:H	8	0.57
(1,935)	1:77:A:THR:HB	1:87:A:SER:H	9	0.57
(1,898)	1:75:A:GLU:HG3	1:90:A:ASN:HA	10	0.57
(1,877)	1:75:A:GLU:HA	1:90:A:ASN:HB2	7	0.57
(1,877)	1:75:A:GLU:HA	1:90:A:ASN:HB3	7	0.57
(1,822)	1:70:A:ALA:H	1:94:A:PHE:HA	9	0.57
(1,611)	1:49:A:PRO:HG2	1:52:A:GLU:H	8	0.57
(1,611)	1:49:A:PRO:HG3	1:52:A:GLU:H	8	0.57
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB1	8	0.57
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB2	8	0.57
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB3	8	0.57
(1,519)	1:32:A:ASP:HB2	1:37:A:ALA:HB1	8	0.57
(1,519)	1:32:A:ASP:HB2	1:37:A:ALA:HB2	8	0.57
(1,519)	1:32:A:ASP:HB2	1:37:A:ALA:HB3	8	0.57
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB1	8	0.57
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB2	8	0.57
(1,519)	1:32:A:ASP:HB3	1:37:A:ALA:HB3	8	0.57
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG11	4	0.57
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG12	4	0.57
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG13	4	0.57
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG21	4	0.57
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG22	4	0.57
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG23	4	0.57
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG11	4	0.57
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG12	4	0.57
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG13	4	0.57
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG21	4	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG22	4	0.57
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG23	4	0.57
(1,434)	1:28:A:ILE:HB	1:41:A:GLU:HA	4	0.57
(1,225)	1:13:A:ASN:HA	1:17:A:LEU:H	6	0.57
(1,225)	1:13:A:ASN:HA	1:17:A:LEU:H	8	0.57
(1,214)	1:12:A:LYS:HG3	1:15:A:TYR:H	5	0.57
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD11	1	0.57
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD12	1	0.57
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD13	1	0.57
(1,162)	1:10:A:SER:HB2	1:13:A:ASN:H	3	0.57
(1,162)	1:10:A:SER:HB3	1:13:A:ASN:H	3	0.57
(1,159)	1:10:A:SER:HB3	1:13:A:ASN:H	7	0.57
(1,158)	1:10:A:SER:HB3	1:12:A:LYS:H	3	0.57
(1,158)	1:10:A:SER:HB3	1:12:A:LYS:H	6	0.57
(1,137)	1:8:A:ASP:HB2	1:9:A:PRO:HA	3	0.57
(1,137)	1:8:A:ASP:HB3	1:9:A:PRO:HA	3	0.57
(1,73)	1:7:A:VAL:HB	1:120:A:SER:HA	2	0.57
(2,2)	1:2:A:ALA:HB1	1:112:A:SER:H	6	0.56
(2,2)	1:2:A:ALA:HB2	1:112:A:SER:H	6	0.56
(2,2)	1:2:A:ALA:HB3	1:112:A:SER:H	6	0.56
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG11	7	0.56
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG12	7	0.56
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG13	7	0.56
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG21	7	0.56
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG22	7	0.56
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG23	7	0.56
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG11	7	0.56
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG12	7	0.56
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG13	7	0.56
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG21	7	0.56
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG22	7	0.56
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG23	7	0.56
(1,1566)	1:133:A:GLU:HG2	1:135:A:SER:H	10	0.56
(1,1566)	1:133:A:GLU:HG3	1:135:A:SER:H	10	0.56
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB2	6	0.56
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB3	6	0.56
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB2	6	0.56
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB3	6	0.56
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG2	6	0.56
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG3	6	0.56
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG2	6	0.56
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG3	6	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG2	6	0.56
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG3	6	0.56
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG2	6	0.56
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG3	6	0.56
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG2	6	0.56
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG3	6	0.56
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG2	6	0.56
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG3	6	0.56
(1,1184)	1:99:A:PRO:HG2	1:100:A:ASP:H	9	0.56
(1,1117)	1:94:A:PHE:HA	1:128:A:GLN:HA	1	0.56
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG21	7	0.56
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG22	7	0.56
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG23	7	0.56
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG21	1	0.56
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG22	1	0.56
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG23	1	0.56
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE2	7	0.56
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE3	7	0.56
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE2	7	0.56
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE3	7	0.56
(1,669)	1:54:A:VAL:HA	1:56:A:GLU:H	6	0.56
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB1	7	0.56
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB2	7	0.56
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB3	7	0.56
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB1	7	0.56
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB2	7	0.56
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB3	7	0.56
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB1	7	0.56
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB2	7	0.56
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB3	7	0.56
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB1	7	0.56
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB2	7	0.56
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB3	7	0.56
(1,576)	1:42:A:LYS:HD2	1:43:A:VAL:H	9	0.56
(1,576)	1:42:A:LYS:HD3	1:43:A:VAL:H	9	0.56
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB2	1	0.56
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB3	1	0.56
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG21	2	0.56
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG22	2	0.56
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG23	2	0.56
(1,511)	1:31:A:ILE:HG21	1:109:A:LEU:HG	2	0.56
(1,511)	1:31:A:ILE:HG22	1:109:A:LEU:HG	2	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:31:A:ILE:HG23	1:109:A:LEU:HG	2	0.56
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD11	1	0.56
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD12	1	0.56
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD13	1	0.56
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD21	1	0.56
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD22	1	0.56
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD23	1	0.56
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD11	1	0.56
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD12	1	0.56
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD13	1	0.56
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD21	1	0.56
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD22	1	0.56
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD23	1	0.56
(1,450)	1:28:A:ILE:HD11	1:70:A:ALA:HA	6	0.56
(1,450)	1:28:A:ILE:HD12	1:70:A:ALA:HA	6	0.56
(1,450)	1:28:A:ILE:HD13	1:70:A:ALA:HA	6	0.56
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD11	9	0.56
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD12	9	0.56
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD13	9	0.56
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD21	9	0.56
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD22	9	0.56
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD23	9	0.56
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD11	9	0.56
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD12	9	0.56
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD13	9	0.56
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD21	9	0.56
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD22	9	0.56
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD23	9	0.56
(1,137)	1:8:A:ASP:HB2	1:9:A:PRO:HA	7	0.56
(1,137)	1:8:A:ASP:HB3	1:9:A:PRO:HA	7	0.56
(1,137)	1:8:A:ASP:HB2	1:9:A:PRO:HA	9	0.56
(1,137)	1:8:A:ASP:HB3	1:9:A:PRO:HA	9	0.56
(1,124)	1:8:A:ASP:HB2	1:39:A:VAL:HB	5	0.56
(1,112)	1:8:A:ASP:H	1:11:A:CYS:HB2	7	0.56
(1,112)	1:8:A:ASP:H	1:11:A:CYS:HB3	7	0.56
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG21	6	0.56
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG22	6	0.56
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG23	6	0.56
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG21	6	0.56
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG22	6	0.56
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG23	6	0.56
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG21	6	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG22	6	0.56
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG23	6	0.56
(1,93)	1:7:A:VAL:HG21	1:38:A:ILE:H	9	0.56
(1,93)	1:7:A:VAL:HG22	1:38:A:ILE:H	9	0.56
(1,93)	1:7:A:VAL:HG23	1:38:A:ILE:H	9	0.56
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG21	7	0.56
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG22	7	0.56
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG23	7	0.56
(1,27)	1:5:A:VAL:HA	1:36:A:THR:HA	2	0.56
(2,35)	1:118:A:LYS:HE3	1:128:A:GLN:HA	5	0.55
(2,34)	1:114:A:VAL:HA	1:117:A:LEU:HA	5	0.55
(2,1)	1:1:A:MET:HA	1:114:A:VAL:HA	4	0.55
(2,1)	1:1:A:MET:HA	1:114:A:VAL:HA	10	0.55
(1,1790)	1:150:A:GLN:HB3	1:152:A:ILE:H	8	0.55
(1,1773)	1:149:A:ASN:HB3	1:151:A:ARG:HA	6	0.55
(1,1757)	1:147:A:MET:HA	1:150:A:GLN:H	6	0.55
(1,1651)	1:140:A:LYS:HD3	1:142:A:VAL:H	2	0.55
(1,1482)	1:121:A:LEU:HG	1:123:A:LEU:HD11	9	0.55
(1,1482)	1:121:A:LEU:HG	1:123:A:LEU:HD12	9	0.55
(1,1482)	1:121:A:LEU:HG	1:123:A:LEU:HD13	9	0.55
(1,1482)	1:121:A:LEU:HG	1:123:A:LEU:HD21	9	0.55
(1,1482)	1:121:A:LEU:HG	1:123:A:LEU:HD22	9	0.55
(1,1482)	1:121:A:LEU:HG	1:123:A:LEU:HD23	9	0.55
(1,1462)	1:120:A:SER:HA	1:122:A:GLY:H	10	0.55
(1,1344)	1:111:A:ALA:HA	1:115:A:ARG:H	2	0.55
(1,1344)	1:111:A:ALA:HA	1:115:A:ARG:H	4	0.55
(1,1333)	1:110:A:TYR:HA	1:114:A:VAL:H	5	0.55
(1,1299)	1:108:A:MET:HB2	1:112:A:SER:H	6	0.55
(1,1286)	1:107:A:ARG:HD2	1:111:A:ALA:HA	1	0.55
(1,1286)	1:107:A:ARG:HD3	1:111:A:ALA:HA	1	0.55
(1,1185)	1:99:A:PRO:HG2	1:102:A:ALA:HA	6	0.55
(1,1174)	1:99:A:PRO:HA	1:102:A:ALA:H	8	0.55
(1,507)	1:31:A:ILE:HG12	1:109:A:LEU:HB2	7	0.55
(1,507)	1:31:A:ILE:HG12	1:109:A:LEU:HB3	7	0.55
(1,507)	1:31:A:ILE:HG13	1:109:A:LEU:HB2	7	0.55
(1,507)	1:31:A:ILE:HG13	1:109:A:LEU:HB3	7	0.55
(1,466)	1:29:A:PHE:HB3	1:41:A:GLU:H	6	0.55
(1,452)	1:28:A:ILE:HD11	1:71:A:ALA:H	4	0.55
(1,452)	1:28:A:ILE:HD12	1:71:A:ALA:H	4	0.55
(1,452)	1:28:A:ILE:HD13	1:71:A:ALA:H	4	0.55
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD2	5	0.55
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD3	5	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD2	5	0.55
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD3	5	0.55
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD2	5	0.55
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD3	5	0.55
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD2	5	0.55
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD3	5	0.55
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD2	5	0.55
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD3	5	0.55
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD2	5	0.55
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD3	5	0.55
(1,208)	1:12:A:LYS:HE2	1:122:A:GLY:H	8	0.55
(1,208)	1:12:A:LYS:HE3	1:122:A:GLY:H	8	0.55
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB2	10	0.55
(1,138)	1:8:A:ASP:HB2	1:9:A:PRO:HB3	10	0.55
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB2	10	0.55
(1,138)	1:8:A:ASP:HB3	1:9:A:PRO:HB3	10	0.55
(1,75)	1:7:A:VAL:HB	1:38:A:ILE:H	7	0.55
(1,73)	1:7:A:VAL:HB	1:120:A:SER:HA	7	0.55
(1,65)	1:7:A:VAL:HA	1:37:A:ALA:HA	2	0.55
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG11	9	0.55
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG12	9	0.55
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG13	9	0.55
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG21	9	0.55
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG22	9	0.55
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG23	9	0.55
(1,33)	1:5:A:VAL:HB	1:7:A:VAL:HA	7	0.55
(1,33)	1:5:A:VAL:HB	1:7:A:VAL:HA	8	0.55
(3,59)	1:143:A:LYS:O	1:147:A:MET:H	3	0.54
(2,31)	1:97:A:TYR:HB2	1:131:A:ALA:HA	9	0.54
(2,31)	1:97:A:TYR:HB3	1:131:A:ALA:HA	9	0.54
(2,28)	1:79:A:GLN:HB3	1:85:A:GLY:H	3	0.54
(2,28)	1:79:A:GLN:HB3	1:85:A:GLY:H	5	0.54
(2,1)	1:1:A:MET:HA	1:114:A:VAL:HA	3	0.54
(1,1744)	1:146:A:LEU:HA	1:150:A:GLN:HA	2	0.54
(1,1587)	1:135:A:SER:HA	1:138:A:ASP:H	1	0.54
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG2	8	0.54
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG3	8	0.54
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG2	8	0.54
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG3	8	0.54
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG2	8	0.54
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG3	8	0.54
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG2	8	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG3	8	0.54
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG2	8	0.54
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG3	8	0.54
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG2	8	0.54
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG3	8	0.54
(1,1220)	1:104:A:VAL:HA	1:107:A:ARG:HB2	9	0.54
(1,1220)	1:104:A:VAL:HA	1:107:A:ARG:HB3	9	0.54
(1,1122)	1:94:A:PHE:HB2	1:118:A:LYS:HE2	9	0.54
(1,1122)	1:94:A:PHE:HB2	1:118:A:LYS:HE3	9	0.54
(1,1122)	1:94:A:PHE:HB3	1:118:A:LYS:HE2	9	0.54
(1,1122)	1:94:A:PHE:HB3	1:118:A:LYS:HE3	9	0.54
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG21	2	0.54
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG22	2	0.54
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG23	2	0.54
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG2	3	0.54
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG3	3	0.54
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG2	10	0.54
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG3	10	0.54
(1,898)	1:75:A:GLU:HG3	1:90:A:ASN:HA	8	0.54
(1,892)	1:75:A:GLU:HG2	1:90:A:ASN:HA	1	0.54
(1,892)	1:75:A:GLU:HG2	1:90:A:ASN:HA	8	0.54
(1,891)	1:75:A:GLU:HG2	1:89:A:LEU:H	7	0.54
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB1	1	0.54
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB2	1	0.54
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB3	1	0.54
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB1	3	0.54
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB2	3	0.54
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB3	3	0.54
(1,494)	1:31:A:ILE:HG12	1:38:A:ILE:HA	4	0.54
(1,454)	1:28:A:ILE:HG12	1:41:A:GLU:HG2	9	0.54
(1,454)	1:28:A:ILE:HG12	1:41:A:GLU:HG3	9	0.54
(1,454)	1:28:A:ILE:HG13	1:41:A:GLU:HG2	9	0.54
(1,454)	1:28:A:ILE:HG13	1:41:A:GLU:HG3	9	0.54
(1,327)	1:18:A:LEU:HD21	1:73:A:ASP:HA	2	0.54
(1,327)	1:18:A:LEU:HD22	1:73:A:ASP:HA	2	0.54
(1,327)	1:18:A:LEU:HD23	1:73:A:ASP:HA	2	0.54
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG11	6	0.54
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG12	6	0.54
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG13	6	0.54
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG21	6	0.54
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG22	6	0.54
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG23	6	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,206)	1:12:A:LYS:HD3	1:15:A:TYR:H	3	0.54
(1,158)	1:10:A:SER:HB3	1:12:A:LYS:H	7	0.54
(1,117)	1:8:A:ASP:H	1:39:A:VAL:HB	2	0.54
(1,93)	1:7:A:VAL:HG21	1:38:A:ILE:H	1	0.54
(1,93)	1:7:A:VAL:HG22	1:38:A:ILE:H	1	0.54
(1,93)	1:7:A:VAL:HG23	1:38:A:ILE:H	1	0.54
(1,83)	1:7:A:VAL:HG11	1:120:A:SER:HA	9	0.54
(1,83)	1:7:A:VAL:HG12	1:120:A:SER:HA	9	0.54
(1,83)	1:7:A:VAL:HG13	1:120:A:SER:HA	9	0.54
(1,73)	1:7:A:VAL:HB	1:120:A:SER:HA	9	0.54
(1,44)	1:6:A:LYS:H	1:37:A:ALA:HA	5	0.54
(2,34)	1:114:A:VAL:HA	1:117:A:LEU:HA	10	0.53
(2,28)	1:79:A:GLN:HB3	1:85:A:GLY:H	7	0.53
(2,28)	1:79:A:GLN:HB3	1:85:A:GLY:H	8	0.53
(2,1)	1:1:A:MET:HA	1:114:A:VAL:HA	5	0.53
(2,1)	1:1:A:MET:HA	1:114:A:VAL:HA	7	0.53
(2,1)	1:1:A:MET:HA	1:114:A:VAL:HA	8	0.53
(1,1803)	1:151:A:ARG:HG2	1:152:A:ILE:H	7	0.53
(1,1803)	1:151:A:ARG:HG3	1:152:A:ILE:H	7	0.53
(1,1779)	1:149:A:ASN:HB2	1:152:A:ILE:H	6	0.53
(1,1779)	1:149:A:ASN:HB3	1:152:A:ILE:H	6	0.53
(1,1587)	1:135:A:SER:HA	1:138:A:ASP:H	10	0.53
(1,1579)	1:134:A:MET:HB2	1:135:A:SER:H	5	0.53
(1,1579)	1:134:A:MET:HB3	1:135:A:SER:H	5	0.53
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD11	1	0.53
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD12	1	0.53
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD13	1	0.53
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD21	1	0.53
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD22	1	0.53
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD23	1	0.53
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB1	1	0.53
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB2	1	0.53
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB3	1	0.53
(1,1117)	1:94:A:PHE:HA	1:128:A:GLN:HA	2	0.53
(1,973)	1:79:A:GLN:HB2	1:85:A:GLY:H	7	0.53
(1,945)	1:78:A:VAL:H	1:86:A:THR:HB	3	0.53
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB2	7	0.53
(1,686)	1:54:A:VAL:HG11	1:138:A:ASP:HB3	7	0.53
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB2	7	0.53
(1,686)	1:54:A:VAL:HG12	1:138:A:ASP:HB3	7	0.53
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB2	7	0.53
(1,686)	1:54:A:VAL:HG13	1:138:A:ASP:HB3	7	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB2	7	0.53
(1,686)	1:54:A:VAL:HG21	1:138:A:ASP:HB3	7	0.53
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB2	7	0.53
(1,686)	1:54:A:VAL:HG22	1:138:A:ASP:HB3	7	0.53
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB2	7	0.53
(1,686)	1:54:A:VAL:HG23	1:138:A:ASP:HB3	7	0.53
(1,685)	1:54:A:VAL:HG11	1:138:A:ASP:HA	1	0.53
(1,685)	1:54:A:VAL:HG12	1:138:A:ASP:HA	1	0.53
(1,685)	1:54:A:VAL:HG13	1:138:A:ASP:HA	1	0.53
(1,685)	1:54:A:VAL:HG21	1:138:A:ASP:HA	1	0.53
(1,685)	1:54:A:VAL:HG22	1:138:A:ASP:HA	1	0.53
(1,685)	1:54:A:VAL:HG23	1:138:A:ASP:HA	1	0.53
(1,659)	1:53:A:PHE:HB2	1:56:A:GLU:H	8	0.53
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD11	3	0.53
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD12	3	0.53
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD13	3	0.53
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD21	3	0.53
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD22	3	0.53
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD23	3	0.53
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD11	3	0.53
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD12	3	0.53
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD13	3	0.53
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD21	3	0.53
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD22	3	0.53
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD23	3	0.53
(1,606)	1:49:A:PRO:HB3	1:52:A:GLU:H	8	0.53
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB1	1	0.53
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB2	1	0.53
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB3	1	0.53
(1,524)	1:33:A:LYS:HG2	1:36:A:THR:HB	2	0.53
(1,277)	1:16:A:ASP:HB2	1:18:A:LEU:H	2	0.53
(1,93)	1:7:A:VAL:HG21	1:38:A:ILE:H	3	0.53
(1,93)	1:7:A:VAL:HG22	1:38:A:ILE:H	3	0.53
(1,93)	1:7:A:VAL:HG23	1:38:A:ILE:H	3	0.53
(1,73)	1:7:A:VAL:HB	1:120:A:SER:HA	10	0.53
(1,28)	1:5:A:VAL:HA	1:36:A:THR:HB	4	0.53
(3,59)	1:143:A:LYS:O	1:147:A:MET:H	10	0.52
(2,28)	1:79:A:GLN:HB3	1:85:A:GLY:H	6	0.52
(1,1778)	1:149:A:ASN:HB2	1:151:A:ARG:HA	2	0.52
(1,1778)	1:149:A:ASN:HB3	1:151:A:ARG:HA	2	0.52
(1,1719)	1:144:A:SER:HA	1:146:A:LEU:H	2	0.52
(1,1719)	1:144:A:SER:HA	1:146:A:LEU:H	5	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1719)	1:144:A:SER:HA	1:146:A:LEU:H	10	0.52
(1,1658)	1:140:A:LYS:HB2	1:142:A:VAL:H	7	0.52
(1,1658)	1:140:A:LYS:HB3	1:142:A:VAL:H	7	0.52
(1,1653)	1:140:A:LYS:HE2	1:142:A:VAL:H	5	0.52
(1,1602)	1:137:A:LEU:H	1:137:A:LEU:HG	9	0.52
(1,1580)	1:134:A:MET:HB2	1:136:A:ASP:H	1	0.52
(1,1580)	1:134:A:MET:HB3	1:136:A:ASP:H	1	0.52
(1,1579)	1:134:A:MET:HB2	1:135:A:SER:H	1	0.52
(1,1579)	1:134:A:MET:HB3	1:135:A:SER:H	1	0.52
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	9	0.52
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	9	0.52
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	9	0.52
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	9	0.52
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	1	0.52
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	1	0.52
(1,1397)	1:115:A:ARG:HA	1:118:A:LYS:HD2	4	0.52
(1,1397)	1:115:A:ARG:HA	1:118:A:LYS:HD3	4	0.52
(1,1397)	1:115:A:ARG:HA	1:118:A:LYS:HD2	9	0.52
(1,1397)	1:115:A:ARG:HA	1:118:A:LYS:HD3	9	0.52
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB2	4	0.52
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB3	4	0.52
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB2	4	0.52
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB3	4	0.52
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB2	4	0.52
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB3	4	0.52
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB2	4	0.52
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB3	4	0.52
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB2	4	0.52
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB3	4	0.52
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB2	4	0.52
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB3	4	0.52
(1,1378)	1:114:A:VAL:HB	1:118:A:LYS:H	1	0.52
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB2	3	0.52
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB3	3	0.52
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB2	3	0.52
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB3	3	0.52
(1,1187)	1:99:A:PRO:HG2	1:132:A:SER:HB3	6	0.52
(1,1186)	1:99:A:PRO:HG2	1:132:A:SER:HA	6	0.52
(1,1184)	1:99:A:PRO:HG2	1:100:A:ASP:H	3	0.52
(1,1165)	1:97:A:TYR:HA	1:131:A:ALA:HA	4	0.52
(1,1145)	1:95:A:VAL:HG11	1:131:A:ALA:HA	9	0.52
(1,1145)	1:95:A:VAL:HG12	1:131:A:ALA:HA	9	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1145)	1:95:A:VAL:HG13	1:131:A:ALA:HA	9	0.52
(1,1145)	1:95:A:VAL:HG21	1:131:A:ALA:HA	9	0.52
(1,1145)	1:95:A:VAL:HG22	1:131:A:ALA:HA	9	0.52
(1,1145)	1:95:A:VAL:HG23	1:131:A:ALA:HA	9	0.52
(1,1082)	1:93:A:ILE:HA	1:127:A:PHE:HA	6	0.52
(1,987)	1:80:A:ARG:H	1:85:A:GLY:H	5	0.52
(1,898)	1:75:A:GLU:HG3	1:90:A:ASN:HA	1	0.52
(1,898)	1:75:A:GLU:HG3	1:90:A:ASN:HA	3	0.52
(1,724)	1:56:A:GLU:HG2	1:58:A:LYS:H	4	0.52
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD2	7	0.52
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD3	7	0.52
(1,669)	1:54:A:VAL:HA	1:56:A:GLU:H	1	0.52
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD11	2	0.52
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD12	2	0.52
(1,495)	1:31:A:ILE:HG12	1:38:A:ILE:HD13	2	0.52
(1,444)	1:28:A:ILE:HG13	1:71:A:ALA:H	6	0.52
(1,434)	1:28:A:ILE:HB	1:41:A:GLU:HA	7	0.52
(1,387)	1:26:A:TYR:HB2	1:73:A:ASP:H	5	0.52
(1,387)	1:26:A:TYR:HB3	1:73:A:ASP:H	5	0.52
(1,214)	1:12:A:LYS:HG3	1:15:A:TYR:H	9	0.52
(1,206)	1:12:A:LYS:HD3	1:15:A:TYR:H	4	0.52
(1,206)	1:12:A:LYS:HD3	1:15:A:TYR:H	5	0.52
(1,206)	1:12:A:LYS:HD3	1:15:A:TYR:H	8	0.52
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD11	1	0.52
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD12	1	0.52
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD13	1	0.52
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD21	1	0.52
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD22	1	0.52
(1,182)	1:11:A:CYS:HB2	1:121:A:LEU:HD23	1	0.52
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD11	1	0.52
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD12	1	0.52
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD13	1	0.52
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD21	1	0.52
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD22	1	0.52
(1,182)	1:11:A:CYS:HB3	1:121:A:LEU:HD23	1	0.52
(1,135)	1:8:A:ASP:HB2	1:39:A:VAL:HB	9	0.52
(1,135)	1:8:A:ASP:HB3	1:39:A:VAL:HB	9	0.52
(1,129)	1:8:A:ASP:HB3	1:39:A:VAL:HB	5	0.52
(1,73)	1:7:A:VAL:HB	1:120:A:SER:HA	5	0.52
(1,72)	1:7:A:VAL:HB	1:117:A:LEU:HA	4	0.52
(1,72)	1:7:A:VAL:HB	1:117:A:LEU:HA	7	0.52
(2,35)	1:118:A:LYS:HE3	1:128:A:GLN:HA	3	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,34)	1:114:A:VAL:HA	1:117:A:LEU:HA	4	0.51
(2,34)	1:114:A:VAL:HA	1:117:A:LEU:HA	6	0.51
(2,34)	1:114:A:VAL:HA	1:117:A:LEU:HA	8	0.51
(2,2)	1:2:A:ALA:HB1	1:112:A:SER:H	5	0.51
(2,2)	1:2:A:ALA:HB2	1:112:A:SER:H	5	0.51
(2,2)	1:2:A:ALA:HB3	1:112:A:SER:H	5	0.51
(2,1)	1:1:A:MET:HA	1:114:A:VAL:HA	9	0.51
(1,1803)	1:151:A:ARG:HG2	1:152:A:ILE:H	4	0.51
(1,1803)	1:151:A:ARG:HG3	1:152:A:ILE:H	4	0.51
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG21	2	0.51
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG22	2	0.51
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG23	2	0.51
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG21	2	0.51
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG22	2	0.51
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG23	2	0.51
(1,1726)	1:144:A:SER:HB3	1:146:A:LEU:H	1	0.51
(1,1725)	1:144:A:SER:HB3	1:145:A:ASP:H	9	0.51
(1,1719)	1:144:A:SER:HA	1:146:A:LEU:H	9	0.51
(1,1718)	1:144:A:SER:H	1:146:A:LEU:H	8	0.51
(1,1718)	1:144:A:SER:H	1:146:A:LEU:H	10	0.51
(1,1709)	1:143:A:LYS:HB2	1:147:A:MET:H	5	0.51
(1,1700)	1:143:A:LYS:H	1:145:A:ASP:H	1	0.51
(1,1669)	1:141:A:SER:HB3	1:143:A:LYS:H	4	0.51
(1,1566)	1:133:A:GLU:HG2	1:135:A:SER:H	9	0.51
(1,1566)	1:133:A:GLU:HG3	1:135:A:SER:H	9	0.51
(1,1440)	1:118:A:LYS:HD2	1:119:A:ALA:H	4	0.51
(1,1440)	1:118:A:LYS:HD3	1:119:A:ALA:H	4	0.51
(1,1260)	1:105:A:ARG:HD2	1:106:A:ARG:H	4	0.51
(1,1260)	1:105:A:ARG:HD3	1:106:A:ARG:H	4	0.51
(1,1255)	1:105:A:ARG:HA	1:109:A:LEU:H	3	0.51
(1,1218)	1:104:A:VAL:HA	1:106:A:ARG:H	7	0.51
(1,1174)	1:99:A:PRO:HA	1:102:A:ALA:H	1	0.51
(1,1173)	1:98:A:CYS:HB2	1:107:A:ARG:HD2	9	0.51
(1,1173)	1:98:A:CYS:HB2	1:107:A:ARG:HD3	9	0.51
(1,1173)	1:98:A:CYS:HB3	1:107:A:ARG:HD2	9	0.51
(1,1173)	1:98:A:CYS:HB3	1:107:A:ARG:HD3	9	0.51
(1,1172)	1:98:A:CYS:HB2	1:107:A:ARG:HA	7	0.51
(1,1172)	1:98:A:CYS:HB3	1:107:A:ARG:HA	7	0.51
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB1	8	0.51
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB2	8	0.51
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB3	8	0.51
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB1	8	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB2	8	0.51
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB3	8	0.51
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG11	9	0.51
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG12	9	0.51
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG13	9	0.51
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG21	9	0.51
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG22	9	0.51
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG23	9	0.51
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG11	9	0.51
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG12	9	0.51
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG13	9	0.51
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG21	9	0.51
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG22	9	0.51
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG23	9	0.51
(1,1065)	1:91:A:LYS:HE3	1:150:A:GLN:H	2	0.51
(1,1027)	1:86:A:THR:HB	1:87:A:SER:H	2	0.51
(1,738)	1:57:A:MET:HG2	1:60:A:LEU:HB2	1	0.51
(1,738)	1:57:A:MET:HG2	1:60:A:LEU:HB3	1	0.51
(1,738)	1:57:A:MET:HG3	1:60:A:LEU:HB2	1	0.51
(1,738)	1:57:A:MET:HG3	1:60:A:LEU:HB3	1	0.51
(1,724)	1:56:A:GLU:HG2	1:58:A:LYS:H	8	0.51
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD2	3	0.51
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD3	3	0.51
(1,528)	1:33:A:LYS:HG3	1:36:A:THR:HB	1	0.51
(1,502)	1:31:A:ILE:HD11	1:109:A:LEU:HA	8	0.51
(1,502)	1:31:A:ILE:HD12	1:109:A:LEU:HA	8	0.51
(1,502)	1:31:A:ILE:HD13	1:109:A:LEU:HA	8	0.51
(1,491)	1:31:A:ILE:HG12	1:109:A:LEU:HA	1	0.51
(1,452)	1:28:A:ILE:HD11	1:71:A:ALA:H	1	0.51
(1,452)	1:28:A:ILE:HD12	1:71:A:ALA:H	1	0.51
(1,452)	1:28:A:ILE:HD13	1:71:A:ALA:H	1	0.51
(1,206)	1:12:A:LYS:HD3	1:15:A:TYR:H	9	0.51
(1,156)	1:10:A:SER:HB2	1:13:A:ASN:H	10	0.51
(1,137)	1:8:A:ASP:HB2	1:9:A:PRO:HA	2	0.51
(1,137)	1:8:A:ASP:HB3	1:9:A:PRO:HA	2	0.51
(1,129)	1:8:A:ASP:HB3	1:39:A:VAL:HB	2	0.51
(1,124)	1:8:A:ASP:HB2	1:39:A:VAL:HB	2	0.51
(1,73)	1:7:A:VAL:HB	1:120:A:SER:HA	3	0.51
(1,60)	1:7:A:VAL:H	1:37:A:ALA:HB1	5	0.51
(1,60)	1:7:A:VAL:H	1:37:A:ALA:HB2	5	0.51
(1,60)	1:7:A:VAL:H	1:37:A:ALA:HB3	5	0.51
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD11	5	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD12	5	0.51
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD13	5	0.51
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD11	5	0.51
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD12	5	0.51
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD13	5	0.51
(1,31)	1:5:A:VAL:HB	1:36:A:THR:HB	10	0.51
(2,28)	1:79:A:GLN:HB3	1:85:A:GLY:H	4	0.5
(1,1808)	1:152:A:ILE:H	1:152:A:ILE:HG12	7	0.5
(1,1808)	1:152:A:ILE:H	1:152:A:ILE:HG13	7	0.5
(1,1762)	1:148:A:SER:H	1:150:A:GLN:H	4	0.5
(1,1726)	1:144:A:SER:HB3	1:146:A:LEU:H	3	0.5
(1,1718)	1:144:A:SER:H	1:146:A:LEU:H	7	0.5
(1,1669)	1:141:A:SER:HB3	1:143:A:LYS:H	10	0.5
(1,1658)	1:140:A:LYS:HB2	1:142:A:VAL:H	3	0.5
(1,1658)	1:140:A:LYS:HB3	1:142:A:VAL:H	3	0.5
(1,1658)	1:140:A:LYS:HB2	1:142:A:VAL:H	5	0.5
(1,1658)	1:140:A:LYS:HB3	1:142:A:VAL:H	5	0.5
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG11	2	0.5
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG12	2	0.5
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG13	2	0.5
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG21	2	0.5
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG22	2	0.5
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG23	2	0.5
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG11	2	0.5
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG12	2	0.5
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG13	2	0.5
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG21	2	0.5
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG22	2	0.5
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG23	2	0.5
(1,1587)	1:135:A:SER:HA	1:138:A:ASP:H	6	0.5
(1,1441)	1:118:A:LYS:HE2	1:119:A:ALA:H	9	0.5
(1,1378)	1:114:A:VAL:HB	1:118:A:LYS:H	5	0.5
(1,1364)	1:113:A:SER:HB2	1:116:A:ALA:H	1	0.5
(1,1322)	1:109:A:LEU:HD21	1:113:A:SER:H	6	0.5
(1,1322)	1:109:A:LEU:HD22	1:113:A:SER:H	6	0.5
(1,1322)	1:109:A:LEU:HD23	1:113:A:SER:H	6	0.5
(1,1220)	1:104:A:VAL:HA	1:107:A:ARG:HB2	5	0.5
(1,1220)	1:104:A:VAL:HA	1:107:A:ARG:HB3	5	0.5
(1,1172)	1:98:A:CYS:HB2	1:107:A:ARG:HA	3	0.5
(1,1172)	1:98:A:CYS:HB3	1:107:A:ARG:HA	3	0.5
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB2	9	0.5
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB3	9	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB2	3	0.5
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB3	3	0.5
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG21	9	0.5
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG22	9	0.5
(1,971)	1:79:A:GLN:HA	1:86:A:THR:HG23	9	0.5
(1,947)	1:78:A:VAL:H	1:87:A:SER:H	5	0.5
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG21	3	0.5
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG22	3	0.5
(1,946)	1:78:A:VAL:H	1:86:A:THR:HG23	3	0.5
(1,940)	1:77:A:THR:HG21	1:87:A:SER:H	3	0.5
(1,940)	1:77:A:THR:HG22	1:87:A:SER:H	3	0.5
(1,940)	1:77:A:THR:HG23	1:87:A:SER:H	3	0.5
(1,909)	1:76:A:VAL:H	1:89:A:LEU:H	4	0.5
(1,909)	1:76:A:VAL:H	1:89:A:LEU:H	6	0.5
(1,736)	1:57:A:MET:HB2	1:60:A:LEU:HG	7	0.5
(1,736)	1:57:A:MET:HB3	1:60:A:LEU:HG	7	0.5
(1,654)	1:53:A:PHE:HA	1:55:A:GLU:H	4	0.5
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG2	5	0.5
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG3	5	0.5
(1,609)	1:49:A:PRO:HG2	1:51:A:ALA:H	8	0.5
(1,609)	1:49:A:PRO:HG3	1:51:A:ALA:H	8	0.5
(1,527)	1:33:A:LYS:HG3	1:36:A:THR:HA	9	0.5
(1,434)	1:28:A:ILE:HB	1:41:A:GLU:HA	6	0.5
(1,256)	1:15:A:TYR:HB2	1:121:A:LEU:HG	3	0.5
(1,206)	1:12:A:LYS:HD3	1:15:A:TYR:H	1	0.5
(1,159)	1:10:A:SER:HB3	1:13:A:ASN:H	8	0.5
(1,156)	1:10:A:SER:HB2	1:13:A:ASN:H	3	0.5
(1,111)	1:7:A:VAL:HG11	1:9:A:PRO:HA	9	0.5
(1,111)	1:7:A:VAL:HG12	1:9:A:PRO:HA	9	0.5
(1,111)	1:7:A:VAL:HG13	1:9:A:PRO:HA	9	0.5
(1,111)	1:7:A:VAL:HG21	1:9:A:PRO:HA	9	0.5
(1,111)	1:7:A:VAL:HG22	1:9:A:PRO:HA	9	0.5
(1,111)	1:7:A:VAL:HG23	1:9:A:PRO:HA	9	0.5
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD11	1	0.5
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD12	1	0.5
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD13	1	0.5
(1,76)	1:7:A:VAL:HB	1:38:A:ILE:HB	6	0.5
(1,73)	1:7:A:VAL:HB	1:120:A:SER:HA	6	0.5
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG11	7	0.5
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG12	7	0.5
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG13	7	0.5
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG21	7	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG22	7	0.5
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG23	7	0.5
(3,27)	1:68:A:ARG:O	1:97:A:TYR:H	8	0.49
(3,9)	1:26:A:TYR:H	1:44:A:GLY:O	10	0.49
(2,3)	1:5:A:VAL:HB	1:117:A:LEU:HG	6	0.49
(2,3)	1:5:A:VAL:HB	1:117:A:LEU:HG	10	0.49
(2,2)	1:2:A:ALA:HB1	1:112:A:SER:H	4	0.49
(2,2)	1:2:A:ALA:HB2	1:112:A:SER:H	4	0.49
(2,2)	1:2:A:ALA:HB3	1:112:A:SER:H	4	0.49
(2,1)	1:1:A:MET:HA	1:114:A:VAL:HA	6	0.49
(1,1756)	1:147:A:MET:HA	1:149:A:ASN:H	5	0.49
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD11	4	0.49
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD12	4	0.49
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD13	4	0.49
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD21	4	0.49
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD22	4	0.49
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD23	4	0.49
(1,1165)	1:97:A:TYR:HA	1:131:A:ALA:HA	7	0.49
(1,1086)	1:93:A:ILE:HB	1:127:A:PHE:H	1	0.49
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG21	3	0.49
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG22	3	0.49
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG23	3	0.49
(1,912)	1:76:A:VAL:HA	1:88:A:THR:HG21	9	0.49
(1,912)	1:76:A:VAL:HA	1:88:A:THR:HG22	9	0.49
(1,912)	1:76:A:VAL:HA	1:88:A:THR:HG23	9	0.49
(1,907)	1:76:A:VAL:H	1:88:A:THR:HB	8	0.49
(1,784)	1:61:A:VAL:HG11	1:66:A:GLU:HG2	7	0.49
(1,784)	1:61:A:VAL:HG12	1:66:A:GLU:HG2	7	0.49
(1,784)	1:61:A:VAL:HG13	1:66:A:GLU:HG2	7	0.49
(1,784)	1:61:A:VAL:HG11	1:66:A:GLU:HG3	7	0.49
(1,784)	1:61:A:VAL:HG12	1:66:A:GLU:HG3	7	0.49
(1,784)	1:61:A:VAL:HG13	1:66:A:GLU:HG3	7	0.49
(1,611)	1:49:A:PRO:HG2	1:52:A:GLU:H	5	0.49
(1,611)	1:49:A:PRO:HG3	1:52:A:GLU:H	5	0.49
(1,607)	1:49:A:PRO:HG2	1:51:A:ALA:HB1	5	0.49
(1,607)	1:49:A:PRO:HG2	1:51:A:ALA:HB2	5	0.49
(1,607)	1:49:A:PRO:HG2	1:51:A:ALA:HB3	5	0.49
(1,607)	1:49:A:PRO:HG3	1:51:A:ALA:HB1	5	0.49
(1,607)	1:49:A:PRO:HG3	1:51:A:ALA:HB2	5	0.49
(1,607)	1:49:A:PRO:HG3	1:51:A:ALA:HB3	5	0.49
(1,604)	1:49:A:PRO:HB3	1:51:A:ALA:H	4	0.49
(1,599)	1:49:A:PRO:HA	1:52:A:GLU:H	8	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG21	5	0.49
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG22	5	0.49
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG23	5	0.49
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD11	8	0.49
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD12	8	0.49
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD13	8	0.49
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG2	1	0.49
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG3	1	0.49
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG2	1	0.49
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG3	1	0.49
(1,464)	1:29:A:PHE:HB2	1:41:A:GLU:H	6	0.49
(1,428)	1:28:A:ILE:H	1:42:A:LYS:HD2	10	0.49
(1,428)	1:28:A:ILE:H	1:42:A:LYS:HD3	10	0.49
(1,206)	1:12:A:LYS:HD3	1:15:A:TYR:H	2	0.49
(1,123)	1:8:A:ASP:HB2	1:39:A:VAL:HA	9	0.49
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG21	10	0.49
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG22	10	0.49
(1,78)	1:7:A:VAL:HB	1:38:A:ILE:HG23	10	0.49
(1,38)	1:5:A:VAL:HG11	1:36:A:THR:HA	5	0.49
(1,38)	1:5:A:VAL:HG12	1:36:A:THR:HA	5	0.49
(1,38)	1:5:A:VAL:HG13	1:36:A:THR:HA	5	0.49
(1,38)	1:5:A:VAL:HG21	1:36:A:THR:HA	5	0.49
(1,38)	1:5:A:VAL:HG22	1:36:A:THR:HA	5	0.49
(1,38)	1:5:A:VAL:HG23	1:36:A:THR:HA	5	0.49
(3,19)	1:29:A:PHE:O	1:69:A:TYR:H	5	0.48
(3,3)	1:8:A:ASP:H	1:38:A:ILE:O	3	0.48
(2,31)	1:97:A:TYR:HB2	1:131:A:ALA:HA	7	0.48
(2,31)	1:97:A:TYR:HB3	1:131:A:ALA:HA	7	0.48
(2,31)	1:97:A:TYR:HB2	1:131:A:ALA:HA	8	0.48
(2,31)	1:97:A:TYR:HB3	1:131:A:ALA:HA	8	0.48
(2,3)	1:5:A:VAL:HB	1:117:A:LEU:HG	7	0.48
(1,1777)	1:149:A:ASN:HB2	1:151:A:ARG:H	1	0.48
(1,1777)	1:149:A:ASN:HB3	1:151:A:ARG:H	1	0.48
(1,1757)	1:147:A:MET:HA	1:150:A:GLN:H	4	0.48
(1,1744)	1:146:A:LEU:HA	1:150:A:GLN:HA	8	0.48
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	10	0.48
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	10	0.48
(1,1398)	1:115:A:ARG:HA	1:119:A:ALA:H	9	0.48
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB1	4	0.48
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB2	4	0.48
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB3	4	0.48
(1,1117)	1:94:A:PHE:HA	1:128:A:GLN:HA	7	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:75:A:GLU:HG3	1:90:A:ASN:HB2	7	0.48
(1,899)	1:75:A:GLU:HG3	1:90:A:ASN:HB3	7	0.48
(1,752)	1:58:A:LYS:HB3	1:59:A:LYS:H	10	0.48
(1,703)	1:55:A:GLU:HA	1:58:A:LYS:HG2	6	0.48
(1,703)	1:55:A:GLU:HA	1:58:A:LYS:HG3	6	0.48
(1,590)	1:45:A:GLU:HB2	1:48:A:ALA:HA	9	0.48
(1,516)	1:32:A:ASP:HB2	1:37:A:ALA:H	10	0.48
(1,507)	1:31:A:ILE:HG12	1:109:A:LEU:HB2	4	0.48
(1,507)	1:31:A:ILE:HG12	1:109:A:LEU:HB3	4	0.48
(1,507)	1:31:A:ILE:HG13	1:109:A:LEU:HB2	4	0.48
(1,507)	1:31:A:ILE:HG13	1:109:A:LEU:HB3	4	0.48
(1,334)	1:19:A:HIS:H	1:21:A:LYS:H	8	0.48
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB1	9	0.48
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB2	9	0.48
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB3	9	0.48
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB1	9	0.48
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB2	9	0.48
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB3	9	0.48
(1,293)	1:17:A:LEU:HA	1:21:A:LYS:HB2	7	0.48
(1,293)	1:17:A:LEU:HA	1:21:A:LYS:HB3	7	0.48
(1,158)	1:10:A:SER:HB3	1:12:A:LYS:H	2	0.48
(1,158)	1:10:A:SER:HB3	1:12:A:LYS:H	9	0.48
(1,108)	1:7:A:VAL:HG11	1:38:A:ILE:HB	5	0.48
(1,108)	1:7:A:VAL:HG12	1:38:A:ILE:HB	5	0.48
(1,108)	1:7:A:VAL:HG13	1:38:A:ILE:HB	5	0.48
(1,108)	1:7:A:VAL:HG21	1:38:A:ILE:HB	5	0.48
(1,108)	1:7:A:VAL:HG22	1:38:A:ILE:HB	5	0.48
(1,108)	1:7:A:VAL:HG23	1:38:A:ILE:HB	5	0.48
(1,94)	1:7:A:VAL:HG21	1:38:A:ILE:HB	6	0.48
(1,94)	1:7:A:VAL:HG22	1:38:A:ILE:HB	6	0.48
(1,94)	1:7:A:VAL:HG23	1:38:A:ILE:HB	6	0.48
(1,83)	1:7:A:VAL:HG11	1:120:A:SER:HA	1	0.48
(1,83)	1:7:A:VAL:HG12	1:120:A:SER:HA	1	0.48
(1,83)	1:7:A:VAL:HG13	1:120:A:SER:HA	1	0.48
(1,76)	1:7:A:VAL:HB	1:38:A:ILE:HB	4	0.48
(1,72)	1:7:A:VAL:HB	1:117:A:LEU:HA	5	0.48
(1,64)	1:7:A:VAL:HA	1:117:A:LEU:HA	1	0.48
(1,48)	1:6:A:LYS:H	1:6:A:LYS:HE2	1	0.48
(1,48)	1:6:A:LYS:H	1:6:A:LYS:HE3	1	0.48
(1,19)	1:4:A:GLY:H	1:5:A:VAL:H	5	0.48
(2,2)	1:2:A:ALA:HB1	1:112:A:SER:H	1	0.47
(2,2)	1:2:A:ALA:HB2	1:112:A:SER:H	1	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:2:A:ALA:HB3	1:112:A:SER:H	1	0.47
(2,2)	1:2:A:ALA:HB1	1:112:A:SER:H	10	0.47
(2,2)	1:2:A:ALA:HB2	1:112:A:SER:H	10	0.47
(2,2)	1:2:A:ALA:HB3	1:112:A:SER:H	10	0.47
(1,1718)	1:144:A:SER:H	1:146:A:LEU:H	1	0.47
(1,1594)	1:135:A:SER:HB2	1:140:A:LYS:HG2	9	0.47
(1,1594)	1:135:A:SER:HB2	1:140:A:LYS:HG3	9	0.47
(1,1594)	1:135:A:SER:HB3	1:140:A:LYS:HG2	9	0.47
(1,1594)	1:135:A:SER:HB3	1:140:A:LYS:HG3	9	0.47
(1,1429)	1:117:A:LEU:HB3	1:119:A:ALA:H	1	0.47
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	5	0.47
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	5	0.47
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	5	0.47
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	5	0.47
(1,1240)	1:104:A:VAL:HG11	1:107:A:ARG:HA	5	0.47
(1,1240)	1:104:A:VAL:HG12	1:107:A:ARG:HA	5	0.47
(1,1240)	1:104:A:VAL:HG13	1:107:A:ARG:HA	5	0.47
(1,1240)	1:104:A:VAL:HG21	1:107:A:ARG:HA	5	0.47
(1,1240)	1:104:A:VAL:HG22	1:107:A:ARG:HA	5	0.47
(1,1240)	1:104:A:VAL:HG23	1:107:A:ARG:HA	5	0.47
(1,1235)	1:104:A:VAL:HG21	1:108:A:MET:H	4	0.47
(1,1235)	1:104:A:VAL:HG22	1:108:A:MET:H	4	0.47
(1,1235)	1:104:A:VAL:HG23	1:108:A:MET:H	4	0.47
(1,1233)	1:104:A:VAL:HG21	1:106:A:ARG:H	6	0.47
(1,1233)	1:104:A:VAL:HG22	1:106:A:ARG:H	6	0.47
(1,1233)	1:104:A:VAL:HG23	1:106:A:ARG:H	6	0.47
(1,1186)	1:99:A:PRO:HG2	1:132:A:SER:HA	9	0.47
(1,1174)	1:99:A:PRO:HA	1:102:A:ALA:H	4	0.47
(1,1086)	1:93:A:ILE:HB	1:127:A:PHE:H	9	0.47
(1,960)	1:78:A:VAL:HG21	1:87:A:SER:HB2	7	0.47
(1,960)	1:78:A:VAL:HG22	1:87:A:SER:HB2	7	0.47
(1,960)	1:78:A:VAL:HG23	1:87:A:SER:HB2	7	0.47
(1,960)	1:78:A:VAL:HG21	1:87:A:SER:HB3	7	0.47
(1,960)	1:78:A:VAL:HG22	1:87:A:SER:HB3	7	0.47
(1,960)	1:78:A:VAL:HG23	1:87:A:SER:HB3	7	0.47
(1,787)	1:61:A:VAL:HG21	1:66:A:GLU:HG3	8	0.47
(1,787)	1:61:A:VAL:HG22	1:66:A:GLU:HG3	8	0.47
(1,787)	1:61:A:VAL:HG23	1:66:A:GLU:HG3	8	0.47
(1,657)	1:53:A:PHE:HA	1:57:A:MET:H	8	0.47
(1,654)	1:53:A:PHE:HA	1:55:A:GLU:H	7	0.47
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG2	3	0.47
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG3	3	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,598)	1:49:A:PRO:HA	1:51:A:ALA:HB1	4	0.47
(1,598)	1:49:A:PRO:HA	1:51:A:ALA:HB2	4	0.47
(1,598)	1:49:A:PRO:HA	1:51:A:ALA:HB3	4	0.47
(1,597)	1:49:A:PRO:HA	1:51:A:ALA:H	4	0.47
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB1	9	0.47
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB2	9	0.47
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB3	9	0.47
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB1	9	0.47
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB2	9	0.47
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB3	9	0.47
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB1	9	0.47
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB2	9	0.47
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB3	9	0.47
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB1	9	0.47
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB2	9	0.47
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB3	9	0.47
(1,214)	1:12:A:LYS:HG3	1:15:A:TYR:H	8	0.47
(1,206)	1:12:A:LYS:HD3	1:15:A:TYR:H	7	0.47
(1,158)	1:10:A:SER:HB3	1:12:A:LYS:H	4	0.47
(1,76)	1:7:A:VAL:HB	1:38:A:ILE:HB	10	0.47
(2,3)	1:5:A:VAL:HB	1:117:A:LEU:HG	5	0.46
(2,1)	1:1:A:MET:HA	1:114:A:VAL:HA	1	0.46
(1,1769)	1:149:A:ASN:H	1:150:A:GLN:H	4	0.46
(1,1721)	1:144:A:SER:HA	1:148:A:SER:H	2	0.46
(1,1718)	1:144:A:SER:H	1:146:A:LEU:H	9	0.46
(1,1669)	1:141:A:SER:HB3	1:143:A:LYS:H	2	0.46
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE2	10	0.46
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE3	10	0.46
(1,1597)	1:136:A:ASP:H	1:138:A:ASP:H	9	0.46
(1,1594)	1:135:A:SER:HB2	1:140:A:LYS:HG2	8	0.46
(1,1594)	1:135:A:SER:HB2	1:140:A:LYS:HG3	8	0.46
(1,1594)	1:135:A:SER:HB3	1:140:A:LYS:HG2	8	0.46
(1,1594)	1:135:A:SER:HB3	1:140:A:LYS:HG3	8	0.46
(1,1571)	1:134:A:MET:H	1:134:A:MET:HG2	3	0.46
(1,1571)	1:134:A:MET:H	1:134:A:MET:HG3	3	0.46
(1,1414)	1:116:A:ALA:HB1	1:120:A:SER:H	2	0.46
(1,1414)	1:116:A:ALA:HB2	1:120:A:SER:H	2	0.46
(1,1414)	1:116:A:ALA:HB3	1:120:A:SER:H	2	0.46
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB2	6	0.46
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB3	6	0.46
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB2	6	0.46
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB3	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB2	6	0.46
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB3	6	0.46
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB2	6	0.46
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB3	6	0.46
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB2	6	0.46
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB3	6	0.46
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB2	6	0.46
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB3	6	0.46
(1,1322)	1:109:A:LEU:HD21	1:113:A:SER:H	9	0.46
(1,1322)	1:109:A:LEU:HD22	1:113:A:SER:H	9	0.46
(1,1322)	1:109:A:LEU:HD23	1:113:A:SER:H	9	0.46
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB2	10	0.46
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB3	10	0.46
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB2	10	0.46
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB3	10	0.46
(1,1240)	1:104:A:VAL:HG11	1:107:A:ARG:HA	9	0.46
(1,1240)	1:104:A:VAL:HG12	1:107:A:ARG:HA	9	0.46
(1,1240)	1:104:A:VAL:HG13	1:107:A:ARG:HA	9	0.46
(1,1240)	1:104:A:VAL:HG21	1:107:A:ARG:HA	9	0.46
(1,1240)	1:104:A:VAL:HG22	1:107:A:ARG:HA	9	0.46
(1,1240)	1:104:A:VAL:HG23	1:107:A:ARG:HA	9	0.46
(1,1235)	1:104:A:VAL:HG21	1:108:A:MET:H	9	0.46
(1,1235)	1:104:A:VAL:HG22	1:108:A:MET:H	9	0.46
(1,1235)	1:104:A:VAL:HG23	1:108:A:MET:H	9	0.46
(1,1205)	1:102:A:ALA:HB1	1:106:A:ARG:HD2	3	0.46
(1,1205)	1:102:A:ALA:HB1	1:106:A:ARG:HD3	3	0.46
(1,1205)	1:102:A:ALA:HB2	1:106:A:ARG:HD2	3	0.46
(1,1205)	1:102:A:ALA:HB2	1:106:A:ARG:HD3	3	0.46
(1,1205)	1:102:A:ALA:HB3	1:106:A:ARG:HD2	3	0.46
(1,1205)	1:102:A:ALA:HB3	1:106:A:ARG:HD3	3	0.46
(1,1165)	1:97:A:TYR:HA	1:131:A:ALA:HA	8	0.46
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG11	4	0.46
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG12	4	0.46
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG13	4	0.46
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG21	4	0.46
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG22	4	0.46
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG23	4	0.46
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG11	4	0.46
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG12	4	0.46
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG13	4	0.46
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG21	4	0.46
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG22	4	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG23	4	0.46
(1,1117)	1:94:A:PHE:HA	1:128:A:GLN:HA	4	0.46
(1,1107)	1:93:A:ILE:HG21	1:146:A:LEU:HA	10	0.46
(1,1107)	1:93:A:ILE:HG22	1:146:A:LEU:HA	10	0.46
(1,1107)	1:93:A:ILE:HG23	1:146:A:LEU:HA	10	0.46
(1,1064)	1:91:A:LYS:HD2	1:92:A:VAL:H	6	0.46
(1,1064)	1:91:A:LYS:HD3	1:92:A:VAL:H	6	0.46
(1,973)	1:79:A:GLN:HB2	1:85:A:GLY:H	5	0.46
(1,898)	1:75:A:GLU:HG3	1:90:A:ASN:HA	5	0.46
(1,896)	1:75:A:GLU:HG3	1:88:A:THR:HG21	6	0.46
(1,896)	1:75:A:GLU:HG3	1:88:A:THR:HG22	6	0.46
(1,896)	1:75:A:GLU:HG3	1:88:A:THR:HG23	6	0.46
(1,892)	1:75:A:GLU:HG2	1:90:A:ASN:HA	4	0.46
(1,892)	1:75:A:GLU:HG2	1:90:A:ASN:HA	5	0.46
(1,883)	1:75:A:GLU:HB3	1:76:A:VAL:H	1	0.46
(1,700)	1:55:A:GLU:HA	1:58:A:LYS:HE2	7	0.46
(1,700)	1:55:A:GLU:HA	1:58:A:LYS:HE3	7	0.46
(1,684)	1:54:A:VAL:HG11	1:138:A:ASP:H	1	0.46
(1,684)	1:54:A:VAL:HG12	1:138:A:ASP:H	1	0.46
(1,684)	1:54:A:VAL:HG13	1:138:A:ASP:H	1	0.46
(1,684)	1:54:A:VAL:HG21	1:138:A:ASP:H	1	0.46
(1,684)	1:54:A:VAL:HG22	1:138:A:ASP:H	1	0.46
(1,684)	1:54:A:VAL:HG23	1:138:A:ASP:H	1	0.46
(1,599)	1:49:A:PRO:HA	1:52:A:GLU:H	10	0.46
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG21	8	0.46
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG22	8	0.46
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG23	8	0.46
(1,331)	1:18:A:LEU:HD11	1:92:A:VAL:HA	4	0.46
(1,331)	1:18:A:LEU:HD12	1:92:A:VAL:HA	4	0.46
(1,331)	1:18:A:LEU:HD13	1:92:A:VAL:HA	4	0.46
(1,331)	1:18:A:LEU:HD21	1:92:A:VAL:HA	4	0.46
(1,331)	1:18:A:LEU:HD22	1:92:A:VAL:HA	4	0.46
(1,331)	1:18:A:LEU:HD23	1:92:A:VAL:HA	4	0.46
(1,264)	1:15:A:TYR:HB3	1:27:A:ILE:HD11	4	0.46
(1,264)	1:15:A:TYR:HB3	1:27:A:ILE:HD12	4	0.46
(1,264)	1:15:A:TYR:HB3	1:27:A:ILE:HD13	4	0.46
(1,124)	1:8:A:ASP:HB2	1:39:A:VAL:HB	9	0.46
(1,93)	1:7:A:VAL:HG21	1:38:A:ILE:H	8	0.46
(1,93)	1:7:A:VAL:HG22	1:38:A:ILE:H	8	0.46
(1,93)	1:7:A:VAL:HG23	1:38:A:ILE:H	8	0.46
(1,75)	1:7:A:VAL:HB	1:38:A:ILE:H	8	0.46
(1,73)	1:7:A:VAL:HB	1:120:A:SER:HA	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG11	2	0.46
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG12	2	0.46
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG13	2	0.46
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG21	2	0.46
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG22	2	0.46
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG23	2	0.46
(1,1773)	1:149:A:ASN:HB3	1:151:A:ARG:HA	7	0.45
(1,1725)	1:144:A:SER:HB3	1:145:A:ASP:H	4	0.45
(1,1721)	1:144:A:SER:HA	1:148:A:SER:H	1	0.45
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD2	6	0.45
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD3	6	0.45
(1,1658)	1:140:A:LYS:HB2	1:142:A:VAL:H	8	0.45
(1,1658)	1:140:A:LYS:HB3	1:142:A:VAL:H	8	0.45
(1,1549)	1:131:A:ALA:H	1:136:A:ASP:HB2	9	0.45
(1,1549)	1:131:A:ALA:H	1:136:A:ASP:HB3	9	0.45
(1,1453)	1:119:A:ALA:HA	1:122:A:GLY:H	2	0.45
(1,1426)	1:117:A:LEU:HB2	1:119:A:ALA:H	1	0.45
(1,1409)	1:116:A:ALA:HA	1:119:A:ALA:HB1	1	0.45
(1,1409)	1:116:A:ALA:HA	1:119:A:ALA:HB2	1	0.45
(1,1409)	1:116:A:ALA:HA	1:119:A:ALA:HB3	1	0.45
(1,1378)	1:114:A:VAL:HB	1:118:A:LYS:H	8	0.45
(1,1344)	1:111:A:ALA:HA	1:115:A:ARG:H	5	0.45
(1,1325)	1:109:A:LEU:HD11	1:112:A:SER:HB2	2	0.45
(1,1325)	1:109:A:LEU:HD11	1:112:A:SER:HB3	2	0.45
(1,1325)	1:109:A:LEU:HD12	1:112:A:SER:HB2	2	0.45
(1,1325)	1:109:A:LEU:HD12	1:112:A:SER:HB3	2	0.45
(1,1325)	1:109:A:LEU:HD13	1:112:A:SER:HB2	2	0.45
(1,1325)	1:109:A:LEU:HD13	1:112:A:SER:HB3	2	0.45
(1,1325)	1:109:A:LEU:HD21	1:112:A:SER:HB2	2	0.45
(1,1325)	1:109:A:LEU:HD21	1:112:A:SER:HB3	2	0.45
(1,1325)	1:109:A:LEU:HD22	1:112:A:SER:HB2	2	0.45
(1,1325)	1:109:A:LEU:HD22	1:112:A:SER:HB3	2	0.45
(1,1325)	1:109:A:LEU:HD23	1:112:A:SER:HB2	2	0.45
(1,1325)	1:109:A:LEU:HD23	1:112:A:SER:HB3	2	0.45
(1,1281)	1:107:A:ARG:HA	1:110:A:TYR:HA	6	0.45
(1,1224)	1:104:A:VAL:HB	1:106:A:ARG:H	8	0.45
(1,1224)	1:104:A:VAL:HB	1:106:A:ARG:H	10	0.45
(1,1165)	1:97:A:TYR:HA	1:131:A:ALA:HA	10	0.45
(1,1145)	1:95:A:VAL:HG11	1:131:A:ALA:HA	8	0.45
(1,1145)	1:95:A:VAL:HG12	1:131:A:ALA:HA	8	0.45
(1,1145)	1:95:A:VAL:HG13	1:131:A:ALA:HA	8	0.45
(1,1145)	1:95:A:VAL:HG21	1:131:A:ALA:HA	8	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1145)	1:95:A:VAL:HG22	1:131:A:ALA:HA	8	0.45
(1,1145)	1:95:A:VAL:HG23	1:131:A:ALA:HA	8	0.45
(1,1118)	1:94:A:PHE:HA	1:128:A:GLN:HB2	4	0.45
(1,1061)	1:91:A:LYS:HA	1:150:A:GLN:HG2	4	0.45
(1,1061)	1:91:A:LYS:HA	1:150:A:GLN:HG3	4	0.45
(1,898)	1:75:A:GLU:HG3	1:90:A:ASN:HA	4	0.45
(1,888)	1:75:A:GLU:HG2	1:76:A:VAL:H	8	0.45
(1,888)	1:75:A:GLU:HG2	1:76:A:VAL:H	9	0.45
(1,736)	1:57:A:MET:HB2	1:60:A:LEU:HG	10	0.45
(1,736)	1:57:A:MET:HB3	1:60:A:LEU:HG	10	0.45
(1,664)	1:53:A:PHE:HB2	1:57:A:MET:H	8	0.45
(1,664)	1:53:A:PHE:HB3	1:57:A:MET:H	8	0.45
(1,608)	1:49:A:PRO:HG2	1:50:A:TYR:H	3	0.45
(1,608)	1:49:A:PRO:HG3	1:50:A:TYR:H	3	0.45
(1,593)	1:45:A:GLU:HB3	1:48:A:ALA:HB1	1	0.45
(1,593)	1:45:A:GLU:HB3	1:48:A:ALA:HB2	1	0.45
(1,593)	1:45:A:GLU:HB3	1:48:A:ALA:HB3	1	0.45
(1,577)	1:42:A:LYS:HB2	1:53:A:PHE:HA	4	0.45
(1,577)	1:42:A:LYS:HB3	1:53:A:PHE:HA	4	0.45
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG21	5	0.45
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG22	5	0.45
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG23	5	0.45
(1,454)	1:28:A:ILE:HG12	1:41:A:GLU:HG2	7	0.45
(1,454)	1:28:A:ILE:HG12	1:41:A:GLU:HG3	7	0.45
(1,454)	1:28:A:ILE:HG13	1:41:A:GLU:HG2	7	0.45
(1,454)	1:28:A:ILE:HG13	1:41:A:GLU:HG3	7	0.45
(1,440)	1:28:A:ILE:HB	1:70:A:ALA:HB1	2	0.45
(1,440)	1:28:A:ILE:HB	1:70:A:ALA:HB2	2	0.45
(1,440)	1:28:A:ILE:HB	1:70:A:ALA:HB3	2	0.45
(1,323)	1:18:A:LEU:HD21	1:71:A:ALA:HA	2	0.45
(1,323)	1:18:A:LEU:HD22	1:71:A:ALA:HA	2	0.45
(1,323)	1:18:A:LEU:HD23	1:71:A:ALA:HA	2	0.45
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG11	1	0.45
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG12	1	0.45
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG13	1	0.45
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG21	1	0.45
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG22	1	0.45
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG23	1	0.45
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG11	1	0.45
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG12	1	0.45
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG13	1	0.45
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG21	1	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG22	1	0.45
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG23	1	0.45
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG11	8	0.45
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG12	8	0.45
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG13	8	0.45
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG21	8	0.45
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG22	8	0.45
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG23	8	0.45
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG11	8	0.45
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG12	8	0.45
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG13	8	0.45
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG21	8	0.45
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG22	8	0.45
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG23	8	0.45
(1,102)	1:7:A:VAL:HG11	1:120:A:SER:HA	6	0.45
(1,102)	1:7:A:VAL:HG12	1:120:A:SER:HA	6	0.45
(1,102)	1:7:A:VAL:HG13	1:120:A:SER:HA	6	0.45
(1,102)	1:7:A:VAL:HG21	1:120:A:SER:HA	6	0.45
(1,102)	1:7:A:VAL:HG22	1:120:A:SER:HA	6	0.45
(1,102)	1:7:A:VAL:HG23	1:120:A:SER:HA	6	0.45
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB2	1	0.45
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB3	1	0.45
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB2	1	0.45
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB3	1	0.45
(3,49)	1:94:A:PHE:H	1:127:A:PHE:O	10	0.44
(3,41)	1:76:A:VAL:H	1:89:A:LEU:O	2	0.44
(3,26)	1:68:A:ARG:N	1:97:A:TYR:O	7	0.44
(3,10)	1:26:A:TYR:N	1:44:A:GLY:O	10	0.44
(2,34)	1:114:A:VAL:HA	1:117:A:LEU:HA	1	0.44
(2,29)	1:86:A:THR:HG21	1:88:A:THR:HA	7	0.44
(2,29)	1:86:A:THR:HG22	1:88:A:THR:HA	7	0.44
(2,29)	1:86:A:THR:HG23	1:88:A:THR:HA	7	0.44
(1,1777)	1:149:A:ASN:HB2	1:151:A:ARG:H	5	0.44
(1,1777)	1:149:A:ASN:HB3	1:151:A:ARG:H	5	0.44
(1,1777)	1:149:A:ASN:HB2	1:151:A:ARG:H	10	0.44
(1,1777)	1:149:A:ASN:HB3	1:151:A:ARG:H	10	0.44
(1,1725)	1:144:A:SER:HB3	1:145:A:ASP:H	6	0.44
(1,1669)	1:141:A:SER:HB3	1:143:A:LYS:H	5	0.44
(1,1669)	1:141:A:SER:HB3	1:143:A:LYS:H	9	0.44
(1,1665)	1:141:A:SER:HA	1:144:A:SER:H	4	0.44
(1,1581)	1:134:A:MET:HG2	1:135:A:SER:H	6	0.44
(1,1581)	1:134:A:MET:HG3	1:135:A:SER:H	6	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1580)	1:134:A:MET:HB2	1:136:A:ASP:H	8	0.44
(1,1580)	1:134:A:MET:HB3	1:136:A:ASP:H	8	0.44
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	3	0.44
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	3	0.44
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	3	0.44
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	3	0.44
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB2	1	0.44
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB3	1	0.44
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB2	1	0.44
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB3	1	0.44
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB2	1	0.44
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB3	1	0.44
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB2	1	0.44
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB3	1	0.44
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB2	1	0.44
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB3	1	0.44
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB2	1	0.44
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB3	1	0.44
(1,1373)	1:114:A:VAL:HA	1:117:A:LEU:HB2	5	0.44
(1,1373)	1:114:A:VAL:HA	1:117:A:LEU:HB3	5	0.44
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD11	6	0.44
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD12	6	0.44
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD13	6	0.44
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD21	6	0.44
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD22	6	0.44
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD23	6	0.44
(1,1356)	1:112:A:SER:HB2	1:116:A:ALA:HB1	9	0.44
(1,1356)	1:112:A:SER:HB2	1:116:A:ALA:HB2	9	0.44
(1,1356)	1:112:A:SER:HB2	1:116:A:ALA:HB3	9	0.44
(1,1356)	1:112:A:SER:HB3	1:116:A:ALA:HB1	9	0.44
(1,1356)	1:112:A:SER:HB3	1:116:A:ALA:HB2	9	0.44
(1,1356)	1:112:A:SER:HB3	1:116:A:ALA:HB3	9	0.44
(1,1333)	1:110:A:TYR:HA	1:114:A:VAL:H	3	0.44
(1,1314)	1:109:A:LEU:HA	1:112:A:SER:H	8	0.44
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB2	9	0.44
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB3	9	0.44
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB2	9	0.44
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB3	9	0.44
(1,1281)	1:107:A:ARG:HA	1:110:A:TYR:HA	9	0.44
(1,1233)	1:104:A:VAL:HG21	1:106:A:ARG:H	1	0.44
(1,1233)	1:104:A:VAL:HG22	1:106:A:ARG:H	1	0.44
(1,1233)	1:104:A:VAL:HG23	1:106:A:ARG:H	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB2	8	0.44
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB3	8	0.44
(1,935)	1:77:A:THR:HB	1:87:A:SER:H	1	0.44
(1,888)	1:75:A:GLU:HG2	1:76:A:VAL:H	10	0.44
(1,885)	1:75:A:GLU:HB3	1:88:A:THR:HB	10	0.44
(1,705)	1:55:A:GLU:HA	1:59:A:LYS:HB3	2	0.44
(1,705)	1:55:A:GLU:HA	1:59:A:LYS:HB3	3	0.44
(1,669)	1:54:A:VAL:HA	1:56:A:GLU:H	4	0.44
(1,669)	1:54:A:VAL:HA	1:56:A:GLU:H	5	0.44
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB1	2	0.44
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB2	2	0.44
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB3	2	0.44
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG21	1	0.44
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG22	1	0.44
(1,529)	1:33:A:LYS:HG3	1:36:A:THR:HG23	1	0.44
(1,528)	1:33:A:LYS:HG3	1:36:A:THR:HB	5	0.44
(1,516)	1:32:A:ASP:HB2	1:37:A:ALA:H	5	0.44
(1,515)	1:31:A:ILE:HG21	1:37:A:ALA:H	4	0.44
(1,515)	1:31:A:ILE:HG22	1:37:A:ALA:H	4	0.44
(1,515)	1:31:A:ILE:HG23	1:37:A:ALA:H	4	0.44
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD11	6	0.44
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD12	6	0.44
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD13	6	0.44
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD21	6	0.44
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD22	6	0.44
(1,508)	1:31:A:ILE:HG12	1:109:A:LEU:HD23	6	0.44
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD11	6	0.44
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD12	6	0.44
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD13	6	0.44
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD21	6	0.44
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD22	6	0.44
(1,508)	1:31:A:ILE:HG13	1:109:A:LEU:HD23	6	0.44
(1,494)	1:31:A:ILE:HG12	1:38:A:ILE:HA	6	0.44
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG2	5	0.44
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG3	5	0.44
(1,323)	1:18:A:LEU:HD21	1:71:A:ALA:HA	3	0.44
(1,323)	1:18:A:LEU:HD22	1:71:A:ALA:HA	3	0.44
(1,323)	1:18:A:LEU:HD23	1:71:A:ALA:HA	3	0.44
(1,302)	1:17:A:LEU:HD21	1:19:A:HIS:H	3	0.44
(1,302)	1:17:A:LEU:HD22	1:19:A:HIS:H	3	0.44
(1,302)	1:17:A:LEU:HD23	1:19:A:HIS:H	3	0.44
(1,281)	1:16:A:ASP:HB3	1:19:A:HIS:H	6	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG11	4	0.44
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG12	4	0.44
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG13	4	0.44
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG21	4	0.44
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG22	4	0.44
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG23	4	0.44
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG11	4	0.44
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG12	4	0.44
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG13	4	0.44
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG21	4	0.44
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG22	4	0.44
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG23	4	0.44
(1,214)	1:12:A:LYS:HG3	1:15:A:TYR:H	3	0.44
(1,161)	1:10:A:SER:HB2	1:12:A:LYS:H	10	0.44
(1,161)	1:10:A:SER:HB3	1:12:A:LYS:H	10	0.44
(1,135)	1:8:A:ASP:HB2	1:39:A:VAL:HB	3	0.44
(1,135)	1:8:A:ASP:HB3	1:39:A:VAL:HB	3	0.44
(1,123)	1:8:A:ASP:HB2	1:39:A:VAL:HA	4	0.44
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG11	3	0.44
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG12	3	0.44
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG13	3	0.44
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG21	3	0.44
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG22	3	0.44
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG23	3	0.44
(1,111)	1:7:A:VAL:HG11	1:9:A:PRO:HA	3	0.44
(1,111)	1:7:A:VAL:HG12	1:9:A:PRO:HA	3	0.44
(1,111)	1:7:A:VAL:HG13	1:9:A:PRO:HA	3	0.44
(1,111)	1:7:A:VAL:HG21	1:9:A:PRO:HA	3	0.44
(1,111)	1:7:A:VAL:HG22	1:9:A:PRO:HA	3	0.44
(1,111)	1:7:A:VAL:HG23	1:9:A:PRO:HA	3	0.44
(1,93)	1:7:A:VAL:HG21	1:38:A:ILE:H	7	0.44
(1,93)	1:7:A:VAL:HG22	1:38:A:ILE:H	7	0.44
(1,93)	1:7:A:VAL:HG23	1:38:A:ILE:H	7	0.44
(1,65)	1:7:A:VAL:HA	1:37:A:ALA:HA	5	0.44
(3,59)	1:143:A:LYS:O	1:147:A:MET:H	9	0.43
(2,6)	1:12:A:LYS:HG2	1:15:A:TYR:H	5	0.43
(2,3)	1:5:A:VAL:HB	1:117:A:LEU:HG	2	0.43
(1,1803)	1:151:A:ARG:HG2	1:152:A:ILE:H	9	0.43
(1,1803)	1:151:A:ARG:HG3	1:152:A:ILE:H	9	0.43
(1,1725)	1:144:A:SER:HB3	1:145:A:ASP:H	7	0.43
(1,1719)	1:144:A:SER:HA	1:146:A:LEU:H	8	0.43
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD2	1	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD3	1	0.43
(1,1669)	1:141:A:SER:HB3	1:143:A:LYS:H	3	0.43
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG11	1	0.43
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG12	1	0.43
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG13	1	0.43
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG21	1	0.43
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG22	1	0.43
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG23	1	0.43
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG11	1	0.43
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG12	1	0.43
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG13	1	0.43
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG21	1	0.43
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG22	1	0.43
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG23	1	0.43
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG11	4	0.43
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG12	4	0.43
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG13	4	0.43
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG21	4	0.43
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG22	4	0.43
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG23	4	0.43
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG11	4	0.43
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG12	4	0.43
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG13	4	0.43
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG21	4	0.43
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG22	4	0.43
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG23	4	0.43
(1,1579)	1:134:A:MET:HB2	1:135:A:SER:H	9	0.43
(1,1579)	1:134:A:MET:HB3	1:135:A:SER:H	9	0.43
(1,1555)	1:132:A:SER:H	1:136:A:ASP:HA	7	0.43
(1,1498)	1:123:A:LEU:H	1:125:A:SER:H	2	0.43
(1,1344)	1:111:A:ALA:HA	1:115:A:ARG:H	3	0.43
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB2	1	0.43
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB3	1	0.43
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB2	1	0.43
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB3	1	0.43
(1,1224)	1:104:A:VAL:HB	1:106:A:ARG:H	2	0.43
(1,1182)	1:99:A:PRO:HB3	1:132:A:SER:HA	7	0.43
(1,1178)	1:99:A:PRO:HB2	1:102:A:ALA:HA	5	0.43
(1,1117)	1:94:A:PHE:HA	1:128:A:GLN:HA	9	0.43
(1,1067)	1:92:A:VAL:H	1:127:A:PHE:H	8	0.43
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	2	0.43
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	2	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	2	0.43
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG11	2	0.43
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG12	2	0.43
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG13	2	0.43
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	2	0.43
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	2	0.43
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	2	0.43
(1,902)	1:75:A:GLU:HG2	1:90:A:ASN:HB2	9	0.43
(1,902)	1:75:A:GLU:HG2	1:90:A:ASN:HB3	9	0.43
(1,902)	1:75:A:GLU:HG3	1:90:A:ASN:HB2	9	0.43
(1,902)	1:75:A:GLU:HG3	1:90:A:ASN:HB3	9	0.43
(1,888)	1:75:A:GLU:HG2	1:76:A:VAL:H	4	0.43
(1,888)	1:75:A:GLU:HG2	1:76:A:VAL:H	7	0.43
(1,884)	1:75:A:GLU:HB3	1:88:A:THR:HA	6	0.43
(1,800)	1:64:A:GLY:H	1:65:A:LYS:H	9	0.43
(1,654)	1:53:A:PHE:HA	1:55:A:GLU:H	3	0.43
(1,611)	1:49:A:PRO:HG2	1:52:A:GLU:H	3	0.43
(1,611)	1:49:A:PRO:HG3	1:52:A:GLU:H	3	0.43
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG11	10	0.43
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG12	10	0.43
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG13	10	0.43
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG21	10	0.43
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG22	10	0.43
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG23	10	0.43
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG11	10	0.43
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG12	10	0.43
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG13	10	0.43
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG21	10	0.43
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG22	10	0.43
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG23	10	0.43
(1,328)	1:18:A:LEU:HD11	1:24:A:HIS:HB2	8	0.43
(1,328)	1:18:A:LEU:HD11	1:24:A:HIS:HB3	8	0.43
(1,328)	1:18:A:LEU:HD12	1:24:A:HIS:HB2	8	0.43
(1,328)	1:18:A:LEU:HD12	1:24:A:HIS:HB3	8	0.43
(1,328)	1:18:A:LEU:HD13	1:24:A:HIS:HB2	8	0.43
(1,328)	1:18:A:LEU:HD13	1:24:A:HIS:HB3	8	0.43
(1,328)	1:18:A:LEU:HD21	1:24:A:HIS:HB2	8	0.43
(1,328)	1:18:A:LEU:HD21	1:24:A:HIS:HB3	8	0.43
(1,328)	1:18:A:LEU:HD22	1:24:A:HIS:HB2	8	0.43
(1,328)	1:18:A:LEU:HD22	1:24:A:HIS:HB3	8	0.43
(1,328)	1:18:A:LEU:HD23	1:24:A:HIS:HB2	8	0.43
(1,328)	1:18:A:LEU:HD23	1:24:A:HIS:HB3	8	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG11	7	0.43
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG12	7	0.43
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG13	7	0.43
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG21	7	0.43
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG22	7	0.43
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG23	7	0.43
(1,75)	1:7:A:VAL:HB	1:38:A:ILE:H	4	0.43
(3,3)	1:8:A:ASP:H	1:38:A:ILE:O	7	0.42
(2,3)	1:5:A:VAL:HB	1:117:A:LEU:HG	3	0.42
(1,1725)	1:144:A:SER:HB3	1:145:A:ASP:H	10	0.42
(1,1721)	1:144:A:SER:HA	1:148:A:SER:H	3	0.42
(1,1719)	1:144:A:SER:HA	1:146:A:LEU:H	1	0.42
(1,1719)	1:144:A:SER:HA	1:146:A:LEU:H	4	0.42
(1,1652)	1:140:A:LYS:HE2	1:141:A:SER:H	3	0.42
(1,1581)	1:134:A:MET:HG2	1:135:A:SER:H	3	0.42
(1,1581)	1:134:A:MET:HG3	1:135:A:SER:H	3	0.42
(1,1581)	1:134:A:MET:HG2	1:135:A:SER:H	7	0.42
(1,1581)	1:134:A:MET:HG3	1:135:A:SER:H	7	0.42
(1,1286)	1:107:A:ARG:HD2	1:111:A:ALA:HA	5	0.42
(1,1286)	1:107:A:ARG:HD3	1:111:A:ALA:HA	5	0.42
(1,1286)	1:107:A:ARG:HD2	1:111:A:ALA:HA	9	0.42
(1,1286)	1:107:A:ARG:HD3	1:111:A:ALA:HA	9	0.42
(1,1239)	1:104:A:VAL:HG11	1:107:A:ARG:H	4	0.42
(1,1239)	1:104:A:VAL:HG12	1:107:A:ARG:H	4	0.42
(1,1239)	1:104:A:VAL:HG13	1:107:A:ARG:H	4	0.42
(1,1239)	1:104:A:VAL:HG21	1:107:A:ARG:H	4	0.42
(1,1239)	1:104:A:VAL:HG22	1:107:A:ARG:H	4	0.42
(1,1239)	1:104:A:VAL:HG23	1:107:A:ARG:H	4	0.42
(1,1196)	1:100:A:ASP:HA	1:132:A:SER:HB3	10	0.42
(1,1187)	1:99:A:PRO:HG2	1:132:A:SER:HB3	4	0.42
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB2	7	0.42
(1,1120)	1:94:A:PHE:HA	1:128:A:GLN:HB3	7	0.42
(1,1114)	1:94:A:PHE:H	1:129:A:VAL:H	4	0.42
(1,1092)	1:93:A:ILE:HG12	1:127:A:PHE:H	3	0.42
(1,1092)	1:93:A:ILE:HG12	1:127:A:PHE:H	9	0.42
(1,960)	1:78:A:VAL:HG21	1:87:A:SER:HB2	8	0.42
(1,960)	1:78:A:VAL:HG22	1:87:A:SER:HB2	8	0.42
(1,960)	1:78:A:VAL:HG23	1:87:A:SER:HB2	8	0.42
(1,960)	1:78:A:VAL:HG21	1:87:A:SER:HB3	8	0.42
(1,960)	1:78:A:VAL:HG22	1:87:A:SER:HB3	8	0.42
(1,960)	1:78:A:VAL:HG23	1:87:A:SER:HB3	8	0.42
(1,883)	1:75:A:GLU:HB3	1:76:A:VAL:H	4	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,883)	1:75:A:GLU:HB3	1:76:A:VAL:H	8	0.42
(1,800)	1:64:A:GLY:H	1:65:A:LYS:H	2	0.42
(1,675)	1:54:A:VAL:HB	1:56:A:GLU:H	8	0.42
(1,606)	1:49:A:PRO:HB3	1:52:A:GLU:H	6	0.42
(1,516)	1:32:A:ASP:HB2	1:37:A:ALA:H	6	0.42
(1,489)	1:31:A:ILE:HA	1:38:A:ILE:HD11	1	0.42
(1,489)	1:31:A:ILE:HA	1:38:A:ILE:HD12	1	0.42
(1,489)	1:31:A:ILE:HA	1:38:A:ILE:HD13	1	0.42
(1,452)	1:28:A:ILE:HD11	1:71:A:ALA:H	5	0.42
(1,452)	1:28:A:ILE:HD12	1:71:A:ALA:H	5	0.42
(1,452)	1:28:A:ILE:HD13	1:71:A:ALA:H	5	0.42
(1,382)	1:26:A:TYR:HB3	1:72:A:VAL:HA	5	0.42
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB1	10	0.42
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB2	10	0.42
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB3	10	0.42
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB1	10	0.42
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB2	10	0.42
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB3	10	0.42
(1,280)	1:16:A:ASP:HB3	1:18:A:LEU:H	8	0.42
(1,226)	1:13:A:ASN:HB2	1:14:A:ALA:H	8	0.42
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG11	4	0.42
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG12	4	0.42
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG13	4	0.42
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG21	4	0.42
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG22	4	0.42
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG23	4	0.42
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD11	9	0.42
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD12	9	0.42
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD13	9	0.42
(1,33)	1:5:A:VAL:HB	1:7:A:VAL:HA	9	0.42
(3,59)	1:143:A:LYS:O	1:147:A:MET:H	7	0.41
(3,3)	1:8:A:ASP:H	1:38:A:ILE:O	9	0.41
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG11	2	0.41
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG12	2	0.41
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG13	2	0.41
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG11	4	0.41
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG12	4	0.41
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG13	4	0.41
(2,2)	1:2:A:ALA:HB1	1:112:A:SER:H	9	0.41
(2,2)	1:2:A:ALA:HB2	1:112:A:SER:H	9	0.41
(2,2)	1:2:A:ALA:HB3	1:112:A:SER:H	9	0.41
(1,1777)	1:149:A:ASN:HB2	1:151:A:ARG:H	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1777)	1:149:A:ASN:HB3	1:151:A:ARG:H	8	0.41
(1,1769)	1:149:A:ASN:H	1:150:A:GLN:H	7	0.41
(1,1745)	1:146:A:LEU:HG	1:147:A:MET:H	1	0.41
(1,1729)	1:145:A:ASP:H	1:146:A:LEU:H	5	0.41
(1,1729)	1:145:A:ASP:H	1:146:A:LEU:H	6	0.41
(1,1658)	1:140:A:LYS:HB2	1:142:A:VAL:H	2	0.41
(1,1658)	1:140:A:LYS:HB3	1:142:A:VAL:H	2	0.41
(1,1649)	1:140:A:LYS:HD2	1:142:A:VAL:H	8	0.41
(1,1580)	1:134:A:MET:HB2	1:136:A:ASP:H	5	0.41
(1,1580)	1:134:A:MET:HB3	1:136:A:ASP:H	5	0.41
(1,1576)	1:134:A:MET:HA	1:138:A:ASP:H	9	0.41
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	7	0.41
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	7	0.41
(1,1410)	1:116:A:ALA:HA	1:120:A:SER:H	6	0.41
(1,1378)	1:114:A:VAL:HB	1:118:A:LYS:H	7	0.41
(1,1375)	1:114:A:VAL:HA	1:118:A:LYS:H	10	0.41
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD11	10	0.41
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD12	10	0.41
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD13	10	0.41
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD21	10	0.41
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD22	10	0.41
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD23	10	0.41
(1,1286)	1:107:A:ARG:HD2	1:111:A:ALA:HA	8	0.41
(1,1286)	1:107:A:ARG:HD3	1:111:A:ALA:HA	8	0.41
(1,1099)	1:93:A:ILE:HD11	1:142:A:VAL:HA	7	0.41
(1,1099)	1:93:A:ILE:HD12	1:142:A:VAL:HA	7	0.41
(1,1099)	1:93:A:ILE:HD13	1:142:A:VAL:HA	7	0.41
(1,1097)	1:93:A:ILE:HD11	1:129:A:VAL:HA	2	0.41
(1,1097)	1:93:A:ILE:HD12	1:129:A:VAL:HA	2	0.41
(1,1097)	1:93:A:ILE:HD13	1:129:A:VAL:HA	2	0.41
(1,1086)	1:93:A:ILE:HB	1:127:A:PHE:H	3	0.41
(1,987)	1:80:A:ARG:H	1:85:A:GLY:H	6	0.41
(1,883)	1:75:A:GLU:HB3	1:76:A:VAL:H	7	0.41
(1,822)	1:70:A:ALA:H	1:94:A:PHE:HA	2	0.41
(1,723)	1:56:A:GLU:HG2	1:57:A:MET:H	9	0.41
(1,664)	1:53:A:PHE:HB2	1:57:A:MET:H	6	0.41
(1,664)	1:53:A:PHE:HB3	1:57:A:MET:H	6	0.41
(1,629)	1:51:A:ALA:HA	1:54:A:VAL:HA	9	0.41
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD11	2	0.41
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD12	2	0.41
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD13	2	0.41
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD21	2	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD22	2	0.41
(1,620)	1:50:A:TYR:HB2	1:137:A:LEU:HD23	2	0.41
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD11	2	0.41
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD12	2	0.41
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD13	2	0.41
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD21	2	0.41
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD22	2	0.41
(1,620)	1:50:A:TYR:HB3	1:137:A:LEU:HD23	2	0.41
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB1	10	0.41
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB2	10	0.41
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB3	10	0.41
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB1	10	0.41
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB2	10	0.41
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB3	10	0.41
(1,600)	1:49:A:PRO:HA	1:53:A:PHE:H	8	0.41
(1,575)	1:42:A:LYS:HB2	1:43:A:VAL:H	1	0.41
(1,575)	1:42:A:LYS:HB3	1:43:A:VAL:H	1	0.41
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG21	3	0.41
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG22	3	0.41
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG23	3	0.41
(1,505)	1:31:A:ILE:HD11	1:32:A:ASP:H	9	0.41
(1,505)	1:31:A:ILE:HD12	1:32:A:ASP:H	9	0.41
(1,505)	1:31:A:ILE:HD13	1:32:A:ASP:H	9	0.41
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD11	5	0.41
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD12	5	0.41
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD13	5	0.41
(1,499)	1:31:A:ILE:HG13	1:38:A:ILE:HB	5	0.41
(1,302)	1:17:A:LEU:HD21	1:19:A:HIS:H	5	0.41
(1,302)	1:17:A:LEU:HD22	1:19:A:HIS:H	5	0.41
(1,302)	1:17:A:LEU:HD23	1:19:A:HIS:H	5	0.41
(1,226)	1:13:A:ASN:HB2	1:14:A:ALA:H	10	0.41
(1,225)	1:13:A:ASN:HA	1:17:A:LEU:H	9	0.41
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD11	4	0.41
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD12	4	0.41
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD13	4	0.41
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD21	4	0.41
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD22	4	0.41
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD23	4	0.41
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD11	4	0.41
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD12	4	0.41
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD13	4	0.41
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD21	4	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD22	4	0.41
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD23	4	0.41
(1,123)	1:8:A:ASP:HB2	1:39:A:VAL:HA	5	0.41
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG11	8	0.41
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG12	8	0.41
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG13	8	0.41
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG21	8	0.41
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG22	8	0.41
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG23	8	0.41
(2,3)	1:5:A:VAL:HB	1:117:A:LEU:HG	1	0.4
(1,1803)	1:151:A:ARG:HG2	1:152:A:ILE:H	6	0.4
(1,1803)	1:151:A:ARG:HG3	1:152:A:ILE:H	6	0.4
(1,1790)	1:150:A:GLN:HB3	1:152:A:ILE:H	4	0.4
(1,1709)	1:143:A:LYS:HB2	1:147:A:MET:H	1	0.4
(1,1700)	1:143:A:LYS:H	1:145:A:ASP:H	5	0.4
(1,1700)	1:143:A:LYS:H	1:145:A:ASP:H	8	0.4
(1,1700)	1:143:A:LYS:H	1:145:A:ASP:H	10	0.4
(1,1699)	1:143:A:LYS:H	1:144:A:SER:H	2	0.4
(1,1594)	1:135:A:SER:HB2	1:140:A:LYS:HG2	10	0.4
(1,1594)	1:135:A:SER:HB2	1:140:A:LYS:HG3	10	0.4
(1,1594)	1:135:A:SER:HB3	1:140:A:LYS:HG2	10	0.4
(1,1594)	1:135:A:SER:HB3	1:140:A:LYS:HG3	10	0.4
(1,1579)	1:134:A:MET:HB2	1:135:A:SER:H	10	0.4
(1,1579)	1:134:A:MET:HB3	1:135:A:SER:H	10	0.4
(1,1436)	1:118:A:LYS:H	1:118:A:LYS:HE2	9	0.4
(1,1436)	1:118:A:LYS:H	1:118:A:LYS:HE3	9	0.4
(1,1419)	1:117:A:LEU:H	1:119:A:ALA:H	1	0.4
(1,1398)	1:115:A:ARG:HA	1:119:A:ALA:H	4	0.4
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB2	10	0.4
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB3	10	0.4
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB2	10	0.4
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB3	10	0.4
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB2	10	0.4
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB3	10	0.4
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB2	10	0.4
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB3	10	0.4
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB2	10	0.4
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB3	10	0.4
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB2	10	0.4
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB3	10	0.4
(1,1208)	1:103:A:PRO:HA	1:107:A:ARG:H	4	0.4
(1,1165)	1:97:A:TYR:HA	1:131:A:ALA:HA	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1117)	1:94:A:PHE:HA	1:128:A:GLN:HA	3	0.4
(1,1114)	1:94:A:PHE:H	1:129:A:VAL:H	6	0.4
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB2	5	0.4
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB3	5	0.4
(1,1087)	1:93:A:ILE:HB	1:127:A:PHE:HB2	10	0.4
(1,1087)	1:93:A:ILE:HB	1:127:A:PHE:HB3	10	0.4
(1,1087)	1:93:A:ILE:HB	1:127:A:PHE:HB2	10	0.4
(1,1087)	1:93:A:ILE:HB	1:127:A:PHE:HB3	10	0.4
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	1	0.4
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	1	0.4
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	1	0.4
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG11	1	0.4
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG12	1	0.4
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG13	1	0.4
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	1	0.4
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	1	0.4
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	1	0.4
(1,883)	1:75:A:GLU:HB3	1:76:A:VAL:H	2	0.4
(1,883)	1:75:A:GLU:HB3	1:76:A:VAL:H	9	0.4
(1,737)	1:57:A:MET:HG2	1:60:A:LEU:HG	5	0.4
(1,737)	1:57:A:MET:HG3	1:60:A:LEU:HG	5	0.4
(1,724)	1:56:A:GLU:HG2	1:58:A:LYS:H	10	0.4
(1,699)	1:55:A:GLU:HA	1:58:A:LYS:HD2	10	0.4
(1,699)	1:55:A:GLU:HA	1:58:A:LYS:HD3	10	0.4
(1,671)	1:54:A:VAL:HA	1:57:A:MET:HA	3	0.4
(1,669)	1:54:A:VAL:HA	1:56:A:GLU:H	8	0.4
(1,655)	1:53:A:PHE:HA	1:56:A:GLU:H	8	0.4
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG21	8	0.4
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG22	8	0.4
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG23	8	0.4
(1,480)	1:30:A:LYS:HB2	1:41:A:GLU:HA	7	0.4
(1,480)	1:30:A:LYS:HB3	1:41:A:GLU:HA	7	0.4
(1,454)	1:28:A:ILE:HG12	1:41:A:GLU:HG2	4	0.4
(1,454)	1:28:A:ILE:HG12	1:41:A:GLU:HG3	4	0.4
(1,454)	1:28:A:ILE:HG13	1:41:A:GLU:HG2	4	0.4
(1,454)	1:28:A:ILE:HG13	1:41:A:GLU:HG3	4	0.4
(1,370)	1:25:A:SER:HB2	1:73:A:ASP:HB2	10	0.4
(1,370)	1:25:A:SER:HB2	1:73:A:ASP:HB3	10	0.4
(1,370)	1:25:A:SER:HB3	1:73:A:ASP:HB2	10	0.4
(1,370)	1:25:A:SER:HB3	1:73:A:ASP:HB3	10	0.4
(1,296)	1:17:A:LEU:HA	1:23:A:GLN:HB2	8	0.4
(1,296)	1:17:A:LEU:HA	1:23:A:GLN:HB3	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,245)	1:14:A:ALA:HB1	1:40:A:VAL:HB	4	0.4
(1,245)	1:14:A:ALA:HB2	1:40:A:VAL:HB	4	0.4
(1,245)	1:14:A:ALA:HB3	1:40:A:VAL:HB	4	0.4
(1,226)	1:13:A:ASN:HB2	1:14:A:ALA:H	3	0.4
(1,214)	1:12:A:LYS:HG3	1:15:A:TYR:H	7	0.4
(1,162)	1:10:A:SER:HB2	1:13:A:ASN:H	7	0.4
(1,162)	1:10:A:SER:HB3	1:13:A:ASN:H	7	0.4
(1,162)	1:10:A:SER:HB2	1:13:A:ASN:H	8	0.4
(1,162)	1:10:A:SER:HB3	1:13:A:ASN:H	8	0.4
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG11	5	0.4
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG12	5	0.4
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG13	5	0.4
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG21	5	0.4
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG22	5	0.4
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG23	5	0.4
(1,108)	1:7:A:VAL:HG11	1:38:A:ILE:HB	8	0.4
(1,108)	1:7:A:VAL:HG12	1:38:A:ILE:HB	8	0.4
(1,108)	1:7:A:VAL:HG13	1:38:A:ILE:HB	8	0.4
(1,108)	1:7:A:VAL:HG21	1:38:A:ILE:HB	8	0.4
(1,108)	1:7:A:VAL:HG22	1:38:A:ILE:HB	8	0.4
(1,108)	1:7:A:VAL:HG23	1:38:A:ILE:HB	8	0.4
(3,4)	1:8:A:ASP:N	1:38:A:ILE:O	5	0.39
(2,6)	1:12:A:LYS:HG2	1:15:A:TYR:H	9	0.39
(1,1799)	1:151:A:ARG:H	1:152:A:ILE:H	9	0.39
(1,1700)	1:143:A:LYS:H	1:145:A:ASP:H	4	0.39
(1,1660)	1:140:A:LYS:HG2	1:142:A:VAL:H	8	0.39
(1,1660)	1:140:A:LYS:HG3	1:142:A:VAL:H	8	0.39
(1,1659)	1:140:A:LYS:HB2	1:143:A:LYS:H	2	0.39
(1,1659)	1:140:A:LYS:HB3	1:143:A:LYS:H	2	0.39
(1,1658)	1:140:A:LYS:HB2	1:142:A:VAL:H	1	0.39
(1,1658)	1:140:A:LYS:HB3	1:142:A:VAL:H	1	0.39
(1,1649)	1:140:A:LYS:HD2	1:142:A:VAL:H	5	0.39
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD2	7	0.39
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD3	7	0.39
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD2	7	0.39
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD3	7	0.39
(1,1579)	1:134:A:MET:HB2	1:135:A:SER:H	4	0.39
(1,1579)	1:134:A:MET:HB3	1:135:A:SER:H	4	0.39
(1,1576)	1:134:A:MET:HA	1:138:A:ASP:H	8	0.39
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	5	0.39
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	5	0.39
(1,1436)	1:118:A:LYS:H	1:118:A:LYS:HE2	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1436)	1:118:A:LYS:H	1:118:A:LYS:HE3	7	0.39
(1,1426)	1:117:A:LEU:HB2	1:119:A:ALA:H	9	0.39
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD11	9	0.39
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD12	9	0.39
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD13	9	0.39
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD21	9	0.39
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD22	9	0.39
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD23	9	0.39
(1,1235)	1:104:A:VAL:HG21	1:108:A:MET:H	7	0.39
(1,1235)	1:104:A:VAL:HG22	1:108:A:MET:H	7	0.39
(1,1235)	1:104:A:VAL:HG23	1:108:A:MET:H	7	0.39
(1,1207)	1:103:A:PRO:HA	1:106:A:ARG:H	7	0.39
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG11	5	0.39
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG12	5	0.39
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG13	5	0.39
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG21	5	0.39
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG22	5	0.39
(1,1161)	1:96:A:GLN:HG2	1:114:A:VAL:HG23	5	0.39
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG11	5	0.39
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG12	5	0.39
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG13	5	0.39
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG21	5	0.39
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG22	5	0.39
(1,1161)	1:96:A:GLN:HG3	1:114:A:VAL:HG23	5	0.39
(1,1118)	1:94:A:PHE:HA	1:128:A:GLN:HB2	2	0.39
(1,1114)	1:94:A:PHE:H	1:129:A:VAL:H	2	0.39
(1,1082)	1:93:A:ILE:HA	1:127:A:PHE:HA	2	0.39
(1,1027)	1:86:A:THR:HB	1:87:A:SER:H	5	0.39
(1,1018)	1:84:A:GLU:HG2	1:85:A:GLY:H	2	0.39
(1,1018)	1:84:A:GLU:HG3	1:85:A:GLY:H	2	0.39
(1,953)	1:78:A:VAL:HB	1:87:A:SER:HB2	8	0.39
(1,953)	1:78:A:VAL:HB	1:87:A:SER:HB3	8	0.39
(1,909)	1:76:A:VAL:H	1:89:A:LEU:H	10	0.39
(1,892)	1:75:A:GLU:HG2	1:90:A:ASN:HA	10	0.39
(1,890)	1:75:A:GLU:HG2	1:88:A:THR:HG21	9	0.39
(1,890)	1:75:A:GLU:HG2	1:88:A:THR:HG22	9	0.39
(1,890)	1:75:A:GLU:HG2	1:88:A:THR:HG23	9	0.39
(1,888)	1:75:A:GLU:HG2	1:76:A:VAL:H	1	0.39
(1,887)	1:75:A:GLU:HB3	1:89:A:LEU:H	9	0.39
(1,886)	1:75:A:GLU:HB3	1:88:A:THR:HG21	9	0.39
(1,886)	1:75:A:GLU:HB3	1:88:A:THR:HG22	9	0.39
(1,886)	1:75:A:GLU:HB3	1:88:A:THR:HG23	9	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,883)	1:75:A:GLU:HB3	1:76:A:VAL:H	10	0.39
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD11	8	0.39
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD12	8	0.39
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD13	8	0.39
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD21	8	0.39
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD22	8	0.39
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD23	8	0.39
(1,800)	1:64:A:GLY:H	1:65:A:LYS:H	1	0.39
(1,751)	1:58:A:LYS:HB2	1:60:A:LEU:H	1	0.39
(1,659)	1:53:A:PHE:HB2	1:56:A:GLU:H	1	0.39
(1,654)	1:53:A:PHE:HA	1:55:A:GLU:H	1	0.39
(1,644)	1:52:A:GLU:HA	1:55:A:GLU:H	6	0.39
(1,590)	1:45:A:GLU:HB2	1:48:A:ALA:HA	2	0.39
(1,521)	1:33:A:LYS:HE2	1:35:A:ASP:H	7	0.39
(1,521)	1:33:A:LYS:HE3	1:35:A:ASP:H	7	0.39
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG11	10	0.39
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG12	10	0.39
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG13	10	0.39
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG21	10	0.39
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG22	10	0.39
(1,484)	1:30:A:LYS:HG2	1:39:A:VAL:HG23	10	0.39
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG11	10	0.39
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG12	10	0.39
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG13	10	0.39
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG21	10	0.39
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG22	10	0.39
(1,484)	1:30:A:LYS:HG3	1:39:A:VAL:HG23	10	0.39
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD2	10	0.39
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD3	10	0.39
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD2	10	0.39
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD3	10	0.39
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD2	10	0.39
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD3	10	0.39
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD2	10	0.39
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD3	10	0.39
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD2	10	0.39
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD3	10	0.39
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD2	10	0.39
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD3	10	0.39
(1,226)	1:13:A:ASN:HB2	1:14:A:ALA:H	5	0.39
(1,181)	1:11:A:CYS:HB3	1:13:A:ASN:H	7	0.39
(1,123)	1:8:A:ASP:HB2	1:39:A:VAL:HA	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:8:A:ASP:HB2	1:10:A:SER:H	10	0.39
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG11	9	0.39
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG12	9	0.39
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG13	9	0.39
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG21	9	0.39
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG22	9	0.39
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG23	9	0.39
(1,108)	1:7:A:VAL:HG11	1:38:A:ILE:HB	7	0.39
(1,108)	1:7:A:VAL:HG12	1:38:A:ILE:HB	7	0.39
(1,108)	1:7:A:VAL:HG13	1:38:A:ILE:HB	7	0.39
(1,108)	1:7:A:VAL:HG21	1:38:A:ILE:HB	7	0.39
(1,108)	1:7:A:VAL:HG22	1:38:A:ILE:HB	7	0.39
(1,108)	1:7:A:VAL:HG23	1:38:A:ILE:HB	7	0.39
(1,102)	1:7:A:VAL:HG11	1:120:A:SER:HA	7	0.39
(1,102)	1:7:A:VAL:HG12	1:120:A:SER:HA	7	0.39
(1,102)	1:7:A:VAL:HG13	1:120:A:SER:HA	7	0.39
(1,102)	1:7:A:VAL:HG21	1:120:A:SER:HA	7	0.39
(1,102)	1:7:A:VAL:HG22	1:120:A:SER:HA	7	0.39
(1,102)	1:7:A:VAL:HG23	1:120:A:SER:HA	7	0.39
(1,41)	1:5:A:VAL:HG11	1:37:A:ALA:HB1	5	0.39
(1,41)	1:5:A:VAL:HG11	1:37:A:ALA:HB2	5	0.39
(1,41)	1:5:A:VAL:HG11	1:37:A:ALA:HB3	5	0.39
(1,41)	1:5:A:VAL:HG12	1:37:A:ALA:HB1	5	0.39
(1,41)	1:5:A:VAL:HG12	1:37:A:ALA:HB2	5	0.39
(1,41)	1:5:A:VAL:HG12	1:37:A:ALA:HB3	5	0.39
(1,41)	1:5:A:VAL:HG13	1:37:A:ALA:HB1	5	0.39
(1,41)	1:5:A:VAL:HG13	1:37:A:ALA:HB2	5	0.39
(1,41)	1:5:A:VAL:HG13	1:37:A:ALA:HB3	5	0.39
(1,41)	1:5:A:VAL:HG21	1:37:A:ALA:HB1	5	0.39
(1,41)	1:5:A:VAL:HG21	1:37:A:ALA:HB2	5	0.39
(1,41)	1:5:A:VAL:HG21	1:37:A:ALA:HB3	5	0.39
(1,41)	1:5:A:VAL:HG22	1:37:A:ALA:HB1	5	0.39
(1,41)	1:5:A:VAL:HG22	1:37:A:ALA:HB2	5	0.39
(1,41)	1:5:A:VAL:HG22	1:37:A:ALA:HB3	5	0.39
(1,41)	1:5:A:VAL:HG23	1:37:A:ALA:HB1	5	0.39
(1,41)	1:5:A:VAL:HG23	1:37:A:ALA:HB2	5	0.39
(1,41)	1:5:A:VAL:HG23	1:37:A:ALA:HB3	5	0.39
(1,33)	1:5:A:VAL:HB	1:7:A:VAL:HA	6	0.39
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG11	6	0.39
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG12	6	0.39
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG13	6	0.39
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG21	6	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG22	6	0.39
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG23	6	0.39
(3,60)	1:143:A:LYS:O	1:147:A:MET:N	10	0.38
(3,50)	1:94:A:PHE:N	1:127:A:PHE:O	10	0.38
(3,27)	1:68:A:ARG:O	1:97:A:TYR:H	9	0.38
(3,7)	1:13:A:ASN:O	1:17:A:LEU:H	2	0.38
(3,3)	1:8:A:ASP:H	1:38:A:ILE:O	8	0.38
(1,1665)	1:141:A:SER:HA	1:144:A:SER:H	3	0.38
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG2	5	0.38
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG3	5	0.38
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG2	5	0.38
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG3	5	0.38
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG2	5	0.38
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG3	5	0.38
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG2	5	0.38
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG3	5	0.38
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG2	5	0.38
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG3	5	0.38
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG2	5	0.38
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG3	5	0.38
(1,1579)	1:134:A:MET:HB2	1:135:A:SER:H	2	0.38
(1,1579)	1:134:A:MET:HB3	1:135:A:SER:H	2	0.38
(1,1575)	1:134:A:MET:HA	1:137:A:LEU:H	3	0.38
(1,1555)	1:132:A:SER:H	1:136:A:ASP:HA	3	0.38
(1,1547)	1:130:A:GLN:HG2	1:131:A:ALA:H	5	0.38
(1,1547)	1:130:A:GLN:HG3	1:131:A:ALA:H	5	0.38
(1,1436)	1:118:A:LYS:H	1:118:A:LYS:HE2	8	0.38
(1,1436)	1:118:A:LYS:H	1:118:A:LYS:HE3	8	0.38
(1,1410)	1:116:A:ALA:HA	1:120:A:SER:H	1	0.38
(1,1239)	1:104:A:VAL:HG11	1:107:A:ARG:H	7	0.38
(1,1239)	1:104:A:VAL:HG12	1:107:A:ARG:H	7	0.38
(1,1239)	1:104:A:VAL:HG13	1:107:A:ARG:H	7	0.38
(1,1239)	1:104:A:VAL:HG21	1:107:A:ARG:H	7	0.38
(1,1239)	1:104:A:VAL:HG22	1:107:A:ARG:H	7	0.38
(1,1239)	1:104:A:VAL:HG23	1:107:A:ARG:H	7	0.38
(1,1235)	1:104:A:VAL:HG21	1:108:A:MET:H	5	0.38
(1,1235)	1:104:A:VAL:HG22	1:108:A:MET:H	5	0.38
(1,1235)	1:104:A:VAL:HG23	1:108:A:MET:H	5	0.38
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB1	2	0.38
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB2	2	0.38
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB3	2	0.38
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB1	7	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB2	7	0.38
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB3	7	0.38
(1,1165)	1:97:A:TYR:HA	1:131:A:ALA:HA	2	0.38
(1,1117)	1:94:A:PHE:HA	1:128:A:GLN:HA	8	0.38
(1,1114)	1:94:A:PHE:H	1:129:A:VAL:H	1	0.38
(1,1099)	1:93:A:ILE:HD11	1:142:A:VAL:HA	10	0.38
(1,1099)	1:93:A:ILE:HD12	1:142:A:VAL:HA	10	0.38
(1,1099)	1:93:A:ILE:HD13	1:142:A:VAL:HA	10	0.38
(1,1067)	1:92:A:VAL:H	1:127:A:PHE:H	5	0.38
(1,1030)	1:87:A:SER:H	1:88:A:THR:H	6	0.38
(1,1003)	1:82:A:GLY:H	1:83:A:ALA:H	2	0.38
(1,985)	1:80:A:ARG:H	1:80:A:ARG:HG2	8	0.38
(1,985)	1:80:A:ARG:H	1:80:A:ARG:HG3	8	0.38
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG21	6	0.38
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG22	6	0.38
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG23	6	0.38
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG2	7	0.38
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG3	7	0.38
(1,889)	1:75:A:GLU:HG2	1:88:A:THR:HB	8	0.38
(1,736)	1:57:A:MET:HB2	1:60:A:LEU:HG	6	0.38
(1,736)	1:57:A:MET:HB3	1:60:A:LEU:HG	6	0.38
(1,700)	1:55:A:GLU:HA	1:58:A:LYS:HE2	3	0.38
(1,700)	1:55:A:GLU:HA	1:58:A:LYS:HE3	3	0.38
(1,697)	1:55:A:GLU:HA	1:57:A:MET:H	1	0.38
(1,697)	1:55:A:GLU:HA	1:57:A:MET:H	3	0.38
(1,671)	1:54:A:VAL:HA	1:57:A:MET:HA	2	0.38
(1,575)	1:42:A:LYS:HB2	1:43:A:VAL:H	3	0.38
(1,575)	1:42:A:LYS:HB3	1:43:A:VAL:H	3	0.38
(1,507)	1:31:A:ILE:HG12	1:109:A:LEU:HB2	10	0.38
(1,507)	1:31:A:ILE:HG12	1:109:A:LEU:HB3	10	0.38
(1,507)	1:31:A:ILE:HG13	1:109:A:LEU:HB2	10	0.38
(1,507)	1:31:A:ILE:HG13	1:109:A:LEU:HB3	10	0.38
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG2	5	0.38
(1,482)	1:30:A:LYS:HB2	1:41:A:GLU:HG3	5	0.38
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG2	5	0.38
(1,482)	1:30:A:LYS:HB3	1:41:A:GLU:HG3	5	0.38
(1,398)	1:27:A:ILE:HA	1:43:A:VAL:HB	2	0.38
(1,385)	1:26:A:TYR:HB2	1:72:A:VAL:HA	2	0.38
(1,385)	1:26:A:TYR:HB3	1:72:A:VAL:HA	2	0.38
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD2	8	0.38
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD3	8	0.38
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD2	8	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD3	8	0.38
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD2	8	0.38
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD3	8	0.38
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD2	8	0.38
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD3	8	0.38
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD2	8	0.38
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD3	8	0.38
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD2	8	0.38
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD3	8	0.38
(1,294)	1:17:A:LEU:HA	1:21:A:LYS:HD2	3	0.38
(1,294)	1:17:A:LEU:HA	1:21:A:LYS:HD3	3	0.38
(1,272)	1:16:A:ASP:HA	1:18:A:LEU:H	8	0.38
(1,255)	1:15:A:TYR:HA	1:19:A:HIS:H	5	0.38
(1,227)	1:13:A:ASN:HB2	1:15:A:TYR:H	8	0.38
(1,226)	1:13:A:ASN:HB2	1:14:A:ALA:H	2	0.38
(1,226)	1:13:A:ASN:HB2	1:14:A:ALA:H	7	0.38
(1,218)	1:12:A:LYS:HG2	1:121:A:LEU:HA	8	0.38
(1,218)	1:12:A:LYS:HG3	1:121:A:LEU:HA	8	0.38
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG11	2	0.38
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG12	2	0.38
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG13	2	0.38
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG21	2	0.38
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG22	2	0.38
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG23	2	0.38
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG11	2	0.38
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG12	2	0.38
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG13	2	0.38
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG21	2	0.38
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG22	2	0.38
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG23	2	0.38
(1,214)	1:12:A:LYS:HG3	1:15:A:TYR:H	4	0.38
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD11	1	0.38
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD12	1	0.38
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD13	1	0.38
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD21	1	0.38
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD22	1	0.38
(1,179)	1:11:A:CYS:HB3	1:121:A:LEU:HD23	1	0.38
(1,158)	1:10:A:SER:HB3	1:12:A:LYS:H	8	0.38
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG11	2	0.38
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG12	2	0.38
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG13	2	0.38
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG21	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG22	2	0.38
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG23	2	0.38
(1,108)	1:7:A:VAL:HG11	1:38:A:ILE:HB	3	0.38
(1,108)	1:7:A:VAL:HG12	1:38:A:ILE:HB	3	0.38
(1,108)	1:7:A:VAL:HG13	1:38:A:ILE:HB	3	0.38
(1,108)	1:7:A:VAL:HG21	1:38:A:ILE:HB	3	0.38
(1,108)	1:7:A:VAL:HG22	1:38:A:ILE:HB	3	0.38
(1,108)	1:7:A:VAL:HG23	1:38:A:ILE:HB	3	0.38
(1,107)	1:7:A:VAL:HG11	1:38:A:ILE:H	5	0.38
(1,107)	1:7:A:VAL:HG12	1:38:A:ILE:H	5	0.38
(1,107)	1:7:A:VAL:HG13	1:38:A:ILE:H	5	0.38
(1,107)	1:7:A:VAL:HG21	1:38:A:ILE:H	5	0.38
(1,107)	1:7:A:VAL:HG22	1:38:A:ILE:H	5	0.38
(1,107)	1:7:A:VAL:HG23	1:38:A:ILE:H	5	0.38
(1,106)	1:7:A:VAL:HG11	1:37:A:ALA:HB1	5	0.38
(1,106)	1:7:A:VAL:HG11	1:37:A:ALA:HB2	5	0.38
(1,106)	1:7:A:VAL:HG11	1:37:A:ALA:HB3	5	0.38
(1,106)	1:7:A:VAL:HG12	1:37:A:ALA:HB1	5	0.38
(1,106)	1:7:A:VAL:HG12	1:37:A:ALA:HB2	5	0.38
(1,106)	1:7:A:VAL:HG12	1:37:A:ALA:HB3	5	0.38
(1,106)	1:7:A:VAL:HG13	1:37:A:ALA:HB1	5	0.38
(1,106)	1:7:A:VAL:HG13	1:37:A:ALA:HB2	5	0.38
(1,106)	1:7:A:VAL:HG13	1:37:A:ALA:HB3	5	0.38
(1,106)	1:7:A:VAL:HG21	1:37:A:ALA:HB1	5	0.38
(1,106)	1:7:A:VAL:HG21	1:37:A:ALA:HB2	5	0.38
(1,106)	1:7:A:VAL:HG21	1:37:A:ALA:HB3	5	0.38
(1,106)	1:7:A:VAL:HG22	1:37:A:ALA:HB1	5	0.38
(1,106)	1:7:A:VAL:HG22	1:37:A:ALA:HB2	5	0.38
(1,106)	1:7:A:VAL:HG22	1:37:A:ALA:HB3	5	0.38
(1,106)	1:7:A:VAL:HG23	1:37:A:ALA:HB1	5	0.38
(1,106)	1:7:A:VAL:HG23	1:37:A:ALA:HB2	5	0.38
(1,106)	1:7:A:VAL:HG23	1:37:A:ALA:HB3	5	0.38
(1,97)	1:7:A:VAL:HG11	1:116:A:ALA:H	4	0.38
(1,97)	1:7:A:VAL:HG12	1:116:A:ALA:H	4	0.38
(1,97)	1:7:A:VAL:HG13	1:116:A:ALA:H	4	0.38
(1,97)	1:7:A:VAL:HG21	1:116:A:ALA:H	4	0.38
(1,97)	1:7:A:VAL:HG22	1:116:A:ALA:H	4	0.38
(1,97)	1:7:A:VAL:HG23	1:116:A:ALA:H	4	0.38
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD11	7	0.38
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD12	7	0.38
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD13	7	0.38
(1,55)	1:6:A:LYS:HE2	1:7:A:VAL:H	7	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:6:A:LYS:HE3	1:7:A:VAL:H	7	0.38
(1,28)	1:5:A:VAL:HA	1:36:A:THR:HB	2	0.38
(1,4)	1:1:A:MET:HA	1:114:A:VAL:HB	9	0.38
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG11	8	0.37
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG12	8	0.37
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG13	8	0.37
(1,1803)	1:151:A:ARG:HG2	1:152:A:ILE:H	2	0.37
(1,1803)	1:151:A:ARG:HG3	1:152:A:ILE:H	2	0.37
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG21	8	0.37
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG22	8	0.37
(1,1781)	1:149:A:ASN:HB2	1:152:A:ILE:HG23	8	0.37
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG21	8	0.37
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG22	8	0.37
(1,1781)	1:149:A:ASN:HB3	1:152:A:ILE:HG23	8	0.37
(1,1756)	1:147:A:MET:HA	1:149:A:ASN:H	1	0.37
(1,1669)	1:141:A:SER:HB3	1:143:A:LYS:H	6	0.37
(1,1658)	1:140:A:LYS:HB2	1:142:A:VAL:H	4	0.37
(1,1658)	1:140:A:LYS:HB3	1:142:A:VAL:H	4	0.37
(1,1658)	1:140:A:LYS:HB2	1:142:A:VAL:H	6	0.37
(1,1658)	1:140:A:LYS:HB3	1:142:A:VAL:H	6	0.37
(1,1655)	1:140:A:LYS:HE3	1:142:A:VAL:H	8	0.37
(1,1580)	1:134:A:MET:HB2	1:136:A:ASP:H	4	0.37
(1,1580)	1:134:A:MET:HB3	1:136:A:ASP:H	4	0.37
(1,1550)	1:131:A:ALA:HA	1:136:A:ASP:HA	3	0.37
(1,1426)	1:117:A:LEU:HB2	1:119:A:ALA:H	10	0.37
(1,1358)	1:113:A:SER:H	1:115:A:ARG:H	4	0.37
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB2	2	0.37
(1,1306)	1:108:A:MET:HG2	1:112:A:SER:HB3	2	0.37
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB2	2	0.37
(1,1306)	1:108:A:MET:HG3	1:112:A:SER:HB3	2	0.37
(1,1298)	1:108:A:MET:HB2	1:110:A:TYR:H	9	0.37
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG2	5	0.37
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG3	5	0.37
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG2	5	0.37
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG3	5	0.37
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG2	5	0.37
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG3	5	0.37
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG2	5	0.37
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG3	5	0.37
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG2	5	0.37
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG3	5	0.37
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG2	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG3	5	0.37
(1,1218)	1:104:A:VAL:HA	1:106:A:ARG:H	9	0.37
(1,1207)	1:103:A:PRO:HA	1:106:A:ARG:H	6	0.37
(1,1178)	1:99:A:PRO:HB2	1:102:A:ALA:HA	4	0.37
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB1	9	0.37
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB2	9	0.37
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB3	9	0.37
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB1	9	0.37
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB2	9	0.37
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB3	9	0.37
(1,1092)	1:93:A:ILE:HG12	1:127:A:PHE:H	8	0.37
(1,1082)	1:93:A:ILE:HA	1:127:A:PHE:HA	1	0.37
(1,1027)	1:86:A:THR:HB	1:87:A:SER:H	3	0.37
(1,1016)	1:84:A:GLU:HA	1:85:A:GLY:H	3	0.37
(1,947)	1:78:A:VAL:H	1:87:A:SER:H	8	0.37
(1,912)	1:76:A:VAL:HA	1:88:A:THR:HG21	8	0.37
(1,912)	1:76:A:VAL:HA	1:88:A:THR:HG22	8	0.37
(1,912)	1:76:A:VAL:HA	1:88:A:THR:HG23	8	0.37
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG2	5	0.37
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG3	5	0.37
(1,909)	1:76:A:VAL:H	1:89:A:LEU:H	7	0.37
(1,888)	1:75:A:GLU:HG2	1:76:A:VAL:H	6	0.37
(1,879)	1:75:A:GLU:HB2	1:88:A:THR:HA	3	0.37
(1,733)	1:57:A:MET:HA	1:61:A:VAL:H	4	0.37
(1,669)	1:54:A:VAL:HA	1:56:A:GLU:H	9	0.37
(1,611)	1:49:A:PRO:HG2	1:52:A:GLU:H	1	0.37
(1,611)	1:49:A:PRO:HG3	1:52:A:GLU:H	1	0.37
(1,608)	1:49:A:PRO:HG2	1:50:A:TYR:H	9	0.37
(1,608)	1:49:A:PRO:HG3	1:50:A:TYR:H	9	0.37
(1,480)	1:30:A:LYS:HB2	1:41:A:GLU:HA	2	0.37
(1,480)	1:30:A:LYS:HB3	1:41:A:GLU:HA	2	0.37
(1,454)	1:28:A:ILE:HG12	1:41:A:GLU:HG2	5	0.37
(1,454)	1:28:A:ILE:HG12	1:41:A:GLU:HG3	5	0.37
(1,454)	1:28:A:ILE:HG13	1:41:A:GLU:HG2	5	0.37
(1,454)	1:28:A:ILE:HG13	1:41:A:GLU:HG3	5	0.37
(1,325)	1:18:A:LEU:HD21	1:72:A:VAL:H	7	0.37
(1,325)	1:18:A:LEU:HD22	1:72:A:VAL:H	7	0.37
(1,325)	1:18:A:LEU:HD23	1:72:A:VAL:H	7	0.37
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD11	5	0.37
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD12	5	0.37
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD13	5	0.37
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD21	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD22	5	0.37
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD23	5	0.37
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD11	5	0.37
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD12	5	0.37
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD13	5	0.37
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD21	5	0.37
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD22	5	0.37
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD23	5	0.37
(1,225)	1:13:A:ASN:HA	1:17:A:LEU:H	4	0.37
(1,214)	1:12:A:LYS:HG3	1:15:A:TYR:H	10	0.37
(1,178)	1:11:A:CYS:HB2	1:13:A:ASN:H	7	0.37
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG21	10	0.37
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG22	10	0.37
(1,95)	1:7:A:VAL:HG21	1:38:A:ILE:HG23	10	0.37
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG21	10	0.37
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG22	10	0.37
(1,95)	1:7:A:VAL:HG22	1:38:A:ILE:HG23	10	0.37
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG21	10	0.37
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG22	10	0.37
(1,95)	1:7:A:VAL:HG23	1:38:A:ILE:HG23	10	0.37
(1,93)	1:7:A:VAL:HG21	1:38:A:ILE:H	4	0.37
(1,93)	1:7:A:VAL:HG22	1:38:A:ILE:H	4	0.37
(1,93)	1:7:A:VAL:HG23	1:38:A:ILE:H	4	0.37
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD11	8	0.37
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD12	8	0.37
(1,77)	1:7:A:VAL:HB	1:38:A:ILE:HD13	8	0.37
(2,34)	1:114:A:VAL:HA	1:117:A:LEU:HA	2	0.36
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG11	5	0.36
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG12	5	0.36
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG13	5	0.36
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG21	5	0.36
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG22	5	0.36
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG23	5	0.36
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD11	7	0.36
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD12	7	0.36
(1,1771)	1:149:A:ASN:HB2	1:152:A:ILE:HD13	7	0.36
(1,1756)	1:147:A:MET:HA	1:149:A:ASN:H	7	0.36
(1,1700)	1:143:A:LYS:H	1:145:A:ASP:H	6	0.36
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD2	2	0.36
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD3	2	0.36
(1,1665)	1:141:A:SER:HA	1:144:A:SER:H	6	0.36
(1,1652)	1:140:A:LYS:HE2	1:141:A:SER:H	4	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1550)	1:131:A:ALA:HA	1:136:A:ASP:HA	6	0.36
(1,1429)	1:117:A:LEU:HB3	1:119:A:ALA:H	9	0.36
(1,1429)	1:117:A:LEU:HB3	1:119:A:ALA:H	10	0.36
(1,1395)	1:115:A:ARG:HA	1:117:A:LEU:HD11	5	0.36
(1,1395)	1:115:A:ARG:HA	1:117:A:LEU:HD12	5	0.36
(1,1395)	1:115:A:ARG:HA	1:117:A:LEU:HD13	5	0.36
(1,1395)	1:115:A:ARG:HA	1:117:A:LEU:HD21	5	0.36
(1,1395)	1:115:A:ARG:HA	1:117:A:LEU:HD22	5	0.36
(1,1395)	1:115:A:ARG:HA	1:117:A:LEU:HD23	5	0.36
(1,1378)	1:114:A:VAL:HB	1:118:A:LYS:H	9	0.36
(1,1356)	1:112:A:SER:HB2	1:116:A:ALA:HB1	7	0.36
(1,1356)	1:112:A:SER:HB2	1:116:A:ALA:HB2	7	0.36
(1,1356)	1:112:A:SER:HB2	1:116:A:ALA:HB3	7	0.36
(1,1356)	1:112:A:SER:HB3	1:116:A:ALA:HB1	7	0.36
(1,1356)	1:112:A:SER:HB3	1:116:A:ALA:HB2	7	0.36
(1,1356)	1:112:A:SER:HB3	1:116:A:ALA:HB3	7	0.36
(1,1324)	1:109:A:LEU:HD11	1:112:A:SER:H	8	0.36
(1,1324)	1:109:A:LEU:HD12	1:112:A:SER:H	8	0.36
(1,1324)	1:109:A:LEU:HD13	1:112:A:SER:H	8	0.36
(1,1324)	1:109:A:LEU:HD21	1:112:A:SER:H	8	0.36
(1,1324)	1:109:A:LEU:HD22	1:112:A:SER:H	8	0.36
(1,1324)	1:109:A:LEU:HD23	1:112:A:SER:H	8	0.36
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	3	0.36
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	3	0.36
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	3	0.36
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	3	0.36
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	4	0.36
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	4	0.36
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	4	0.36
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	4	0.36
(1,1281)	1:107:A:ARG:HA	1:110:A:TYR:HA	2	0.36
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG2	9	0.36
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG3	9	0.36
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG2	9	0.36
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG3	9	0.36
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG2	9	0.36
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG3	9	0.36
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG2	9	0.36
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG3	9	0.36
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG2	9	0.36
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG3	9	0.36
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG2	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG3	9	0.36
(1,1208)	1:103:A:PRO:HA	1:107:A:ARG:H	9	0.36
(1,1189)	1:99:A:PRO:HG3	1:102:A:ALA:HA	4	0.36
(1,1117)	1:94:A:PHE:HA	1:128:A:GLN:HA	6	0.36
(1,1086)	1:93:A:ILE:HB	1:127:A:PHE:H	7	0.36
(1,1061)	1:91:A:LYS:HA	1:150:A:GLN:HG2	5	0.36
(1,1061)	1:91:A:LYS:HA	1:150:A:GLN:HG3	5	0.36
(1,988)	1:80:A:ARG:HA	1:81:A:GLN:H	9	0.36
(1,947)	1:78:A:VAL:H	1:87:A:SER:H	6	0.36
(1,935)	1:77:A:THR:HB	1:87:A:SER:H	4	0.36
(1,737)	1:57:A:MET:HG2	1:60:A:LEU:HG	9	0.36
(1,737)	1:57:A:MET:HG3	1:60:A:LEU:HG	9	0.36
(1,685)	1:54:A:VAL:HG11	1:138:A:ASP:HA	5	0.36
(1,685)	1:54:A:VAL:HG12	1:138:A:ASP:HA	5	0.36
(1,685)	1:54:A:VAL:HG13	1:138:A:ASP:HA	5	0.36
(1,685)	1:54:A:VAL:HG21	1:138:A:ASP:HA	5	0.36
(1,685)	1:54:A:VAL:HG22	1:138:A:ASP:HA	5	0.36
(1,685)	1:54:A:VAL:HG23	1:138:A:ASP:HA	5	0.36
(1,675)	1:54:A:VAL:HB	1:56:A:GLU:H	5	0.36
(1,654)	1:53:A:PHE:HA	1:55:A:GLU:H	8	0.36
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG2	10	0.36
(1,645)	1:52:A:GLU:HA	1:55:A:GLU:HG3	10	0.36
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG2	4	0.36
(1,621)	1:50:A:TYR:HB2	1:143:A:LYS:HG3	4	0.36
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG2	4	0.36
(1,621)	1:50:A:TYR:HB3	1:143:A:LYS:HG3	4	0.36
(1,608)	1:49:A:PRO:HG2	1:50:A:TYR:H	1	0.36
(1,608)	1:49:A:PRO:HG3	1:50:A:TYR:H	1	0.36
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB1	5	0.36
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB2	5	0.36
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB3	5	0.36
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD11	6	0.36
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD12	6	0.36
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD13	6	0.36
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD21	6	0.36
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD22	6	0.36
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD23	6	0.36
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB1	10	0.36
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB2	10	0.36
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB3	10	0.36
(1,384)	1:26:A:TYR:HB2	1:71:A:ALA:H	6	0.36
(1,384)	1:26:A:TYR:HB3	1:71:A:ALA:H	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	1:13:A:ASN:HB2	1:14:A:ALA:H	1	0.36
(1,117)	1:8:A:ASP:H	1:39:A:VAL:HB	3	0.36
(1,108)	1:7:A:VAL:HG11	1:38:A:ILE:HB	9	0.36
(1,108)	1:7:A:VAL:HG12	1:38:A:ILE:HB	9	0.36
(1,108)	1:7:A:VAL:HG13	1:38:A:ILE:HB	9	0.36
(1,108)	1:7:A:VAL:HG21	1:38:A:ILE:HB	9	0.36
(1,108)	1:7:A:VAL:HG22	1:38:A:ILE:HB	9	0.36
(1,108)	1:7:A:VAL:HG23	1:38:A:ILE:HB	9	0.36
(1,31)	1:5:A:VAL:HB	1:36:A:THR:HB	8	0.36
(1,16)	1:3:A:SER:H	1:4:A:GLY:H	9	0.36
(3,10)	1:26:A:TYR:N	1:44:A:GLY:O	7	0.35
(3,9)	1:26:A:TYR:H	1:44:A:GLY:O	4	0.35
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG11	7	0.35
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG12	7	0.35
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG13	7	0.35
(2,6)	1:12:A:LYS:HG2	1:15:A:TYR:H	8	0.35
(1,1777)	1:149:A:ASN:HB2	1:151:A:ARG:H	3	0.35
(1,1777)	1:149:A:ASN:HB3	1:151:A:ARG:H	3	0.35
(1,1725)	1:144:A:SER:HB3	1:145:A:ASP:H	3	0.35
(1,1725)	1:144:A:SER:HB3	1:145:A:ASP:H	5	0.35
(1,1594)	1:135:A:SER:HB2	1:140:A:LYS:HG2	7	0.35
(1,1594)	1:135:A:SER:HB2	1:140:A:LYS:HG3	7	0.35
(1,1594)	1:135:A:SER:HB3	1:140:A:LYS:HG2	7	0.35
(1,1594)	1:135:A:SER:HB3	1:140:A:LYS:HG3	7	0.35
(1,1580)	1:134:A:MET:HB2	1:136:A:ASP:H	2	0.35
(1,1580)	1:134:A:MET:HB3	1:136:A:ASP:H	2	0.35
(1,1547)	1:130:A:GLN:HG2	1:131:A:ALA:H	9	0.35
(1,1547)	1:130:A:GLN:HG3	1:131:A:ALA:H	9	0.35
(1,1410)	1:116:A:ALA:HA	1:120:A:SER:H	5	0.35
(1,1382)	1:114:A:VAL:HG21	1:116:A:ALA:H	7	0.35
(1,1382)	1:114:A:VAL:HG22	1:116:A:ALA:H	7	0.35
(1,1382)	1:114:A:VAL:HG23	1:116:A:ALA:H	7	0.35
(1,1378)	1:114:A:VAL:HB	1:118:A:LYS:H	2	0.35
(1,1187)	1:99:A:PRO:HG2	1:132:A:SER:HB3	3	0.35
(1,1186)	1:99:A:PRO:HG2	1:132:A:SER:HA	10	0.35
(1,1174)	1:99:A:PRO:HA	1:102:A:ALA:H	7	0.35
(1,1165)	1:97:A:TYR:HA	1:131:A:ALA:HA	5	0.35
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG11	5	0.35
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG12	5	0.35
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG13	5	0.35
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG21	5	0.35
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG22	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1159)	1:96:A:GLN:HB2	1:114:A:VAL:HG23	5	0.35
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG11	5	0.35
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG12	5	0.35
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG13	5	0.35
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG21	5	0.35
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG22	5	0.35
(1,1159)	1:96:A:GLN:HB3	1:114:A:VAL:HG23	5	0.35
(1,1118)	1:94:A:PHE:HA	1:128:A:GLN:HB2	10	0.35
(1,1117)	1:94:A:PHE:HA	1:128:A:GLN:HA	5	0.35
(1,1109)	1:94:A:PHE:H	1:127:A:PHE:H	10	0.35
(1,1092)	1:93:A:ILE:HG12	1:127:A:PHE:H	2	0.35
(1,1016)	1:84:A:GLU:HA	1:85:A:GLY:H	5	0.35
(1,960)	1:78:A:VAL:HG21	1:87:A:SER:HB2	2	0.35
(1,960)	1:78:A:VAL:HG22	1:87:A:SER:HB2	2	0.35
(1,960)	1:78:A:VAL:HG23	1:87:A:SER:HB2	2	0.35
(1,960)	1:78:A:VAL:HG21	1:87:A:SER:HB3	2	0.35
(1,960)	1:78:A:VAL:HG22	1:87:A:SER:HB3	2	0.35
(1,960)	1:78:A:VAL:HG23	1:87:A:SER:HB3	2	0.35
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG21	8	0.35
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG22	8	0.35
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG23	8	0.35
(1,886)	1:75:A:GLU:HB3	1:88:A:THR:HG21	8	0.35
(1,886)	1:75:A:GLU:HB3	1:88:A:THR:HG22	8	0.35
(1,886)	1:75:A:GLU:HB3	1:88:A:THR:HG23	8	0.35
(1,883)	1:75:A:GLU:HB3	1:76:A:VAL:H	6	0.35
(1,756)	1:58:A:LYS:HD3	1:59:A:LYS:H	9	0.35
(1,751)	1:58:A:LYS:HB2	1:60:A:LEU:H	8	0.35
(1,605)	1:49:A:PRO:HB3	1:51:A:ALA:HB1	10	0.35
(1,605)	1:49:A:PRO:HB3	1:51:A:ALA:HB2	10	0.35
(1,605)	1:49:A:PRO:HB3	1:51:A:ALA:HB3	10	0.35
(1,509)	1:31:A:ILE:HG21	1:109:A:LEU:H	2	0.35
(1,509)	1:31:A:ILE:HG22	1:109:A:LEU:H	2	0.35
(1,509)	1:31:A:ILE:HG23	1:109:A:LEU:H	2	0.35
(1,335)	1:19:A:HIS:HA	1:21:A:LYS:H	4	0.35
(1,335)	1:19:A:HIS:HA	1:21:A:LYS:H	7	0.35
(1,277)	1:16:A:ASP:HB2	1:18:A:LEU:H	10	0.35
(1,206)	1:12:A:LYS:HD3	1:15:A:TYR:H	6	0.35
(1,158)	1:10:A:SER:HB3	1:12:A:LYS:H	1	0.35
(1,94)	1:7:A:VAL:HG21	1:38:A:ILE:HB	10	0.35
(1,94)	1:7:A:VAL:HG22	1:38:A:ILE:HB	10	0.35
(1,94)	1:7:A:VAL:HG23	1:38:A:ILE:HB	10	0.35
(1,64)	1:7:A:VAL:HA	1:117:A:LEU:HA	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:5:A:VAL:HA	1:36:A:THR:HA	1	0.35
(1,1778)	1:149:A:ASN:HB2	1:151:A:ARG:HA	6	0.34
(1,1778)	1:149:A:ASN:HB3	1:151:A:ARG:HA	6	0.34
(1,1757)	1:147:A:MET:HA	1:150:A:GLN:H	10	0.34
(1,1740)	1:146:A:LEU:H	1:148:A:SER:H	6	0.34
(1,1719)	1:144:A:SER:HA	1:146:A:LEU:H	7	0.34
(1,1718)	1:144:A:SER:H	1:146:A:LEU:H	3	0.34
(1,1703)	1:143:A:LYS:HA	1:146:A:LEU:HA	7	0.34
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG11	8	0.34
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG12	8	0.34
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG13	8	0.34
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG21	8	0.34
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG22	8	0.34
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG23	8	0.34
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG11	8	0.34
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG12	8	0.34
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG13	8	0.34
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG21	8	0.34
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG22	8	0.34
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG23	8	0.34
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE2	3	0.34
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE3	3	0.34
(1,1436)	1:118:A:LYS:H	1:118:A:LYS:HE2	3	0.34
(1,1436)	1:118:A:LYS:H	1:118:A:LYS:HE3	3	0.34
(1,1436)	1:118:A:LYS:H	1:118:A:LYS:HE2	5	0.34
(1,1436)	1:118:A:LYS:H	1:118:A:LYS:HE3	5	0.34
(1,1366)	1:113:A:SER:HB3	1:116:A:ALA:H	1	0.34
(1,1364)	1:113:A:SER:HB2	1:116:A:ALA:H	3	0.34
(1,1325)	1:109:A:LEU:HD11	1:112:A:SER:HB2	6	0.34
(1,1325)	1:109:A:LEU:HD11	1:112:A:SER:HB3	6	0.34
(1,1325)	1:109:A:LEU:HD12	1:112:A:SER:HB2	6	0.34
(1,1325)	1:109:A:LEU:HD12	1:112:A:SER:HB3	6	0.34
(1,1325)	1:109:A:LEU:HD13	1:112:A:SER:HB2	6	0.34
(1,1325)	1:109:A:LEU:HD13	1:112:A:SER:HB3	6	0.34
(1,1325)	1:109:A:LEU:HD21	1:112:A:SER:HB2	6	0.34
(1,1325)	1:109:A:LEU:HD21	1:112:A:SER:HB3	6	0.34
(1,1325)	1:109:A:LEU:HD22	1:112:A:SER:HB2	6	0.34
(1,1325)	1:109:A:LEU:HD22	1:112:A:SER:HB3	6	0.34
(1,1325)	1:109:A:LEU:HD23	1:112:A:SER:HB2	6	0.34
(1,1325)	1:109:A:LEU:HD23	1:112:A:SER:HB3	6	0.34
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	5	0.34
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	5	0.34
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	5	0.34
(1,1174)	1:99:A:PRO:HA	1:102:A:ALA:H	9	0.34
(1,1109)	1:94:A:PHE:H	1:127:A:PHE:H	7	0.34
(1,1086)	1:93:A:ILE:HB	1:127:A:PHE:H	2	0.34
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG21	9	0.34
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG22	9	0.34
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG23	9	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	8	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	8	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	8	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG11	8	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG12	8	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG13	8	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	8	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	8	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	8	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	10	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	10	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	10	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG11	10	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG12	10	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG13	10	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	10	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	10	0.34
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	10	0.34
(1,769)	1:60:A:LEU:H	1:60:A:LEU:HG	9	0.34
(1,741)	1:58:A:LYS:H	1:58:A:LYS:HD2	1	0.34
(1,741)	1:58:A:LYS:H	1:58:A:LYS:HD3	1	0.34
(1,741)	1:58:A:LYS:H	1:58:A:LYS:HD2	6	0.34
(1,741)	1:58:A:LYS:H	1:58:A:LYS:HD3	6	0.34
(1,643)	1:52:A:GLU:HA	1:54:A:VAL:H	4	0.34
(1,608)	1:49:A:PRO:HG2	1:50:A:TYR:H	8	0.34
(1,608)	1:49:A:PRO:HG3	1:50:A:TYR:H	8	0.34
(1,575)	1:42:A:LYS:HB2	1:43:A:VAL:H	8	0.34
(1,575)	1:42:A:LYS:HB3	1:43:A:VAL:H	8	0.34
(1,515)	1:31:A:ILE:HG21	1:37:A:ALA:H	7	0.34
(1,515)	1:31:A:ILE:HG22	1:37:A:ALA:H	7	0.34
(1,515)	1:31:A:ILE:HG23	1:37:A:ALA:H	7	0.34
(1,507)	1:31:A:ILE:HG12	1:109:A:LEU:HB2	6	0.34
(1,507)	1:31:A:ILE:HG12	1:109:A:LEU:HB3	6	0.34
(1,507)	1:31:A:ILE:HG13	1:109:A:LEU:HB2	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,507)	1:31:A:ILE:HG13	1:109:A:LEU:HB3	6	0.34
(1,452)	1:28:A:ILE:HD11	1:71:A:ALA:H	8	0.34
(1,452)	1:28:A:ILE:HD12	1:71:A:ALA:H	8	0.34
(1,452)	1:28:A:ILE:HD13	1:71:A:ALA:H	8	0.34
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB1	1	0.34
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB2	1	0.34
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB3	1	0.34
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB1	6	0.34
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB2	6	0.34
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB3	6	0.34
(1,384)	1:26:A:TYR:HB2	1:71:A:ALA:H	2	0.34
(1,384)	1:26:A:TYR:HB3	1:71:A:ALA:H	2	0.34
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB1	6	0.34
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB2	6	0.34
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB3	6	0.34
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB1	6	0.34
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB2	6	0.34
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB3	6	0.34
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD11	2	0.34
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD12	2	0.34
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD13	2	0.34
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD21	2	0.34
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD22	2	0.34
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD23	2	0.34
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD11	2	0.34
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD12	2	0.34
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD13	2	0.34
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD21	2	0.34
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD22	2	0.34
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD23	2	0.34
(1,237)	1:14:A:ALA:HA	1:18:A:LEU:H	6	0.34
(1,227)	1:13:A:ASN:HB2	1:15:A:TYR:H	5	0.34
(1,224)	1:13:A:ASN:HA	1:16:A:ASP:H	10	0.34
(1,159)	1:10:A:SER:HB3	1:13:A:ASN:H	1	0.34
(1,156)	1:10:A:SER:HB2	1:13:A:ASN:H	8	0.34
(1,105)	1:7:A:VAL:HG11	1:37:A:ALA:HA	5	0.34
(1,105)	1:7:A:VAL:HG12	1:37:A:ALA:HA	5	0.34
(1,105)	1:7:A:VAL:HG13	1:37:A:ALA:HA	5	0.34
(1,105)	1:7:A:VAL:HG21	1:37:A:ALA:HA	5	0.34
(1,105)	1:7:A:VAL:HG22	1:37:A:ALA:HA	5	0.34
(1,105)	1:7:A:VAL:HG23	1:37:A:ALA:HA	5	0.34
(1,27)	1:5:A:VAL:HA	1:36:A:THR:HA	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:3:A:SER:H	1:4:A:GLY:H	8	0.34
(2,31)	1:97:A:TYR:HB2	1:131:A:ALA:HA	6	0.33
(2,31)	1:97:A:TYR:HB3	1:131:A:ALA:HA	6	0.33
(2,29)	1:86:A:THR:HG21	1:88:A:THR:HA	2	0.33
(2,29)	1:86:A:THR:HG22	1:88:A:THR:HA	2	0.33
(2,29)	1:86:A:THR:HG23	1:88:A:THR:HA	2	0.33
(2,5)	1:12:A:LYS:HG2	1:121:A:LEU:HD21	4	0.33
(2,5)	1:12:A:LYS:HG2	1:121:A:LEU:HD22	4	0.33
(2,5)	1:12:A:LYS:HG2	1:121:A:LEU:HD23	4	0.33
(1,1699)	1:143:A:LYS:H	1:144:A:SER:H	7	0.33
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD2	7	0.33
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD3	7	0.33
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG2	1	0.33
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG3	1	0.33
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG2	1	0.33
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG3	1	0.33
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG2	1	0.33
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG3	1	0.33
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG2	1	0.33
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG3	1	0.33
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG2	1	0.33
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG3	1	0.33
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG2	1	0.33
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG3	1	0.33
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE2	5	0.33
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE3	5	0.33
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	9	0.33
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	9	0.33
(1,1441)	1:118:A:LYS:HE2	1:119:A:ALA:H	8	0.33
(1,1382)	1:114:A:VAL:HG21	1:116:A:ALA:H	9	0.33
(1,1382)	1:114:A:VAL:HG22	1:116:A:ALA:H	9	0.33
(1,1382)	1:114:A:VAL:HG23	1:116:A:ALA:H	9	0.33
(1,1316)	1:109:A:LEU:HA	1:113:A:SER:H	3	0.33
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	9	0.33
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	9	0.33
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	9	0.33
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	9	0.33
(1,1185)	1:99:A:PRO:HG2	1:102:A:ALA:HA	7	0.33
(1,1180)	1:99:A:PRO:HB2	1:132:A:SER:HB2	9	0.33
(1,1180)	1:99:A:PRO:HB2	1:132:A:SER:HB3	9	0.33
(1,1165)	1:97:A:TYR:HA	1:131:A:ALA:HA	6	0.33
(1,1112)	1:94:A:PHE:H	1:128:A:GLN:HG2	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1112)	1:94:A:PHE:H	1:128:A:GLN:HG3	1	0.33
(1,1052)	1:89:A:LEU:HD21	1:90:A:ASN:H	7	0.33
(1,1052)	1:89:A:LEU:HD22	1:90:A:ASN:H	7	0.33
(1,1052)	1:89:A:LEU:HD23	1:90:A:ASN:H	7	0.33
(1,985)	1:80:A:ARG:H	1:80:A:ARG:HG2	9	0.33
(1,985)	1:80:A:ARG:H	1:80:A:ARG:HG3	9	0.33
(1,892)	1:75:A:GLU:HG2	1:90:A:ASN:HA	7	0.33
(1,822)	1:70:A:ALA:H	1:94:A:PHE:HA	7	0.33
(1,736)	1:57:A:MET:HB2	1:60:A:LEU:HG	2	0.33
(1,736)	1:57:A:MET:HB3	1:60:A:LEU:HG	2	0.33
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD2	8	0.33
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD3	8	0.33
(1,704)	1:55:A:GLU:HA	1:59:A:LYS:H	1	0.33
(1,689)	1:54:A:VAL:HG11	1:57:A:MET:H	1	0.33
(1,689)	1:54:A:VAL:HG12	1:57:A:MET:H	1	0.33
(1,689)	1:54:A:VAL:HG13	1:57:A:MET:H	1	0.33
(1,689)	1:54:A:VAL:HG21	1:57:A:MET:H	1	0.33
(1,689)	1:54:A:VAL:HG22	1:57:A:MET:H	1	0.33
(1,689)	1:54:A:VAL:HG23	1:57:A:MET:H	1	0.33
(1,675)	1:54:A:VAL:HB	1:56:A:GLU:H	1	0.33
(1,671)	1:54:A:VAL:HA	1:57:A:MET:HA	7	0.33
(1,669)	1:54:A:VAL:HA	1:56:A:GLU:H	3	0.33
(1,527)	1:33:A:LYS:HG3	1:36:A:THR:HA	1	0.33
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD11	9	0.33
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD12	9	0.33
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD13	9	0.33
(1,452)	1:28:A:ILE:HD11	1:71:A:ALA:H	2	0.33
(1,452)	1:28:A:ILE:HD12	1:71:A:ALA:H	2	0.33
(1,452)	1:28:A:ILE:HD13	1:71:A:ALA:H	2	0.33
(1,434)	1:28:A:ILE:HB	1:41:A:GLU:HA	5	0.33
(1,428)	1:28:A:ILE:H	1:42:A:LYS:HD2	4	0.33
(1,428)	1:28:A:ILE:H	1:42:A:LYS:HD3	4	0.33
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB1	9	0.33
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB2	9	0.33
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB3	9	0.33
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG11	5	0.33
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG12	5	0.33
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG13	5	0.33
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG21	5	0.33
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG22	5	0.33
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG23	5	0.33
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG11	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG12	5	0.33
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG13	5	0.33
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG21	5	0.33
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG22	5	0.33
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG23	5	0.33
(1,329)	1:18:A:LEU:HD11	1:27:A:ILE:HA	8	0.33
(1,329)	1:18:A:LEU:HD12	1:27:A:ILE:HA	8	0.33
(1,329)	1:18:A:LEU:HD13	1:27:A:ILE:HA	8	0.33
(1,329)	1:18:A:LEU:HD21	1:27:A:ILE:HA	8	0.33
(1,329)	1:18:A:LEU:HD22	1:27:A:ILE:HA	8	0.33
(1,329)	1:18:A:LEU:HD23	1:27:A:ILE:HA	8	0.33
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD2	2	0.33
(1,303)	1:17:A:LEU:HD11	1:21:A:LYS:HD3	2	0.33
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD2	2	0.33
(1,303)	1:17:A:LEU:HD12	1:21:A:LYS:HD3	2	0.33
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD2	2	0.33
(1,303)	1:17:A:LEU:HD13	1:21:A:LYS:HD3	2	0.33
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD2	2	0.33
(1,303)	1:17:A:LEU:HD21	1:21:A:LYS:HD3	2	0.33
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD2	2	0.33
(1,303)	1:17:A:LEU:HD22	1:21:A:LYS:HD3	2	0.33
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD2	2	0.33
(1,303)	1:17:A:LEU:HD23	1:21:A:LYS:HD3	2	0.33
(1,302)	1:17:A:LEU:HD21	1:19:A:HIS:H	7	0.33
(1,302)	1:17:A:LEU:HD22	1:19:A:HIS:H	7	0.33
(1,302)	1:17:A:LEU:HD23	1:19:A:HIS:H	7	0.33
(1,281)	1:16:A:ASP:HB3	1:19:A:HIS:H	9	0.33
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG11	5	0.33
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG12	5	0.33
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG13	5	0.33
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG21	5	0.33
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG22	5	0.33
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG23	5	0.33
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG11	5	0.33
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG12	5	0.33
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG13	5	0.33
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG21	5	0.33
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG22	5	0.33
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG23	5	0.33
(1,214)	1:12:A:LYS:HG3	1:15:A:TYR:H	1	0.33
(1,91)	1:7:A:VAL:HG21	1:120:A:SER:HA	7	0.33
(1,91)	1:7:A:VAL:HG22	1:120:A:SER:HA	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:7:A:VAL:HG23	1:120:A:SER:HA	7	0.33
(1,47)	1:6:A:LYS:H	1:6:A:LYS:HD2	8	0.33
(1,47)	1:6:A:LYS:H	1:6:A:LYS:HD3	8	0.33
(1,46)	1:6:A:LYS:H	1:38:A:ILE:H	6	0.33
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG11	6	0.33
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG12	6	0.33
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG13	6	0.33
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG21	6	0.33
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG22	6	0.33
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG23	6	0.33
(1,33)	1:5:A:VAL:HB	1:7:A:VAL:HA	4	0.33
(1,31)	1:5:A:VAL:HB	1:36:A:THR:HB	4	0.33
(3,59)	1:143:A:LYS:O	1:147:A:MET:H	2	0.32
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG11	5	0.32
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG12	5	0.32
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG13	5	0.32
(2,6)	1:12:A:LYS:HG2	1:15:A:TYR:H	3	0.32
(1,1769)	1:149:A:ASN:H	1:150:A:GLN:H	1	0.32
(1,1740)	1:146:A:LEU:H	1:148:A:SER:H	3	0.32
(1,1703)	1:143:A:LYS:HA	1:146:A:LEU:HA	4	0.32
(1,1669)	1:141:A:SER:HB3	1:143:A:LYS:H	8	0.32
(1,1658)	1:140:A:LYS:HB2	1:142:A:VAL:H	9	0.32
(1,1658)	1:140:A:LYS:HB3	1:142:A:VAL:H	9	0.32
(1,1579)	1:134:A:MET:HB2	1:135:A:SER:H	8	0.32
(1,1579)	1:134:A:MET:HB3	1:135:A:SER:H	8	0.32
(1,1549)	1:131:A:ALA:H	1:136:A:ASP:HB2	6	0.32
(1,1549)	1:131:A:ALA:H	1:136:A:ASP:HB3	6	0.32
(1,1440)	1:118:A:LYS:HD2	1:119:A:ALA:H	10	0.32
(1,1440)	1:118:A:LYS:HD3	1:119:A:ALA:H	10	0.32
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB2	2	0.32
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB3	2	0.32
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB2	2	0.32
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB3	2	0.32
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB2	2	0.32
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB3	2	0.32
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB2	2	0.32
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB3	2	0.32
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB2	2	0.32
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB3	2	0.32
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB2	2	0.32
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB3	2	0.32
(1,1382)	1:114:A:VAL:HG21	1:116:A:ALA:H	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1382)	1:114:A:VAL:HG22	1:116:A:ALA:H	3	0.32
(1,1382)	1:114:A:VAL:HG23	1:116:A:ALA:H	3	0.32
(1,1333)	1:110:A:TYR:HA	1:114:A:VAL:H	2	0.32
(1,1322)	1:109:A:LEU:HD21	1:113:A:SER:H	1	0.32
(1,1322)	1:109:A:LEU:HD22	1:113:A:SER:H	1	0.32
(1,1322)	1:109:A:LEU:HD23	1:113:A:SER:H	1	0.32
(1,1313)	1:109:A:LEU:HA	1:111:A:ALA:H	2	0.32
(1,1293)	1:108:A:MET:HA	1:110:A:TYR:H	9	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	1	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	1	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	1	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	1	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	2	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	2	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	2	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	2	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	6	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	6	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	6	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	6	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	10	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	10	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	10	0.32
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	10	0.32
(1,1218)	1:104:A:VAL:HA	1:106:A:ARG:H	10	0.32
(1,1190)	1:99:A:PRO:HG3	1:132:A:SER:HA	6	0.32
(1,1189)	1:99:A:PRO:HG3	1:102:A:ALA:HA	1	0.32
(1,1179)	1:99:A:PRO:HB2	1:132:A:SER:HA	7	0.32
(1,1118)	1:94:A:PHE:HA	1:128:A:GLN:HB2	1	0.32
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB2	9	0.32
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB3	9	0.32
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD11	10	0.32
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD12	10	0.32
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD13	10	0.32
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD21	10	0.32
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD22	10	0.32
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD23	10	0.32
(1,1052)	1:89:A:LEU:HD21	1:90:A:ASN:H	2	0.32
(1,1052)	1:89:A:LEU:HD22	1:90:A:ASN:H	2	0.32
(1,1052)	1:89:A:LEU:HD23	1:90:A:ASN:H	2	0.32
(1,1033)	1:88:A:THR:H	1:88:A:THR:HB	6	0.32
(1,947)	1:78:A:VAL:H	1:87:A:SER:H	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,944)	1:78:A:VAL:H	1:79:A:GLN:H	9	0.32
(1,899)	1:75:A:GLU:HG3	1:90:A:ASN:HB2	9	0.32
(1,899)	1:75:A:GLU:HG3	1:90:A:ASN:HB3	9	0.32
(1,885)	1:75:A:GLU:HB3	1:88:A:THR:HB	1	0.32
(1,820)	1:69:A:TYR:HA	1:96:A:GLN:HG2	3	0.32
(1,820)	1:69:A:TYR:HA	1:96:A:GLN:HG3	3	0.32
(1,820)	1:69:A:TYR:HA	1:96:A:GLN:HG2	4	0.32
(1,820)	1:69:A:TYR:HA	1:96:A:GLN:HG3	4	0.32
(1,741)	1:58:A:LYS:H	1:58:A:LYS:HD2	9	0.32
(1,741)	1:58:A:LYS:H	1:58:A:LYS:HD3	9	0.32
(1,736)	1:57:A:MET:HB2	1:60:A:LEU:HG	5	0.32
(1,736)	1:57:A:MET:HB3	1:60:A:LEU:HG	5	0.32
(1,725)	1:56:A:GLU:HG3	1:57:A:MET:H	8	0.32
(1,724)	1:56:A:GLU:HG2	1:58:A:LYS:H	6	0.32
(1,723)	1:56:A:GLU:HG2	1:57:A:MET:H	2	0.32
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE2	8	0.32
(1,715)	1:55:A:GLU:HG2	1:58:A:LYS:HE3	8	0.32
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE2	8	0.32
(1,715)	1:55:A:GLU:HG3	1:58:A:LYS:HE3	8	0.32
(1,704)	1:55:A:GLU:HA	1:59:A:LYS:H	4	0.32
(1,704)	1:55:A:GLU:HA	1:59:A:LYS:H	10	0.32
(1,654)	1:53:A:PHE:HA	1:55:A:GLU:H	2	0.32
(1,629)	1:51:A:ALA:HA	1:54:A:VAL:HA	1	0.32
(1,608)	1:49:A:PRO:HG2	1:50:A:TYR:H	7	0.32
(1,608)	1:49:A:PRO:HG3	1:50:A:TYR:H	7	0.32
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB1	6	0.32
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB2	6	0.32
(1,517)	1:32:A:ASP:HB2	1:37:A:ALA:HB3	6	0.32
(1,515)	1:31:A:ILE:HG21	1:37:A:ALA:H	6	0.32
(1,515)	1:31:A:ILE:HG22	1:37:A:ALA:H	6	0.32
(1,515)	1:31:A:ILE:HG23	1:37:A:ALA:H	6	0.32
(1,498)	1:31:A:ILE:HG13	1:38:A:ILE:HA	1	0.32
(1,494)	1:31:A:ILE:HG12	1:38:A:ILE:HA	8	0.32
(1,489)	1:31:A:ILE:HA	1:38:A:ILE:HD11	9	0.32
(1,489)	1:31:A:ILE:HA	1:38:A:ILE:HD12	9	0.32
(1,489)	1:31:A:ILE:HA	1:38:A:ILE:HD13	9	0.32
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG2	1	0.32
(1,474)	1:30:A:LYS:HA	1:41:A:GLU:HG3	1	0.32
(1,426)	1:28:A:ILE:H	1:42:A:LYS:HA	6	0.32
(1,379)	1:26:A:TYR:HB2	1:72:A:VAL:HA	10	0.32
(1,327)	1:18:A:LEU:HD21	1:73:A:ASP:HA	1	0.32
(1,327)	1:18:A:LEU:HD22	1:73:A:ASP:HA	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:18:A:LEU:HD23	1:73:A:ASP:HA	1	0.32
(1,327)	1:18:A:LEU:HD21	1:73:A:ASP:HA	8	0.32
(1,327)	1:18:A:LEU:HD22	1:73:A:ASP:HA	8	0.32
(1,327)	1:18:A:LEU:HD23	1:73:A:ASP:HA	8	0.32
(1,280)	1:16:A:ASP:HB3	1:18:A:LEU:H	6	0.32
(1,256)	1:15:A:TYR:HB2	1:121:A:LEU:HG	1	0.32
(1,237)	1:14:A:ALA:HA	1:18:A:LEU:H	4	0.32
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG11	5	0.32
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG12	5	0.32
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG13	5	0.32
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG21	5	0.32
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG22	5	0.32
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG23	5	0.32
(1,214)	1:12:A:LYS:HG3	1:15:A:TYR:H	2	0.32
(1,213)	1:12:A:LYS:HG3	1:14:A:ALA:H	6	0.32
(1,159)	1:10:A:SER:HB3	1:13:A:ASN:H	2	0.32
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG11	7	0.32
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG12	7	0.32
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG13	7	0.32
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG21	7	0.32
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG22	7	0.32
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG23	7	0.32
(1,116)	1:8:A:ASP:H	1:39:A:VAL:HA	7	0.32
(1,94)	1:7:A:VAL:HG21	1:38:A:ILE:HB	4	0.32
(1,94)	1:7:A:VAL:HG22	1:38:A:ILE:HB	4	0.32
(1,94)	1:7:A:VAL:HG23	1:38:A:ILE:HB	4	0.32
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG21	1	0.32
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG22	1	0.32
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG23	1	0.32
(2,30)	1:91:A:LYS:HE2	1:92:A:VAL:H	5	0.31
(2,30)	1:91:A:LYS:HE3	1:92:A:VAL:H	5	0.31
(2,6)	1:12:A:LYS:HG2	1:15:A:TYR:H	10	0.31
(2,5)	1:12:A:LYS:HG2	1:121:A:LEU:HD21	2	0.31
(2,5)	1:12:A:LYS:HG2	1:121:A:LEU:HD22	2	0.31
(2,5)	1:12:A:LYS:HG2	1:121:A:LEU:HD23	2	0.31
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG21	5	0.31
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG22	5	0.31
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG23	5	0.31
(1,1757)	1:147:A:MET:HA	1:150:A:GLN:H	2	0.31
(1,1729)	1:145:A:ASP:H	1:146:A:LEU:H	7	0.31
(1,1729)	1:145:A:ASP:H	1:146:A:LEU:H	8	0.31
(1,1725)	1:144:A:SER:HB3	1:145:A:ASP:H	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1699)	1:143:A:LYS:H	1:144:A:SER:H	4	0.31
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD2	3	0.31
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD3	3	0.31
(1,1659)	1:140:A:LYS:HB2	1:143:A:LYS:H	4	0.31
(1,1659)	1:140:A:LYS:HB3	1:143:A:LYS:H	4	0.31
(1,1587)	1:135:A:SER:HA	1:138:A:ASP:H	4	0.31
(1,1462)	1:120:A:SER:HA	1:122:A:GLY:H	6	0.31
(1,1397)	1:115:A:ARG:HA	1:118:A:LYS:HD2	10	0.31
(1,1397)	1:115:A:ARG:HA	1:118:A:LYS:HD3	10	0.31
(1,1333)	1:110:A:TYR:HA	1:114:A:VAL:H	8	0.31
(1,1301)	1:108:A:MET:HB3	1:110:A:TYR:H	7	0.31
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	8	0.31
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	8	0.31
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG2	8	0.31
(1,1290)	1:108:A:MET:H	1:108:A:MET:HG3	8	0.31
(1,1234)	1:104:A:VAL:HG21	1:107:A:ARG:H	9	0.31
(1,1234)	1:104:A:VAL:HG22	1:107:A:ARG:H	9	0.31
(1,1234)	1:104:A:VAL:HG23	1:107:A:ARG:H	9	0.31
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB1	10	0.31
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB2	10	0.31
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB3	10	0.31
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB1	10	0.31
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB2	10	0.31
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB3	10	0.31
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB1	3	0.31
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB2	3	0.31
(1,1169)	1:97:A:TYR:HB3	1:131:A:ALA:HB3	3	0.31
(1,1162)	1:96:A:GLN:HG2	1:130:A:GLN:HA	9	0.31
(1,1162)	1:96:A:GLN:HG3	1:130:A:GLN:HA	9	0.31
(1,1016)	1:84:A:GLU:HA	1:85:A:GLY:H	7	0.31
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG21	7	0.31
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG22	7	0.31
(1,974)	1:79:A:GLN:HB2	1:86:A:THR:HG23	7	0.31
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	4	0.31
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	4	0.31
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	4	0.31
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG11	4	0.31
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG12	4	0.31
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG13	4	0.31
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	4	0.31
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	4	0.31
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,915)	1:76:A:VAL:HG11	1:143:A:LYS:HG2	2	0.31
(1,915)	1:76:A:VAL:HG12	1:143:A:LYS:HG2	2	0.31
(1,915)	1:76:A:VAL:HG13	1:143:A:LYS:HG2	2	0.31
(1,915)	1:76:A:VAL:HG11	1:143:A:LYS:HG3	2	0.31
(1,915)	1:76:A:VAL:HG12	1:143:A:LYS:HG3	2	0.31
(1,915)	1:76:A:VAL:HG13	1:143:A:LYS:HG3	2	0.31
(1,893)	1:75:A:GLU:HG2	1:90:A:ASN:HB2	9	0.31
(1,893)	1:75:A:GLU:HG2	1:90:A:ASN:HB3	9	0.31
(1,885)	1:75:A:GLU:HB3	1:88:A:THR:HB	5	0.31
(1,884)	1:75:A:GLU:HB3	1:88:A:THR:HA	9	0.31
(1,822)	1:70:A:ALA:H	1:94:A:PHE:HA	3	0.31
(1,700)	1:55:A:GLU:HA	1:58:A:LYS:HE2	6	0.31
(1,700)	1:55:A:GLU:HA	1:58:A:LYS:HE3	6	0.31
(1,659)	1:53:A:PHE:HB2	1:56:A:GLU:H	4	0.31
(1,580)	1:42:A:LYS:HG2	1:56:A:GLU:HG2	1	0.31
(1,580)	1:42:A:LYS:HG2	1:56:A:GLU:HG3	1	0.31
(1,580)	1:42:A:LYS:HG3	1:56:A:GLU:HG2	1	0.31
(1,580)	1:42:A:LYS:HG3	1:56:A:GLU:HG3	1	0.31
(1,515)	1:31:A:ILE:HG21	1:37:A:ALA:H	3	0.31
(1,515)	1:31:A:ILE:HG22	1:37:A:ALA:H	3	0.31
(1,515)	1:31:A:ILE:HG23	1:37:A:ALA:H	3	0.31
(1,511)	1:31:A:ILE:HG21	1:109:A:LEU:HG	10	0.31
(1,511)	1:31:A:ILE:HG22	1:109:A:LEU:HG	10	0.31
(1,511)	1:31:A:ILE:HG23	1:109:A:LEU:HG	10	0.31
(1,453)	1:28:A:ILE:HG12	1:41:A:GLU:HB2	10	0.31
(1,453)	1:28:A:ILE:HG12	1:41:A:GLU:HB3	10	0.31
(1,453)	1:28:A:ILE:HG13	1:41:A:GLU:HB2	10	0.31
(1,453)	1:28:A:ILE:HG13	1:41:A:GLU:HB3	10	0.31
(1,451)	1:28:A:ILE:HD11	1:70:A:ALA:HB1	6	0.31
(1,451)	1:28:A:ILE:HD11	1:70:A:ALA:HB2	6	0.31
(1,451)	1:28:A:ILE:HD11	1:70:A:ALA:HB3	6	0.31
(1,451)	1:28:A:ILE:HD12	1:70:A:ALA:HB1	6	0.31
(1,451)	1:28:A:ILE:HD12	1:70:A:ALA:HB2	6	0.31
(1,451)	1:28:A:ILE:HD12	1:70:A:ALA:HB3	6	0.31
(1,451)	1:28:A:ILE:HD13	1:70:A:ALA:HB1	6	0.31
(1,451)	1:28:A:ILE:HD13	1:70:A:ALA:HB2	6	0.31
(1,451)	1:28:A:ILE:HD13	1:70:A:ALA:HB3	6	0.31
(1,335)	1:19:A:HIS:HA	1:21:A:LYS:H	5	0.31
(1,319)	1:18:A:LEU:HD11	1:72:A:VAL:H	4	0.31
(1,319)	1:18:A:LEU:HD12	1:72:A:VAL:H	4	0.31
(1,319)	1:18:A:LEU:HD13	1:72:A:VAL:H	4	0.31
(1,237)	1:14:A:ALA:HA	1:18:A:LEU:H	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,186)	1:12:A:LYS:H	1:121:A:LEU:HG	7	0.31
(1,181)	1:11:A:CYS:HB3	1:13:A:ASN:H	3	0.31
(1,116)	1:8:A:ASP:H	1:39:A:VAL:HA	9	0.31
(1,102)	1:7:A:VAL:HG11	1:120:A:SER:HA	8	0.31
(1,102)	1:7:A:VAL:HG12	1:120:A:SER:HA	8	0.31
(1,102)	1:7:A:VAL:HG13	1:120:A:SER:HA	8	0.31
(1,102)	1:7:A:VAL:HG21	1:120:A:SER:HA	8	0.31
(1,102)	1:7:A:VAL:HG22	1:120:A:SER:HA	8	0.31
(1,102)	1:7:A:VAL:HG23	1:120:A:SER:HA	8	0.31
(3,60)	1:143:A:LYS:O	1:147:A:MET:N	9	0.3
(2,35)	1:118:A:LYS:HE3	1:128:A:GLN:HA	9	0.3
(2,2)	1:2:A:ALA:HB1	1:112:A:SER:H	3	0.3
(2,2)	1:2:A:ALA:HB2	1:112:A:SER:H	3	0.3
(2,2)	1:2:A:ALA:HB3	1:112:A:SER:H	3	0.3
(1,1700)	1:143:A:LYS:H	1:145:A:ASP:H	9	0.3
(1,1555)	1:132:A:SER:H	1:136:A:ASP:HA	2	0.3
(1,1440)	1:118:A:LYS:HD2	1:119:A:ALA:H	6	0.3
(1,1440)	1:118:A:LYS:HD3	1:119:A:ALA:H	6	0.3
(1,1426)	1:117:A:LEU:HB2	1:119:A:ALA:H	3	0.3
(1,1398)	1:115:A:ARG:HA	1:119:A:ALA:H	1	0.3
(1,1378)	1:114:A:VAL:HB	1:118:A:LYS:H	3	0.3
(1,1364)	1:113:A:SER:HB2	1:116:A:ALA:H	9	0.3
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG2	2	0.3
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG3	2	0.3
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG2	2	0.3
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG3	2	0.3
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG2	2	0.3
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG3	2	0.3
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG2	2	0.3
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG3	2	0.3
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG2	2	0.3
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG3	2	0.3
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG2	2	0.3
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG3	2	0.3
(1,1174)	1:99:A:PRO:HA	1:102:A:ALA:H	5	0.3
(1,1172)	1:98:A:CYS:HB2	1:107:A:ARG:HA	2	0.3
(1,1172)	1:98:A:CYS:HB3	1:107:A:ARG:HA	2	0.3
(1,1122)	1:94:A:PHE:HB2	1:118:A:LYS:HE2	7	0.3
(1,1122)	1:94:A:PHE:HB2	1:118:A:LYS:HE3	7	0.3
(1,1122)	1:94:A:PHE:HB3	1:118:A:LYS:HE2	7	0.3
(1,1122)	1:94:A:PHE:HB3	1:118:A:LYS:HE3	7	0.3
(1,1099)	1:93:A:ILE:HD11	1:142:A:VAL:HA	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1099)	1:93:A:ILE:HD12	1:142:A:VAL:HA	6	0.3
(1,1099)	1:93:A:ILE:HD13	1:142:A:VAL:HA	6	0.3
(1,1086)	1:93:A:ILE:HB	1:127:A:PHE:H	4	0.3
(1,1082)	1:93:A:ILE:HA	1:127:A:PHE:HA	10	0.3
(1,1048)	1:89:A:LEU:HG	1:90:A:ASN:H	9	0.3
(1,973)	1:79:A:GLN:HB2	1:85:A:GLY:H	6	0.3
(1,955)	1:78:A:VAL:HG11	1:80:A:ARG:HG2	5	0.3
(1,955)	1:78:A:VAL:HG12	1:80:A:ARG:HG2	5	0.3
(1,955)	1:78:A:VAL:HG13	1:80:A:ARG:HG2	5	0.3
(1,955)	1:78:A:VAL:HG11	1:80:A:ARG:HG3	5	0.3
(1,955)	1:78:A:VAL:HG12	1:80:A:ARG:HG3	5	0.3
(1,955)	1:78:A:VAL:HG13	1:80:A:ARG:HG3	5	0.3
(1,955)	1:78:A:VAL:HG11	1:80:A:ARG:HG2	10	0.3
(1,955)	1:78:A:VAL:HG12	1:80:A:ARG:HG2	10	0.3
(1,955)	1:78:A:VAL:HG13	1:80:A:ARG:HG2	10	0.3
(1,955)	1:78:A:VAL:HG11	1:80:A:ARG:HG3	10	0.3
(1,955)	1:78:A:VAL:HG12	1:80:A:ARG:HG3	10	0.3
(1,955)	1:78:A:VAL:HG13	1:80:A:ARG:HG3	10	0.3
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	3	0.3
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	3	0.3
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	3	0.3
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG11	3	0.3
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG12	3	0.3
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG13	3	0.3
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	3	0.3
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	3	0.3
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	3	0.3
(1,882)	1:75:A:GLU:HB2	1:89:A:LEU:H	5	0.3
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD11	7	0.3
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD12	7	0.3
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD13	7	0.3
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD21	7	0.3
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD22	7	0.3
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD23	7	0.3
(1,682)	1:54:A:VAL:HG21	1:57:A:MET:H	1	0.3
(1,682)	1:54:A:VAL:HG22	1:57:A:MET:H	1	0.3
(1,682)	1:54:A:VAL:HG23	1:57:A:MET:H	1	0.3
(1,608)	1:49:A:PRO:HG2	1:50:A:TYR:H	5	0.3
(1,608)	1:49:A:PRO:HG3	1:50:A:TYR:H	5	0.3
(1,575)	1:42:A:LYS:HB2	1:43:A:VAL:H	7	0.3
(1,575)	1:42:A:LYS:HB3	1:43:A:VAL:H	7	0.3
(1,527)	1:33:A:LYS:HG3	1:36:A:THR:HA	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,515)	1:31:A:ILE:HG21	1:37:A:ALA:H	10	0.3
(1,515)	1:31:A:ILE:HG22	1:37:A:ALA:H	10	0.3
(1,515)	1:31:A:ILE:HG23	1:37:A:ALA:H	10	0.3
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD11	6	0.3
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD12	6	0.3
(1,500)	1:31:A:ILE:HG13	1:38:A:ILE:HD13	6	0.3
(1,453)	1:28:A:ILE:HG12	1:41:A:GLU:HB2	6	0.3
(1,453)	1:28:A:ILE:HG12	1:41:A:GLU:HB3	6	0.3
(1,453)	1:28:A:ILE:HG13	1:41:A:GLU:HB2	6	0.3
(1,453)	1:28:A:ILE:HG13	1:41:A:GLU:HB3	6	0.3
(1,280)	1:16:A:ASP:HB3	1:18:A:LEU:H	1	0.3
(1,277)	1:16:A:ASP:HB2	1:18:A:LEU:H	3	0.3
(1,214)	1:12:A:LYS:HG3	1:15:A:TYR:H	6	0.3
(1,181)	1:11:A:CYS:HB3	1:13:A:ASN:H	1	0.3
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD11	9	0.3
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD12	9	0.3
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD13	9	0.3
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD21	9	0.3
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD22	9	0.3
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD23	9	0.3
(1,159)	1:10:A:SER:HB3	1:13:A:ASN:H	9	0.3
(1,135)	1:8:A:ASP:HB2	1:39:A:VAL:HB	7	0.3
(1,135)	1:8:A:ASP:HB3	1:39:A:VAL:HB	7	0.3
(1,112)	1:8:A:ASP:H	1:11:A:CYS:HB2	6	0.3
(1,112)	1:8:A:ASP:H	1:11:A:CYS:HB3	6	0.3
(1,54)	1:6:A:LYS:HD2	1:7:A:VAL:H	10	0.3
(1,54)	1:6:A:LYS:HD3	1:7:A:VAL:H	10	0.3
(1,44)	1:6:A:LYS:H	1:37:A:ALA:HA	6	0.3
(3,59)	1:143:A:LYS:O	1:147:A:MET:H	6	0.29
(2,6)	1:12:A:LYS:HG2	1:15:A:TYR:H	7	0.29
(1,1769)	1:149:A:ASN:H	1:150:A:GLN:H	6	0.29
(1,1719)	1:144:A:SER:HA	1:146:A:LEU:H	3	0.29
(1,1717)	1:144:A:SER:H	1:145:A:ASP:H	1	0.29
(1,1699)	1:143:A:LYS:H	1:144:A:SER:H	9	0.29
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD2	4	0.29
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD3	4	0.29
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD2	10	0.29
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD3	10	0.29
(1,1652)	1:140:A:LYS:HE2	1:141:A:SER:H	2	0.29
(1,1589)	1:135:A:SER:HA	1:140:A:LYS:HE2	5	0.29
(1,1421)	1:117:A:LEU:HA	1:120:A:SER:H	9	0.29
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB2	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB2	3	0.29
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB2	3	0.29
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB3	3	0.29
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB3	3	0.29
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB3	3	0.29
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB2	3	0.29
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB3	3	0.29
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB2	3	0.29
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB3	3	0.29
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB2	3	0.29
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB3	3	0.29
(1,1398)	1:115:A:ARG:HA	1:119:A:ALA:H	10	0.29
(1,1397)	1:115:A:ARG:HA	1:118:A:LYS:HD2	1	0.29
(1,1397)	1:115:A:ARG:HA	1:118:A:LYS:HD3	1	0.29
(1,1382)	1:114:A:VAL:HG21	1:116:A:ALA:H	6	0.29
(1,1382)	1:114:A:VAL:HG22	1:116:A:ALA:H	6	0.29
(1,1382)	1:114:A:VAL:HG23	1:116:A:ALA:H	6	0.29
(1,1204)	1:102:A:ALA:HB1	1:103:A:PRO:HG2	3	0.29
(1,1204)	1:102:A:ALA:HB1	1:103:A:PRO:HG3	3	0.29
(1,1204)	1:102:A:ALA:HB2	1:103:A:PRO:HG2	3	0.29
(1,1204)	1:102:A:ALA:HB2	1:103:A:PRO:HG3	3	0.29
(1,1204)	1:102:A:ALA:HB3	1:103:A:PRO:HG2	3	0.29
(1,1204)	1:102:A:ALA:HB3	1:103:A:PRO:HG3	3	0.29
(1,1118)	1:94:A:PHE:HA	1:128:A:GLN:HB2	6	0.29
(1,1114)	1:94:A:PHE:H	1:129:A:VAL:H	9	0.29
(1,1092)	1:93:A:ILE:HG12	1:127:A:PHE:H	1	0.29
(1,1030)	1:87:A:SER:H	1:88:A:THR:H	7	0.29
(1,1016)	1:84:A:GLU:HA	1:85:A:GLY:H	4	0.29
(1,1016)	1:84:A:GLU:HA	1:85:A:GLY:H	6	0.29
(1,947)	1:78:A:VAL:H	1:87:A:SER:H	2	0.29
(1,921)	1:76:A:VAL:HG11	1:143:A:LYS:HG2	9	0.29
(1,921)	1:76:A:VAL:HG11	1:143:A:LYS:HG3	9	0.29
(1,921)	1:76:A:VAL:HG12	1:143:A:LYS:HG2	9	0.29
(1,921)	1:76:A:VAL:HG12	1:143:A:LYS:HG3	9	0.29
(1,921)	1:76:A:VAL:HG13	1:143:A:LYS:HG2	9	0.29
(1,921)	1:76:A:VAL:HG13	1:143:A:LYS:HG3	9	0.29
(1,921)	1:76:A:VAL:HG21	1:143:A:LYS:HG2	9	0.29
(1,921)	1:76:A:VAL:HG21	1:143:A:LYS:HG3	9	0.29
(1,921)	1:76:A:VAL:HG22	1:143:A:LYS:HG2	9	0.29
(1,921)	1:76:A:VAL:HG22	1:143:A:LYS:HG3	9	0.29
(1,921)	1:76:A:VAL:HG23	1:143:A:LYS:HG2	9	0.29
(1,921)	1:76:A:VAL:HG23	1:143:A:LYS:HG3	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,915)	1:76:A:VAL:HG11	1:143:A:LYS:HG2	10	0.29
(1,915)	1:76:A:VAL:HG12	1:143:A:LYS:HG2	10	0.29
(1,915)	1:76:A:VAL:HG13	1:143:A:LYS:HG2	10	0.29
(1,915)	1:76:A:VAL:HG11	1:143:A:LYS:HG3	10	0.29
(1,915)	1:76:A:VAL:HG12	1:143:A:LYS:HG3	10	0.29
(1,915)	1:76:A:VAL:HG13	1:143:A:LYS:HG3	10	0.29
(1,753)	1:58:A:LYS:HB3	1:60:A:LEU:H	4	0.29
(1,676)	1:54:A:VAL:HB	1:57:A:MET:H	3	0.29
(1,671)	1:54:A:VAL:HA	1:57:A:MET:HA	1	0.29
(1,661)	1:53:A:PHE:HB3	1:56:A:GLU:H	6	0.29
(1,659)	1:53:A:PHE:HB2	1:56:A:GLU:H	7	0.29
(1,636)	1:51:A:ALA:HB1	1:54:A:VAL:H	9	0.29
(1,636)	1:51:A:ALA:HB2	1:54:A:VAL:H	9	0.29
(1,636)	1:51:A:ALA:HB3	1:54:A:VAL:H	9	0.29
(1,597)	1:49:A:PRO:HA	1:51:A:ALA:H	10	0.29
(1,575)	1:42:A:LYS:HB2	1:43:A:VAL:H	5	0.29
(1,575)	1:42:A:LYS:HB3	1:43:A:VAL:H	5	0.29
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB2	6	0.29
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB3	6	0.29
(1,510)	1:31:A:ILE:HG21	1:109:A:LEU:HA	1	0.29
(1,510)	1:31:A:ILE:HG22	1:109:A:LEU:HA	1	0.29
(1,510)	1:31:A:ILE:HG23	1:109:A:LEU:HA	1	0.29
(1,450)	1:28:A:ILE:HD11	1:70:A:ALA:HA	8	0.29
(1,450)	1:28:A:ILE:HD12	1:70:A:ALA:HA	8	0.29
(1,450)	1:28:A:ILE:HD13	1:70:A:ALA:HA	8	0.29
(1,428)	1:28:A:ILE:H	1:42:A:LYS:HD2	1	0.29
(1,428)	1:28:A:ILE:H	1:42:A:LYS:HD3	1	0.29
(1,385)	1:26:A:TYR:HB2	1:72:A:VAL:HA	10	0.29
(1,385)	1:26:A:TYR:HB3	1:72:A:VAL:HA	10	0.29
(1,315)	1:18:A:LEU:HB2	1:73:A:ASP:HB2	8	0.29
(1,315)	1:18:A:LEU:HB2	1:73:A:ASP:HB3	8	0.29
(1,315)	1:18:A:LEU:HB3	1:73:A:ASP:HB2	8	0.29
(1,315)	1:18:A:LEU:HB3	1:73:A:ASP:HB3	8	0.29
(1,290)	1:17:A:LEU:HA	1:19:A:HIS:H	1	0.29
(1,280)	1:16:A:ASP:HB3	1:18:A:LEU:H	4	0.29
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD11	1	0.29
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD12	1	0.29
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD13	1	0.29
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD21	1	0.29
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD22	1	0.29
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD23	1	0.29
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD11	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD12	1	0.29
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD13	1	0.29
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD21	1	0.29
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD22	1	0.29
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD23	1	0.29
(1,256)	1:15:A:TYR:HB2	1:121:A:LEU:HG	5	0.29
(1,243)	1:14:A:ALA:HB1	1:27:A:ILE:HB	10	0.29
(1,243)	1:14:A:ALA:HB2	1:27:A:ILE:HB	10	0.29
(1,243)	1:14:A:ALA:HB3	1:27:A:ILE:HB	10	0.29
(1,227)	1:13:A:ASN:HB2	1:15:A:TYR:H	9	0.29
(1,178)	1:11:A:CYS:HB2	1:13:A:ASN:H	3	0.29
(1,161)	1:10:A:SER:HB2	1:12:A:LYS:H	5	0.29
(1,161)	1:10:A:SER:HB3	1:12:A:LYS:H	5	0.29
(1,51)	1:6:A:LYS:HA	1:37:A:ALA:HA	4	0.29
(1,31)	1:5:A:VAL:HB	1:36:A:THR:HB	7	0.29
(3,25)	1:68:A:ARG:H	1:97:A:TYR:O	7	0.28
(3,20)	1:29:A:PHE:O	1:69:A:TYR:N	4	0.28
(3,4)	1:8:A:ASP:N	1:38:A:ILE:O	3	0.28
(3,3)	1:8:A:ASP:H	1:38:A:ILE:O	2	0.28
(2,27)	1:78:A:VAL:HB	1:87:A:SER:HA	3	0.28
(2,7)	1:15:A:TYR:H	1:43:A:VAL:HG11	8	0.28
(2,7)	1:15:A:TYR:H	1:43:A:VAL:HG12	8	0.28
(2,7)	1:15:A:TYR:H	1:43:A:VAL:HG13	8	0.28
(2,7)	1:15:A:TYR:H	1:43:A:VAL:HG21	8	0.28
(2,7)	1:15:A:TYR:H	1:43:A:VAL:HG22	8	0.28
(2,7)	1:15:A:TYR:H	1:43:A:VAL:HG23	8	0.28
(1,1790)	1:150:A:GLN:HB3	1:152:A:ILE:H	10	0.28
(1,1778)	1:149:A:ASN:HB2	1:151:A:ARG:HA	7	0.28
(1,1778)	1:149:A:ASN:HB3	1:151:A:ARG:HA	7	0.28
(1,1774)	1:149:A:ASN:HB3	1:152:A:ILE:HD11	8	0.28
(1,1774)	1:149:A:ASN:HB3	1:152:A:ILE:HD12	8	0.28
(1,1774)	1:149:A:ASN:HB3	1:152:A:ILE:HD13	8	0.28
(1,1757)	1:147:A:MET:HA	1:150:A:GLN:H	1	0.28
(1,1729)	1:145:A:ASP:H	1:146:A:LEU:H	4	0.28
(1,1630)	1:139:A:GLU:HB2	1:142:A:VAL:H	5	0.28
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG2	2	0.28
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG3	2	0.28
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG2	2	0.28
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG3	2	0.28
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG2	2	0.28
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG3	2	0.28
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG2	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG3	2	0.28
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG2	2	0.28
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG3	2	0.28
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG2	2	0.28
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG3	2	0.28
(1,1550)	1:131:A:ALA:HA	1:136:A:ASP:HA	10	0.28
(1,1426)	1:117:A:LEU:HB2	1:119:A:ALA:H	6	0.28
(1,1373)	1:114:A:VAL:HA	1:117:A:LEU:HB2	8	0.28
(1,1373)	1:114:A:VAL:HA	1:117:A:LEU:HB3	8	0.28
(1,1293)	1:108:A:MET:HA	1:110:A:TYR:H	2	0.28
(1,1225)	1:104:A:VAL:HB	1:107:A:ARG:H	4	0.28
(1,1107)	1:93:A:ILE:HG21	1:146:A:LEU:HA	6	0.28
(1,1107)	1:93:A:ILE:HG22	1:146:A:LEU:HA	6	0.28
(1,1107)	1:93:A:ILE:HG23	1:146:A:LEU:HA	6	0.28
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD11	7	0.28
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD12	7	0.28
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD13	7	0.28
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD21	7	0.28
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD22	7	0.28
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD23	7	0.28
(1,1065)	1:91:A:LYS:HE3	1:150:A:GLN:H	5	0.28
(1,1030)	1:87:A:SER:H	1:88:A:THR:H	8	0.28
(1,949)	1:78:A:VAL:HA	1:87:A:SER:HB2	8	0.28
(1,949)	1:78:A:VAL:HA	1:87:A:SER:HB3	8	0.28
(1,949)	1:78:A:VAL:HA	1:87:A:SER:HB2	8	0.28
(1,949)	1:78:A:VAL:HA	1:87:A:SER:HB3	8	0.28
(1,947)	1:78:A:VAL:H	1:87:A:SER:H	10	0.28
(1,944)	1:78:A:VAL:H	1:79:A:GLN:H	5	0.28
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	5	0.28
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	5	0.28
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	5	0.28
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG11	5	0.28
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG12	5	0.28
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG13	5	0.28
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	5	0.28
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	5	0.28
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	5	0.28
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	7	0.28
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	7	0.28
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	7	0.28
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG11	7	0.28
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG12	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG13	7	0.28
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	7	0.28
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	7	0.28
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	7	0.28
(1,882)	1:75:A:GLU:HB2	1:89:A:LEU:H	10	0.28
(1,723)	1:56:A:GLU:HG2	1:57:A:MET:H	3	0.28
(1,723)	1:56:A:GLU:HG2	1:57:A:MET:H	8	0.28
(1,682)	1:54:A:VAL:HG21	1:57:A:MET:H	3	0.28
(1,682)	1:54:A:VAL:HG22	1:57:A:MET:H	3	0.28
(1,682)	1:54:A:VAL:HG23	1:57:A:MET:H	3	0.28
(1,677)	1:54:A:VAL:HB	1:58:A:LYS:H	5	0.28
(1,669)	1:54:A:VAL:HA	1:56:A:GLU:H	7	0.28
(1,669)	1:54:A:VAL:HA	1:56:A:GLU:H	10	0.28
(1,600)	1:49:A:PRO:HA	1:53:A:PHE:H	6	0.28
(1,593)	1:45:A:GLU:HB3	1:48:A:ALA:HB1	9	0.28
(1,593)	1:45:A:GLU:HB3	1:48:A:ALA:HB2	9	0.28
(1,593)	1:45:A:GLU:HB3	1:48:A:ALA:HB3	9	0.28
(1,579)	1:42:A:LYS:HG2	1:56:A:GLU:HB2	3	0.28
(1,579)	1:42:A:LYS:HG2	1:56:A:GLU:HB3	3	0.28
(1,579)	1:42:A:LYS:HG3	1:56:A:GLU:HB2	3	0.28
(1,579)	1:42:A:LYS:HG3	1:56:A:GLU:HB3	3	0.28
(1,429)	1:28:A:ILE:H	1:42:A:LYS:HG2	10	0.28
(1,429)	1:28:A:ILE:H	1:42:A:LYS:HG3	10	0.28
(1,334)	1:19:A:HIS:H	1:21:A:LYS:H	2	0.28
(1,327)	1:18:A:LEU:HD21	1:73:A:ASP:HA	10	0.28
(1,327)	1:18:A:LEU:HD22	1:73:A:ASP:HA	10	0.28
(1,327)	1:18:A:LEU:HD23	1:73:A:ASP:HA	10	0.28
(1,321)	1:18:A:LEU:HD11	1:73:A:ASP:HA	7	0.28
(1,321)	1:18:A:LEU:HD12	1:73:A:ASP:HA	7	0.28
(1,321)	1:18:A:LEU:HD13	1:73:A:ASP:HA	7	0.28
(1,289)	1:17:A:LEU:H	1:23:A:GLN:HB2	3	0.28
(1,289)	1:17:A:LEU:H	1:23:A:GLN:HB3	3	0.28
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG11	7	0.28
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG12	7	0.28
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG13	7	0.28
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG21	7	0.28
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG22	7	0.28
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG23	7	0.28
(1,226)	1:13:A:ASN:HB2	1:14:A:ALA:H	6	0.28
(1,213)	1:12:A:LYS:HG3	1:14:A:ALA:H	2	0.28
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD11	1	0.28
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD12	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD13	1	0.28
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD21	1	0.28
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD22	1	0.28
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD23	1	0.28
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB2	6	0.28
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB3	6	0.28
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB2	6	0.28
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB3	6	0.28
(1,51)	1:6:A:LYS:HA	1:37:A:ALA:HA	6	0.28
(2,39)	1:135:A:SER:HA	1:140:A:LYS:HE3	5	0.27
(2,34)	1:114:A:VAL:HA	1:117:A:LEU:HA	3	0.27
(2,6)	1:12:A:LYS:HG2	1:15:A:TYR:H	4	0.27
(1,1780)	1:149:A:ASN:HB2	1:152:A:ILE:HD11	7	0.27
(1,1780)	1:149:A:ASN:HB2	1:152:A:ILE:HD12	7	0.27
(1,1780)	1:149:A:ASN:HB2	1:152:A:ILE:HD13	7	0.27
(1,1780)	1:149:A:ASN:HB3	1:152:A:ILE:HD11	7	0.27
(1,1780)	1:149:A:ASN:HB3	1:152:A:ILE:HD12	7	0.27
(1,1780)	1:149:A:ASN:HB3	1:152:A:ILE:HD13	7	0.27
(1,1769)	1:149:A:ASN:H	1:150:A:GLN:H	10	0.27
(1,1747)	1:146:A:LEU:HB2	1:147:A:MET:H	3	0.27
(1,1747)	1:146:A:LEU:HB3	1:147:A:MET:H	3	0.27
(1,1702)	1:143:A:LYS:HA	1:146:A:LEU:H	6	0.27
(1,1700)	1:143:A:LYS:H	1:145:A:ASP:H	3	0.27
(1,1652)	1:140:A:LYS:HE2	1:141:A:SER:H	10	0.27
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG2	6	0.27
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG3	6	0.27
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG2	6	0.27
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG3	6	0.27
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG2	6	0.27
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG3	6	0.27
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG2	6	0.27
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG3	6	0.27
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG2	6	0.27
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG3	6	0.27
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG2	6	0.27
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG3	6	0.27
(1,1597)	1:136:A:ASP:H	1:138:A:ASP:H	3	0.27
(1,1597)	1:136:A:ASP:H	1:138:A:ASP:H	10	0.27
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	2	0.27
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	2	0.27
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	2	0.27
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1436)	1:118:A:LYS:H	1:118:A:LYS:HE2	2	0.27
(1,1436)	1:118:A:LYS:H	1:118:A:LYS:HE3	2	0.27
(1,1429)	1:117:A:LEU:HB3	1:119:A:ALA:H	6	0.27
(1,1366)	1:113:A:SER:HB3	1:116:A:ALA:H	7	0.27
(1,1364)	1:113:A:SER:HB2	1:116:A:ALA:H	6	0.27
(1,1316)	1:109:A:LEU:HA	1:113:A:SER:H	10	0.27
(1,1236)	1:104:A:VAL:HG21	1:108:A:MET:HB2	1	0.27
(1,1236)	1:104:A:VAL:HG22	1:108:A:MET:HB2	1	0.27
(1,1236)	1:104:A:VAL:HG23	1:108:A:MET:HB2	1	0.27
(1,1236)	1:104:A:VAL:HG21	1:108:A:MET:HB3	1	0.27
(1,1236)	1:104:A:VAL:HG22	1:108:A:MET:HB3	1	0.27
(1,1236)	1:104:A:VAL:HG23	1:108:A:MET:HB3	1	0.27
(1,1218)	1:104:A:VAL:HA	1:106:A:ARG:H	8	0.27
(1,1186)	1:99:A:PRO:HG2	1:132:A:SER:HA	7	0.27
(1,1099)	1:93:A:ILE:HD11	1:142:A:VAL:HA	3	0.27
(1,1099)	1:93:A:ILE:HD12	1:142:A:VAL:HA	3	0.27
(1,1099)	1:93:A:ILE:HD13	1:142:A:VAL:HA	3	0.27
(1,982)	1:80:A:ARG:H	1:80:A:ARG:HD2	9	0.27
(1,982)	1:80:A:ARG:H	1:80:A:ARG:HD3	9	0.27
(1,953)	1:78:A:VAL:HB	1:87:A:SER:HB2	7	0.27
(1,953)	1:78:A:VAL:HB	1:87:A:SER:HB3	7	0.27
(1,944)	1:78:A:VAL:H	1:79:A:GLN:H	1	0.27
(1,938)	1:77:A:THR:HB	1:88:A:THR:HG21	9	0.27
(1,938)	1:77:A:THR:HB	1:88:A:THR:HG22	9	0.27
(1,938)	1:77:A:THR:HB	1:88:A:THR:HG23	9	0.27
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	6	0.27
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	6	0.27
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	6	0.27
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG11	6	0.27
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG12	6	0.27
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG13	6	0.27
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	6	0.27
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	6	0.27
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	6	0.27
(1,887)	1:75:A:GLU:HB3	1:89:A:LEU:H	8	0.27
(1,885)	1:75:A:GLU:HB3	1:88:A:THR:HB	4	0.27
(1,883)	1:75:A:GLU:HB3	1:76:A:VAL:H	5	0.27
(1,882)	1:75:A:GLU:HB2	1:89:A:LEU:H	4	0.27
(1,880)	1:75:A:GLU:HB2	1:88:A:THR:HB	10	0.27
(1,703)	1:55:A:GLU:HA	1:58:A:LYS:HG2	1	0.27
(1,703)	1:55:A:GLU:HA	1:58:A:LYS:HG3	1	0.27
(1,689)	1:54:A:VAL:HG11	1:57:A:MET:H	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,689)	1:54:A:VAL:HG12	1:57:A:MET:H	3	0.27
(1,689)	1:54:A:VAL:HG13	1:57:A:MET:H	3	0.27
(1,689)	1:54:A:VAL:HG21	1:57:A:MET:H	3	0.27
(1,689)	1:54:A:VAL:HG22	1:57:A:MET:H	3	0.27
(1,689)	1:54:A:VAL:HG23	1:57:A:MET:H	3	0.27
(1,682)	1:54:A:VAL:HG21	1:57:A:MET:H	6	0.27
(1,682)	1:54:A:VAL:HG22	1:57:A:MET:H	6	0.27
(1,682)	1:54:A:VAL:HG23	1:57:A:MET:H	6	0.27
(1,676)	1:54:A:VAL:HB	1:57:A:MET:H	1	0.27
(1,657)	1:53:A:PHE:HA	1:57:A:MET:H	6	0.27
(1,654)	1:53:A:PHE:HA	1:55:A:GLU:H	10	0.27
(1,598)	1:49:A:PRO:HA	1:51:A:ALA:HB1	5	0.27
(1,598)	1:49:A:PRO:HA	1:51:A:ALA:HB2	5	0.27
(1,598)	1:49:A:PRO:HA	1:51:A:ALA:HB3	5	0.27
(1,453)	1:28:A:ILE:HG12	1:41:A:GLU:HB2	4	0.27
(1,453)	1:28:A:ILE:HG12	1:41:A:GLU:HB3	4	0.27
(1,453)	1:28:A:ILE:HG13	1:41:A:GLU:HB2	4	0.27
(1,453)	1:28:A:ILE:HG13	1:41:A:GLU:HB3	4	0.27
(1,366)	1:25:A:SER:H	1:73:A:ASP:H	1	0.27
(1,366)	1:25:A:SER:H	1:73:A:ASP:H	7	0.27
(1,302)	1:17:A:LEU:HD21	1:19:A:HIS:H	4	0.27
(1,302)	1:17:A:LEU:HD22	1:19:A:HIS:H	4	0.27
(1,302)	1:17:A:LEU:HD23	1:19:A:HIS:H	4	0.27
(1,283)	1:16:A:ASP:HB2	1:18:A:LEU:H	2	0.27
(1,283)	1:16:A:ASP:HB3	1:18:A:LEU:H	2	0.27
(1,283)	1:16:A:ASP:HB2	1:18:A:LEU:H	5	0.27
(1,283)	1:16:A:ASP:HB3	1:18:A:LEU:H	5	0.27
(1,255)	1:15:A:TYR:HA	1:19:A:HIS:H	10	0.27
(1,227)	1:13:A:ASN:HB2	1:15:A:TYR:H	1	0.27
(1,226)	1:13:A:ASN:HB2	1:14:A:ALA:H	9	0.27
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD11	7	0.27
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD12	7	0.27
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD13	7	0.27
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD21	7	0.27
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD22	7	0.27
(1,166)	1:11:A:CYS:H	1:121:A:LEU:HD23	7	0.27
(1,156)	1:10:A:SER:HB2	1:13:A:ASN:H	7	0.27
(1,129)	1:8:A:ASP:HB3	1:39:A:VAL:HB	4	0.27
(1,116)	1:8:A:ASP:H	1:39:A:VAL:HA	4	0.27
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG21	2	0.27
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG22	2	0.27
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG23	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG21	3	0.27
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG22	3	0.27
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG23	3	0.27
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG21	6	0.27
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG22	6	0.27
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG23	6	0.27
(1,65)	1:7:A:VAL:HA	1:37:A:ALA:HA	3	0.27
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG11	4	0.27
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG12	4	0.27
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG13	4	0.27
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG21	4	0.27
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG22	4	0.27
(1,34)	1:5:A:VAL:HB	1:7:A:VAL:HG23	4	0.27
(3,10)	1:26:A:TYR:N	1:44:A:GLY:O	9	0.26
(3,8)	1:13:A:ASN:O	1:17:A:LEU:N	2	0.26
(2,27)	1:78:A:VAL:HB	1:87:A:SER:HA	1	0.26
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG11	6	0.26
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG12	6	0.26
(2,26)	1:77:A:THR:HB	1:78:A:VAL:HG13	6	0.26
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG11	1	0.26
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG12	1	0.26
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG13	1	0.26
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG21	1	0.26
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG22	1	0.26
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG23	1	0.26
(1,1717)	1:144:A:SER:H	1:145:A:ASP:H	10	0.26
(1,1700)	1:143:A:LYS:H	1:145:A:ASP:H	7	0.26
(1,1699)	1:143:A:LYS:H	1:144:A:SER:H	8	0.26
(1,1597)	1:136:A:ASP:H	1:138:A:ASP:H	1	0.26
(1,1597)	1:136:A:ASP:H	1:138:A:ASP:H	6	0.26
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	8	0.26
(1,1449)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	8	0.26
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	8	0.26
(1,1449)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	8	0.26
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB2	2	0.26
(1,1445)	1:118:A:LYS:HG2	1:128:A:GLN:HB3	2	0.26
(1,1414)	1:116:A:ALA:HB1	1:120:A:SER:H	5	0.26
(1,1414)	1:116:A:ALA:HB2	1:120:A:SER:H	5	0.26
(1,1414)	1:116:A:ALA:HB3	1:120:A:SER:H	5	0.26
(1,1402)	1:115:A:ARG:HB2	1:118:A:LYS:H	5	0.26
(1,1402)	1:115:A:ARG:HB3	1:118:A:LYS:H	5	0.26
(1,1382)	1:114:A:VAL:HG21	1:116:A:ALA:H	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1382)	1:114:A:VAL:HG22	1:116:A:ALA:H	1	0.26
(1,1382)	1:114:A:VAL:HG23	1:116:A:ALA:H	1	0.26
(1,1382)	1:114:A:VAL:HG21	1:116:A:ALA:H	2	0.26
(1,1382)	1:114:A:VAL:HG22	1:116:A:ALA:H	2	0.26
(1,1382)	1:114:A:VAL:HG23	1:116:A:ALA:H	2	0.26
(1,1364)	1:113:A:SER:HB2	1:116:A:ALA:H	2	0.26
(1,1316)	1:109:A:LEU:HA	1:113:A:SER:H	2	0.26
(1,1313)	1:109:A:LEU:HA	1:111:A:ALA:H	8	0.26
(1,1234)	1:104:A:VAL:HG21	1:107:A:ARG:H	5	0.26
(1,1234)	1:104:A:VAL:HG22	1:107:A:ARG:H	5	0.26
(1,1234)	1:104:A:VAL:HG23	1:107:A:ARG:H	5	0.26
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB2	8	0.26
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB3	8	0.26
(1,1086)	1:93:A:ILE:HB	1:127:A:PHE:H	6	0.26
(1,1061)	1:91:A:LYS:HA	1:150:A:GLN:HG2	3	0.26
(1,1061)	1:91:A:LYS:HA	1:150:A:GLN:HG3	3	0.26
(1,944)	1:78:A:VAL:H	1:79:A:GLN:H	4	0.26
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD11	1	0.26
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD12	1	0.26
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD13	1	0.26
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD21	1	0.26
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD22	1	0.26
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD23	1	0.26
(1,858)	1:74:A:VAL:H	1:74:A:VAL:HB	9	0.26
(1,769)	1:60:A:LEU:H	1:60:A:LEU:HG	8	0.26
(1,742)	1:58:A:LYS:H	1:58:A:LYS:HE2	5	0.26
(1,742)	1:58:A:LYS:H	1:58:A:LYS:HE3	5	0.26
(1,725)	1:56:A:GLU:HG3	1:57:A:MET:H	6	0.26
(1,692)	1:54:A:VAL:HG11	1:58:A:LYS:HE2	1	0.26
(1,692)	1:54:A:VAL:HG11	1:58:A:LYS:HE3	1	0.26
(1,692)	1:54:A:VAL:HG12	1:58:A:LYS:HE2	1	0.26
(1,692)	1:54:A:VAL:HG12	1:58:A:LYS:HE3	1	0.26
(1,692)	1:54:A:VAL:HG13	1:58:A:LYS:HE2	1	0.26
(1,692)	1:54:A:VAL:HG13	1:58:A:LYS:HE3	1	0.26
(1,692)	1:54:A:VAL:HG21	1:58:A:LYS:HE2	1	0.26
(1,692)	1:54:A:VAL:HG21	1:58:A:LYS:HE3	1	0.26
(1,692)	1:54:A:VAL:HG22	1:58:A:LYS:HE2	1	0.26
(1,692)	1:54:A:VAL:HG22	1:58:A:LYS:HE3	1	0.26
(1,692)	1:54:A:VAL:HG23	1:58:A:LYS:HE2	1	0.26
(1,692)	1:54:A:VAL:HG23	1:58:A:LYS:HE3	1	0.26
(1,683)	1:54:A:VAL:HG21	1:58:A:LYS:H	5	0.26
(1,683)	1:54:A:VAL:HG22	1:58:A:LYS:H	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,683)	1:54:A:VAL:HG23	1:58:A:LYS:H	5	0.26
(1,664)	1:53:A:PHE:HB2	1:57:A:MET:H	7	0.26
(1,664)	1:53:A:PHE:HB3	1:57:A:MET:H	7	0.26
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB1	3	0.26
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB2	3	0.26
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB3	3	0.26
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB1	3	0.26
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB2	3	0.26
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB3	3	0.26
(1,597)	1:49:A:PRO:HA	1:51:A:ALA:H	5	0.26
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB1	4	0.26
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB2	4	0.26
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB3	4	0.26
(1,450)	1:28:A:ILE:HD11	1:70:A:ALA:HA	4	0.26
(1,450)	1:28:A:ILE:HD12	1:70:A:ALA:HA	4	0.26
(1,450)	1:28:A:ILE:HD13	1:70:A:ALA:HA	4	0.26
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB1	8	0.26
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB2	8	0.26
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB3	8	0.26
(1,296)	1:17:A:LEU:HA	1:23:A:GLN:HB2	9	0.26
(1,296)	1:17:A:LEU:HA	1:23:A:GLN:HB3	9	0.26
(1,281)	1:16:A:ASP:HB3	1:19:A:HIS:H	1	0.26
(1,272)	1:16:A:ASP:HA	1:18:A:LEU:H	6	0.26
(1,264)	1:15:A:TYR:HB3	1:27:A:ILE:HD11	8	0.26
(1,264)	1:15:A:TYR:HB3	1:27:A:ILE:HD12	8	0.26
(1,264)	1:15:A:TYR:HB3	1:27:A:ILE:HD13	8	0.26
(1,243)	1:14:A:ALA:HB1	1:27:A:ILE:HB	2	0.26
(1,243)	1:14:A:ALA:HB2	1:27:A:ILE:HB	2	0.26
(1,243)	1:14:A:ALA:HB3	1:27:A:ILE:HB	2	0.26
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG11	3	0.26
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG12	3	0.26
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG13	3	0.26
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG21	3	0.26
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG22	3	0.26
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG23	3	0.26
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG11	3	0.26
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG12	3	0.26
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG13	3	0.26
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG21	3	0.26
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG22	3	0.26
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG23	3	0.26
(1,178)	1:11:A:CYS:HB2	1:13:A:ASN:H	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,155)	1:10:A:SER:HB2	1:12:A:LYS:H	10	0.26
(1,116)	1:8:A:ASP:H	1:39:A:VAL:HA	2	0.26
(1,108)	1:7:A:VAL:HG11	1:38:A:ILE:HB	2	0.26
(1,108)	1:7:A:VAL:HG12	1:38:A:ILE:HB	2	0.26
(1,108)	1:7:A:VAL:HG13	1:38:A:ILE:HB	2	0.26
(1,108)	1:7:A:VAL:HG21	1:38:A:ILE:HB	2	0.26
(1,108)	1:7:A:VAL:HG22	1:38:A:ILE:HB	2	0.26
(1,108)	1:7:A:VAL:HG23	1:38:A:ILE:HB	2	0.26
(1,107)	1:7:A:VAL:HG11	1:38:A:ILE:H	9	0.26
(1,107)	1:7:A:VAL:HG12	1:38:A:ILE:H	9	0.26
(1,107)	1:7:A:VAL:HG13	1:38:A:ILE:H	9	0.26
(1,107)	1:7:A:VAL:HG21	1:38:A:ILE:H	9	0.26
(1,107)	1:7:A:VAL:HG22	1:38:A:ILE:H	9	0.26
(1,107)	1:7:A:VAL:HG23	1:38:A:ILE:H	9	0.26
(3,60)	1:143:A:LYS:O	1:147:A:MET:N	3	0.25
(3,7)	1:13:A:ASN:O	1:17:A:LEU:H	9	0.25
(2,27)	1:78:A:VAL:HB	1:87:A:SER:HA	10	0.25
(2,6)	1:12:A:LYS:HG2	1:15:A:TYR:H	2	0.25
(1,1769)	1:149:A:ASN:H	1:150:A:GLN:H	2	0.25
(1,1730)	1:145:A:ASP:H	1:147:A:MET:H	8	0.25
(1,1729)	1:145:A:ASP:H	1:146:A:LEU:H	1	0.25
(1,1723)	1:144:A:SER:HB2	1:146:A:LEU:H	6	0.25
(1,1717)	1:144:A:SER:H	1:145:A:ASP:H	5	0.25
(1,1717)	1:144:A:SER:H	1:145:A:ASP:H	6	0.25
(1,1699)	1:143:A:LYS:H	1:144:A:SER:H	6	0.25
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD2	5	0.25
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD3	5	0.25
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD2	9	0.25
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD3	9	0.25
(1,1659)	1:140:A:LYS:HB2	1:143:A:LYS:H	3	0.25
(1,1659)	1:140:A:LYS:HB3	1:143:A:LYS:H	3	0.25
(1,1659)	1:140:A:LYS:HB2	1:143:A:LYS:H	6	0.25
(1,1659)	1:140:A:LYS:HB3	1:143:A:LYS:H	6	0.25
(1,1552)	1:131:A:ALA:HB1	1:136:A:ASP:HA	6	0.25
(1,1552)	1:131:A:ALA:HB2	1:136:A:ASP:HA	6	0.25
(1,1552)	1:131:A:ALA:HB3	1:136:A:ASP:HA	6	0.25
(1,1549)	1:131:A:ALA:H	1:136:A:ASP:HB2	1	0.25
(1,1549)	1:131:A:ALA:H	1:136:A:ASP:HB3	1	0.25
(1,1441)	1:118:A:LYS:HE2	1:119:A:ALA:H	10	0.25
(1,1426)	1:117:A:LEU:HB2	1:119:A:ALA:H	8	0.25
(1,1288)	1:107:A:ARG:HG2	1:109:A:LEU:H	1	0.25
(1,1288)	1:107:A:ARG:HG3	1:109:A:LEU:H	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1241)	1:104:A:VAL:HG11	1:107:A:ARG:HB2	3	0.25
(1,1241)	1:104:A:VAL:HG11	1:107:A:ARG:HB3	3	0.25
(1,1241)	1:104:A:VAL:HG12	1:107:A:ARG:HB2	3	0.25
(1,1241)	1:104:A:VAL:HG12	1:107:A:ARG:HB3	3	0.25
(1,1241)	1:104:A:VAL:HG13	1:107:A:ARG:HB2	3	0.25
(1,1241)	1:104:A:VAL:HG13	1:107:A:ARG:HB3	3	0.25
(1,1241)	1:104:A:VAL:HG21	1:107:A:ARG:HB2	3	0.25
(1,1241)	1:104:A:VAL:HG21	1:107:A:ARG:HB3	3	0.25
(1,1241)	1:104:A:VAL:HG22	1:107:A:ARG:HB2	3	0.25
(1,1241)	1:104:A:VAL:HG22	1:107:A:ARG:HB3	3	0.25
(1,1241)	1:104:A:VAL:HG23	1:107:A:ARG:HB2	3	0.25
(1,1241)	1:104:A:VAL:HG23	1:107:A:ARG:HB3	3	0.25
(1,1205)	1:102:A:ALA:HB1	1:106:A:ARG:HD2	7	0.25
(1,1205)	1:102:A:ALA:HB1	1:106:A:ARG:HD3	7	0.25
(1,1205)	1:102:A:ALA:HB2	1:106:A:ARG:HD2	7	0.25
(1,1205)	1:102:A:ALA:HB2	1:106:A:ARG:HD3	7	0.25
(1,1205)	1:102:A:ALA:HB3	1:106:A:ARG:HD2	7	0.25
(1,1205)	1:102:A:ALA:HB3	1:106:A:ARG:HD3	7	0.25
(1,1189)	1:99:A:PRO:HG3	1:102:A:ALA:HA	10	0.25
(1,1186)	1:99:A:PRO:HG2	1:132:A:SER:HA	2	0.25
(1,1027)	1:86:A:THR:HB	1:87:A:SER:H	10	0.25
(1,1015)	1:84:A:GLU:H	1:85:A:GLY:H	2	0.25
(1,962)	1:78:A:VAL:HG11	1:87:A:SER:HB2	6	0.25
(1,962)	1:78:A:VAL:HG11	1:87:A:SER:HB3	6	0.25
(1,962)	1:78:A:VAL:HG12	1:87:A:SER:HB2	6	0.25
(1,962)	1:78:A:VAL:HG12	1:87:A:SER:HB3	6	0.25
(1,962)	1:78:A:VAL:HG13	1:87:A:SER:HB2	6	0.25
(1,962)	1:78:A:VAL:HG13	1:87:A:SER:HB3	6	0.25
(1,962)	1:78:A:VAL:HG21	1:87:A:SER:HB2	6	0.25
(1,962)	1:78:A:VAL:HG21	1:87:A:SER:HB3	6	0.25
(1,962)	1:78:A:VAL:HG22	1:87:A:SER:HB2	6	0.25
(1,962)	1:78:A:VAL:HG22	1:87:A:SER:HB3	6	0.25
(1,962)	1:78:A:VAL:HG23	1:87:A:SER:HB2	6	0.25
(1,962)	1:78:A:VAL:HG23	1:87:A:SER:HB3	6	0.25
(1,948)	1:78:A:VAL:HA	1:79:A:GLN:H	1	0.25
(1,948)	1:78:A:VAL:HA	1:79:A:GLN:H	10	0.25
(1,944)	1:78:A:VAL:H	1:79:A:GLN:H	3	0.25
(1,944)	1:78:A:VAL:H	1:79:A:GLN:H	7	0.25
(1,944)	1:78:A:VAL:H	1:79:A:GLN:H	10	0.25
(1,930)	1:77:A:THR:HA	1:78:A:VAL:HB	1	0.25
(1,851)	1:73:A:ASP:HA	1:91:A:LYS:H	1	0.25
(1,682)	1:54:A:VAL:HG21	1:57:A:MET:H	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,682)	1:54:A:VAL:HG22	1:57:A:MET:H	7	0.25
(1,682)	1:54:A:VAL:HG23	1:57:A:MET:H	7	0.25
(1,675)	1:54:A:VAL:HB	1:56:A:GLU:H	4	0.25
(1,629)	1:51:A:ALA:HA	1:54:A:VAL:HA	8	0.25
(1,426)	1:28:A:ILE:H	1:42:A:LYS:HA	4	0.25
(1,404)	1:27:A:ILE:HB	1:71:A:ALA:HB1	1	0.25
(1,404)	1:27:A:ILE:HB	1:71:A:ALA:HB2	1	0.25
(1,404)	1:27:A:ILE:HB	1:71:A:ALA:HB3	1	0.25
(1,331)	1:18:A:LEU:HD11	1:92:A:VAL:HA	1	0.25
(1,331)	1:18:A:LEU:HD12	1:92:A:VAL:HA	1	0.25
(1,331)	1:18:A:LEU:HD13	1:92:A:VAL:HA	1	0.25
(1,331)	1:18:A:LEU:HD21	1:92:A:VAL:HA	1	0.25
(1,331)	1:18:A:LEU:HD22	1:92:A:VAL:HA	1	0.25
(1,331)	1:18:A:LEU:HD23	1:92:A:VAL:HA	1	0.25
(1,292)	1:17:A:LEU:HA	1:21:A:LYS:H	2	0.25
(1,162)	1:10:A:SER:HB2	1:13:A:ASN:H	1	0.25
(1,162)	1:10:A:SER:HB3	1:13:A:ASN:H	1	0.25
(1,162)	1:10:A:SER:HB2	1:13:A:ASN:H	9	0.25
(1,162)	1:10:A:SER:HB3	1:13:A:ASN:H	9	0.25
(1,161)	1:10:A:SER:HB2	1:12:A:LYS:H	6	0.25
(1,161)	1:10:A:SER:HB3	1:12:A:LYS:H	6	0.25
(1,159)	1:10:A:SER:HB3	1:13:A:ASN:H	5	0.25
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG11	8	0.25
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG12	8	0.25
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG13	8	0.25
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG21	8	0.25
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG22	8	0.25
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG23	8	0.25
(1,73)	1:7:A:VAL:HB	1:120:A:SER:HA	4	0.25
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG11	5	0.25
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG12	5	0.25
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG13	5	0.25
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG21	5	0.25
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG22	5	0.25
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG23	5	0.25
(1,4)	1:1:A:MET:HA	1:114:A:VAL:HB	4	0.25
(3,4)	1:8:A:ASP:N	1:38:A:ILE:O	4	0.24
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG11	6	0.24
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG12	6	0.24
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG13	6	0.24
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG21	6	0.24
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG22	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG23	6	0.24
(2,3)	1:5:A:VAL:HB	1:117:A:LEU:HG	8	0.24
(1,1747)	1:146:A:LEU:HB2	1:147:A:MET:H	5	0.24
(1,1747)	1:146:A:LEU:HB3	1:147:A:MET:H	5	0.24
(1,1725)	1:144:A:SER:HB3	1:145:A:ASP:H	1	0.24
(1,1712)	1:143:A:LYS:HB3	1:147:A:MET:H	10	0.24
(1,1704)	1:143:A:LYS:HA	1:146:A:LEU:HB2	7	0.24
(1,1704)	1:143:A:LYS:HA	1:146:A:LEU:HB3	7	0.24
(1,1699)	1:143:A:LYS:H	1:144:A:SER:H	1	0.24
(1,1699)	1:143:A:LYS:H	1:144:A:SER:H	10	0.24
(1,1669)	1:141:A:SER:HB3	1:143:A:LYS:H	7	0.24
(1,1660)	1:140:A:LYS:HG2	1:142:A:VAL:H	7	0.24
(1,1660)	1:140:A:LYS:HG3	1:142:A:VAL:H	7	0.24
(1,1658)	1:140:A:LYS:HB2	1:142:A:VAL:H	10	0.24
(1,1658)	1:140:A:LYS:HB3	1:142:A:VAL:H	10	0.24
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG11	10	0.24
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG12	10	0.24
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG13	10	0.24
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG21	10	0.24
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG22	10	0.24
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG23	10	0.24
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG11	10	0.24
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG12	10	0.24
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG13	10	0.24
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG21	10	0.24
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG22	10	0.24
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG23	10	0.24
(1,1594)	1:135:A:SER:HB2	1:140:A:LYS:HG2	1	0.24
(1,1594)	1:135:A:SER:HB2	1:140:A:LYS:HG3	1	0.24
(1,1594)	1:135:A:SER:HB3	1:140:A:LYS:HG2	1	0.24
(1,1594)	1:135:A:SER:HB3	1:140:A:LYS:HG3	1	0.24
(1,1414)	1:116:A:ALA:HB1	1:120:A:SER:H	1	0.24
(1,1414)	1:116:A:ALA:HB2	1:120:A:SER:H	1	0.24
(1,1414)	1:116:A:ALA:HB3	1:120:A:SER:H	1	0.24
(1,1405)	1:116:A:ALA:H	1:117:A:LEU:H	1	0.24
(1,1396)	1:115:A:ARG:HA	1:118:A:LYS:H	9	0.24
(1,1366)	1:113:A:SER:HB3	1:116:A:ALA:H	10	0.24
(1,1325)	1:109:A:LEU:HD11	1:112:A:SER:HB2	3	0.24
(1,1325)	1:109:A:LEU:HD11	1:112:A:SER:HB3	3	0.24
(1,1325)	1:109:A:LEU:HD12	1:112:A:SER:HB2	3	0.24
(1,1325)	1:109:A:LEU:HD12	1:112:A:SER:HB3	3	0.24
(1,1325)	1:109:A:LEU:HD13	1:112:A:SER:HB2	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1325)	1:109:A:LEU:HD13	1:112:A:SER:HB3	3	0.24
(1,1325)	1:109:A:LEU:HD21	1:112:A:SER:HB2	3	0.24
(1,1325)	1:109:A:LEU:HD21	1:112:A:SER:HB3	3	0.24
(1,1325)	1:109:A:LEU:HD22	1:112:A:SER:HB2	3	0.24
(1,1325)	1:109:A:LEU:HD22	1:112:A:SER:HB3	3	0.24
(1,1325)	1:109:A:LEU:HD23	1:112:A:SER:HB2	3	0.24
(1,1325)	1:109:A:LEU:HD23	1:112:A:SER:HB3	3	0.24
(1,1242)	1:104:A:VAL:HG11	1:107:A:ARG:HD2	8	0.24
(1,1242)	1:104:A:VAL:HG11	1:107:A:ARG:HD3	8	0.24
(1,1242)	1:104:A:VAL:HG12	1:107:A:ARG:HD2	8	0.24
(1,1242)	1:104:A:VAL:HG12	1:107:A:ARG:HD3	8	0.24
(1,1242)	1:104:A:VAL:HG13	1:107:A:ARG:HD2	8	0.24
(1,1242)	1:104:A:VAL:HG13	1:107:A:ARG:HD3	8	0.24
(1,1242)	1:104:A:VAL:HG21	1:107:A:ARG:HD2	8	0.24
(1,1242)	1:104:A:VAL:HG21	1:107:A:ARG:HD3	8	0.24
(1,1242)	1:104:A:VAL:HG22	1:107:A:ARG:HD2	8	0.24
(1,1242)	1:104:A:VAL:HG22	1:107:A:ARG:HD3	8	0.24
(1,1242)	1:104:A:VAL:HG23	1:107:A:ARG:HD2	8	0.24
(1,1242)	1:104:A:VAL:HG23	1:107:A:ARG:HD3	8	0.24
(1,1190)	1:99:A:PRO:HG3	1:132:A:SER:HA	4	0.24
(1,1174)	1:99:A:PRO:HA	1:102:A:ALA:H	2	0.24
(1,1172)	1:98:A:CYS:HB2	1:107:A:ARG:HA	4	0.24
(1,1172)	1:98:A:CYS:HB3	1:107:A:ARG:HA	4	0.24
(1,1165)	1:97:A:TYR:HA	1:131:A:ALA:HA	3	0.24
(1,1107)	1:93:A:ILE:HG21	1:146:A:LEU:HA	1	0.24
(1,1107)	1:93:A:ILE:HG22	1:146:A:LEU:HA	1	0.24
(1,1107)	1:93:A:ILE:HG23	1:146:A:LEU:HA	1	0.24
(1,1086)	1:93:A:ILE:HB	1:127:A:PHE:H	8	0.24
(1,1052)	1:89:A:LEU:HD21	1:90:A:ASN:H	4	0.24
(1,1052)	1:89:A:LEU:HD22	1:90:A:ASN:H	4	0.24
(1,1052)	1:89:A:LEU:HD23	1:90:A:ASN:H	4	0.24
(1,1050)	1:89:A:LEU:HD11	1:90:A:ASN:H	6	0.24
(1,1050)	1:89:A:LEU:HD12	1:90:A:ASN:H	6	0.24
(1,1050)	1:89:A:LEU:HD13	1:90:A:ASN:H	6	0.24
(1,1050)	1:89:A:LEU:HD11	1:90:A:ASN:H	9	0.24
(1,1050)	1:89:A:LEU:HD12	1:90:A:ASN:H	9	0.24
(1,1050)	1:89:A:LEU:HD13	1:90:A:ASN:H	9	0.24
(1,1014)	1:84:A:GLU:H	1:84:A:GLU:HB2	2	0.24
(1,1014)	1:84:A:GLU:H	1:84:A:GLU:HB3	2	0.24
(1,994)	1:80:A:ARG:HG2	1:86:A:THR:HA	8	0.24
(1,994)	1:80:A:ARG:HG3	1:86:A:THR:HA	8	0.24
(1,948)	1:78:A:VAL:HA	1:79:A:GLN:H	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,882)	1:75:A:GLU:HB2	1:89:A:LEU:H	3	0.24
(1,749)	1:58:A:LYS:HA	1:62:A:GLU:H	7	0.24
(1,725)	1:56:A:GLU:HG3	1:57:A:MET:H	9	0.24
(1,724)	1:56:A:GLU:HG2	1:58:A:LYS:H	9	0.24
(1,708)	1:55:A:GLU:HB2	1:57:A:MET:H	2	0.24
(1,684)	1:54:A:VAL:HG11	1:138:A:ASP:H	7	0.24
(1,684)	1:54:A:VAL:HG12	1:138:A:ASP:H	7	0.24
(1,684)	1:54:A:VAL:HG13	1:138:A:ASP:H	7	0.24
(1,684)	1:54:A:VAL:HG21	1:138:A:ASP:H	7	0.24
(1,684)	1:54:A:VAL:HG22	1:138:A:ASP:H	7	0.24
(1,684)	1:54:A:VAL:HG23	1:138:A:ASP:H	7	0.24
(1,675)	1:54:A:VAL:HB	1:56:A:GLU:H	6	0.24
(1,655)	1:53:A:PHE:HA	1:56:A:GLU:H	1	0.24
(1,654)	1:53:A:PHE:HA	1:55:A:GLU:H	9	0.24
(1,644)	1:52:A:GLU:HA	1:55:A:GLU:H	4	0.24
(1,629)	1:51:A:ALA:HA	1:54:A:VAL:HA	10	0.24
(1,616)	1:50:A:TYR:HA	1:52:A:GLU:H	7	0.24
(1,607)	1:49:A:PRO:HG2	1:51:A:ALA:HB1	9	0.24
(1,607)	1:49:A:PRO:HG2	1:51:A:ALA:HB2	9	0.24
(1,607)	1:49:A:PRO:HG2	1:51:A:ALA:HB3	9	0.24
(1,607)	1:49:A:PRO:HG3	1:51:A:ALA:HB1	9	0.24
(1,607)	1:49:A:PRO:HG3	1:51:A:ALA:HB2	9	0.24
(1,607)	1:49:A:PRO:HG3	1:51:A:ALA:HB3	9	0.24
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB1	4	0.24
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB2	4	0.24
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB3	4	0.24
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG21	10	0.24
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG22	10	0.24
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG23	10	0.24
(1,480)	1:30:A:LYS:HB2	1:41:A:GLU:HA	3	0.24
(1,480)	1:30:A:LYS:HB3	1:41:A:GLU:HA	3	0.24
(1,452)	1:28:A:ILE:HD11	1:71:A:ALA:H	3	0.24
(1,452)	1:28:A:ILE:HD12	1:71:A:ALA:H	3	0.24
(1,452)	1:28:A:ILE:HD13	1:71:A:ALA:H	3	0.24
(1,366)	1:25:A:SER:H	1:73:A:ASP:H	9	0.24
(1,302)	1:17:A:LEU:HD21	1:19:A:HIS:H	10	0.24
(1,302)	1:17:A:LEU:HD22	1:19:A:HIS:H	10	0.24
(1,302)	1:17:A:LEU:HD23	1:19:A:HIS:H	10	0.24
(1,291)	1:17:A:LEU:HA	1:20:A:ASN:H	10	0.24
(1,289)	1:17:A:LEU:H	1:23:A:GLN:HB2	4	0.24
(1,289)	1:17:A:LEU:H	1:23:A:GLN:HB3	4	0.24
(1,280)	1:16:A:ASP:HB3	1:18:A:LEU:H	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD11	4	0.24
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD12	4	0.24
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD13	4	0.24
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD21	4	0.24
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD22	4	0.24
(1,265)	1:15:A:TYR:HB2	1:121:A:LEU:HD23	4	0.24
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD11	4	0.24
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD12	4	0.24
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD13	4	0.24
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD21	4	0.24
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD22	4	0.24
(1,265)	1:15:A:TYR:HB3	1:121:A:LEU:HD23	4	0.24
(1,227)	1:13:A:ASN:HB2	1:15:A:TYR:H	3	0.24
(1,162)	1:10:A:SER:HB2	1:13:A:ASN:H	2	0.24
(1,162)	1:10:A:SER:HB3	1:13:A:ASN:H	2	0.24
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG11	4	0.24
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG12	4	0.24
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG13	4	0.24
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG21	4	0.24
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG22	4	0.24
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG23	4	0.24
(1,133)	1:8:A:ASP:HB2	1:11:A:CYS:HB2	3	0.24
(1,133)	1:8:A:ASP:HB2	1:11:A:CYS:HB3	3	0.24
(1,133)	1:8:A:ASP:HB3	1:11:A:CYS:HB2	3	0.24
(1,133)	1:8:A:ASP:HB3	1:11:A:CYS:HB3	3	0.24
(1,117)	1:8:A:ASP:H	1:39:A:VAL:HB	8	0.24
(1,83)	1:7:A:VAL:HG11	1:120:A:SER:HA	10	0.24
(1,83)	1:7:A:VAL:HG12	1:120:A:SER:HA	10	0.24
(1,83)	1:7:A:VAL:HG13	1:120:A:SER:HA	10	0.24
(1,4)	1:1:A:MET:HA	1:114:A:VAL:HB	8	0.24
(2,6)	1:12:A:LYS:HG2	1:15:A:TYR:H	1	0.23
(2,2)	1:2:A:ALA:HB1	1:112:A:SER:H	8	0.23
(2,2)	1:2:A:ALA:HB2	1:112:A:SER:H	8	0.23
(2,2)	1:2:A:ALA:HB3	1:112:A:SER:H	8	0.23
(1,1808)	1:152:A:ILE:H	1:152:A:ILE:HG12	6	0.23
(1,1808)	1:152:A:ILE:H	1:152:A:ILE:HG13	6	0.23
(1,1790)	1:150:A:GLN:HB3	1:152:A:ILE:H	1	0.23
(1,1777)	1:149:A:ASN:HB2	1:151:A:ARG:H	2	0.23
(1,1777)	1:149:A:ASN:HB3	1:151:A:ARG:H	2	0.23
(1,1756)	1:147:A:MET:HA	1:149:A:ASN:H	6	0.23
(1,1756)	1:147:A:MET:HA	1:149:A:ASN:H	10	0.23
(1,1747)	1:146:A:LEU:HB2	1:147:A:MET:H	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1747)	1:146:A:LEU:HB3	1:147:A:MET:H	6	0.23
(1,1720)	1:144:A:SER:HA	1:147:A:MET:H	10	0.23
(1,1669)	1:141:A:SER:HB3	1:143:A:LYS:H	1	0.23
(1,1651)	1:140:A:LYS:HD3	1:142:A:VAL:H	10	0.23
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG2	8	0.23
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG3	8	0.23
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG2	8	0.23
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG3	8	0.23
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG2	8	0.23
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG3	8	0.23
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG2	8	0.23
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG3	8	0.23
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG2	8	0.23
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG3	8	0.23
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG2	8	0.23
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG3	8	0.23
(1,1426)	1:117:A:LEU:HB2	1:119:A:ALA:H	2	0.23
(1,1375)	1:114:A:VAL:HA	1:118:A:LYS:H	6	0.23
(1,1358)	1:113:A:SER:H	1:115:A:ARG:H	8	0.23
(1,1315)	1:109:A:LEU:HA	1:112:A:SER:HB2	9	0.23
(1,1315)	1:109:A:LEU:HA	1:112:A:SER:HB3	9	0.23
(1,1314)	1:109:A:LEU:HA	1:112:A:SER:H	2	0.23
(1,1313)	1:109:A:LEU:HA	1:111:A:ALA:H	3	0.23
(1,1244)	1:104:A:VAL:HG11	1:108:A:MET:HB2	1	0.23
(1,1244)	1:104:A:VAL:HG11	1:108:A:MET:HB3	1	0.23
(1,1244)	1:104:A:VAL:HG12	1:108:A:MET:HB2	1	0.23
(1,1244)	1:104:A:VAL:HG12	1:108:A:MET:HB3	1	0.23
(1,1244)	1:104:A:VAL:HG13	1:108:A:MET:HB2	1	0.23
(1,1244)	1:104:A:VAL:HG13	1:108:A:MET:HB3	1	0.23
(1,1244)	1:104:A:VAL:HG21	1:108:A:MET:HB2	1	0.23
(1,1244)	1:104:A:VAL:HG21	1:108:A:MET:HB3	1	0.23
(1,1244)	1:104:A:VAL:HG22	1:108:A:MET:HB2	1	0.23
(1,1244)	1:104:A:VAL:HG22	1:108:A:MET:HB3	1	0.23
(1,1244)	1:104:A:VAL:HG23	1:108:A:MET:HB2	1	0.23
(1,1244)	1:104:A:VAL:HG23	1:108:A:MET:HB3	1	0.23
(1,1225)	1:104:A:VAL:HB	1:107:A:ARG:H	7	0.23
(1,1094)	1:93:A:ILE:HG13	1:127:A:PHE:H	9	0.23
(1,1052)	1:89:A:LEU:HD21	1:90:A:ASN:H	5	0.23
(1,1052)	1:89:A:LEU:HD22	1:90:A:ASN:H	5	0.23
(1,1052)	1:89:A:LEU:HD23	1:90:A:ASN:H	5	0.23
(1,1050)	1:89:A:LEU:HD11	1:90:A:ASN:H	8	0.23
(1,1050)	1:89:A:LEU:HD12	1:90:A:ASN:H	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1050)	1:89:A:LEU:HD13	1:90:A:ASN:H	8	0.23
(1,1033)	1:88:A:THR:H	1:88:A:THR:HB	7	0.23
(1,1027)	1:86:A:THR:HB	1:87:A:SER:H	4	0.23
(1,948)	1:78:A:VAL:HA	1:79:A:GLN:H	3	0.23
(1,907)	1:76:A:VAL:H	1:88:A:THR:HB	9	0.23
(1,895)	1:75:A:GLU:HG3	1:88:A:THR:HB	6	0.23
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD11	4	0.23
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD12	4	0.23
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD13	4	0.23
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD21	4	0.23
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD22	4	0.23
(1,869)	1:75:A:GLU:H	1:146:A:LEU:HD23	4	0.23
(1,784)	1:61:A:VAL:HG11	1:66:A:GLU:HG2	6	0.23
(1,784)	1:61:A:VAL:HG12	1:66:A:GLU:HG2	6	0.23
(1,784)	1:61:A:VAL:HG13	1:66:A:GLU:HG2	6	0.23
(1,784)	1:61:A:VAL:HG11	1:66:A:GLU:HG3	6	0.23
(1,784)	1:61:A:VAL:HG12	1:66:A:GLU:HG3	6	0.23
(1,784)	1:61:A:VAL:HG13	1:66:A:GLU:HG3	6	0.23
(1,689)	1:54:A:VAL:HG11	1:57:A:MET:H	5	0.23
(1,689)	1:54:A:VAL:HG12	1:57:A:MET:H	5	0.23
(1,689)	1:54:A:VAL:HG13	1:57:A:MET:H	5	0.23
(1,689)	1:54:A:VAL:HG21	1:57:A:MET:H	5	0.23
(1,689)	1:54:A:VAL:HG22	1:57:A:MET:H	5	0.23
(1,689)	1:54:A:VAL:HG23	1:57:A:MET:H	5	0.23
(1,683)	1:54:A:VAL:HG21	1:58:A:LYS:H	2	0.23
(1,683)	1:54:A:VAL:HG22	1:58:A:LYS:H	2	0.23
(1,683)	1:54:A:VAL:HG23	1:58:A:LYS:H	2	0.23
(1,671)	1:54:A:VAL:HA	1:57:A:MET:HA	6	0.23
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB1	6	0.23
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB2	6	0.23
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB3	6	0.23
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB1	6	0.23
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB2	6	0.23
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB3	6	0.23
(1,590)	1:45:A:GLU:HB2	1:48:A:ALA:HA	1	0.23
(1,516)	1:32:A:ASP:HB2	1:37:A:ALA:H	3	0.23
(1,494)	1:31:A:ILE:HG12	1:38:A:ILE:HA	3	0.23
(1,466)	1:29:A:PHE:HB3	1:41:A:GLU:H	2	0.23
(1,464)	1:29:A:PHE:HB2	1:41:A:GLU:H	2	0.23
(1,458)	1:29:A:PHE:H	1:70:A:ALA:HB1	2	0.23
(1,458)	1:29:A:PHE:H	1:70:A:ALA:HB2	2	0.23
(1,458)	1:29:A:PHE:H	1:70:A:ALA:HB3	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,426)	1:28:A:ILE:H	1:42:A:LYS:HA	7	0.23
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB1	4	0.23
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB2	4	0.23
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB3	4	0.23
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB1	4	0.23
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB2	4	0.23
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB3	4	0.23
(1,227)	1:13:A:ASN:HB2	1:15:A:TYR:H	10	0.23
(1,195)	1:12:A:LYS:HA	1:16:A:ASP:H	1	0.23
(1,123)	1:8:A:ASP:HB2	1:39:A:VAL:HA	2	0.23
(1,97)	1:7:A:VAL:HG11	1:116:A:ALA:H	6	0.23
(1,97)	1:7:A:VAL:HG12	1:116:A:ALA:H	6	0.23
(1,97)	1:7:A:VAL:HG13	1:116:A:ALA:H	6	0.23
(1,97)	1:7:A:VAL:HG21	1:116:A:ALA:H	6	0.23
(1,97)	1:7:A:VAL:HG22	1:116:A:ALA:H	6	0.23
(1,97)	1:7:A:VAL:HG23	1:116:A:ALA:H	6	0.23
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG21	10	0.23
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG22	10	0.23
(1,70)	1:7:A:VAL:HA	1:38:A:ILE:HG23	10	0.23
(2,30)	1:91:A:LYS:HE2	1:92:A:VAL:H	3	0.22
(2,30)	1:91:A:LYS:HE3	1:92:A:VAL:H	3	0.22
(2,29)	1:86:A:THR:HG21	1:88:A:THR:HA	5	0.22
(2,29)	1:86:A:THR:HG22	1:88:A:THR:HA	5	0.22
(2,29)	1:86:A:THR:HG23	1:88:A:THR:HA	5	0.22
(2,1)	1:1:A:MET:HA	1:114:A:VAL:HA	2	0.22
(1,1799)	1:151:A:ARG:H	1:152:A:ILE:H	2	0.22
(1,1787)	1:150:A:GLN:HB2	1:151:A:ARG:H	3	0.22
(1,1780)	1:149:A:ASN:HB2	1:152:A:ILE:HD11	8	0.22
(1,1780)	1:149:A:ASN:HB2	1:152:A:ILE:HD12	8	0.22
(1,1780)	1:149:A:ASN:HB2	1:152:A:ILE:HD13	8	0.22
(1,1780)	1:149:A:ASN:HB3	1:152:A:ILE:HD11	8	0.22
(1,1780)	1:149:A:ASN:HB3	1:152:A:ILE:HD12	8	0.22
(1,1780)	1:149:A:ASN:HB3	1:152:A:ILE:HD13	8	0.22
(1,1740)	1:146:A:LEU:H	1:148:A:SER:H	2	0.22
(1,1740)	1:146:A:LEU:H	1:148:A:SER:H	10	0.22
(1,1717)	1:144:A:SER:H	1:145:A:ASP:H	4	0.22
(1,1699)	1:143:A:LYS:H	1:144:A:SER:H	3	0.22
(1,1699)	1:143:A:LYS:H	1:144:A:SER:H	5	0.22
(1,1627)	1:139:A:GLU:HA	1:143:A:LYS:HE2	6	0.22
(1,1627)	1:139:A:GLU:HA	1:143:A:LYS:HE3	6	0.22
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE2	1	0.22
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE3	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1441)	1:118:A:LYS:HE2	1:119:A:ALA:H	3	0.22
(1,1441)	1:118:A:LYS:HE2	1:119:A:ALA:H	5	0.22
(1,1433)	1:117:A:LEU:HD11	1:120:A:SER:H	3	0.22
(1,1433)	1:117:A:LEU:HD12	1:120:A:SER:H	3	0.22
(1,1433)	1:117:A:LEU:HD13	1:120:A:SER:H	3	0.22
(1,1433)	1:117:A:LEU:HD21	1:120:A:SER:H	3	0.22
(1,1433)	1:117:A:LEU:HD22	1:120:A:SER:H	3	0.22
(1,1433)	1:117:A:LEU:HD23	1:120:A:SER:H	3	0.22
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB2	3	0.22
(1,1387)	1:114:A:VAL:HG11	1:117:A:LEU:HB3	3	0.22
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB2	3	0.22
(1,1387)	1:114:A:VAL:HG12	1:117:A:LEU:HB3	3	0.22
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB2	3	0.22
(1,1387)	1:114:A:VAL:HG13	1:117:A:LEU:HB3	3	0.22
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB2	3	0.22
(1,1387)	1:114:A:VAL:HG21	1:117:A:LEU:HB3	3	0.22
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB2	3	0.22
(1,1387)	1:114:A:VAL:HG22	1:117:A:LEU:HB3	3	0.22
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB2	3	0.22
(1,1387)	1:114:A:VAL:HG23	1:117:A:LEU:HB3	3	0.22
(1,1322)	1:109:A:LEU:HD21	1:113:A:SER:H	4	0.22
(1,1322)	1:109:A:LEU:HD22	1:113:A:SER:H	4	0.22
(1,1322)	1:109:A:LEU:HD23	1:113:A:SER:H	4	0.22
(1,1288)	1:107:A:ARG:HG2	1:109:A:LEU:H	2	0.22
(1,1288)	1:107:A:ARG:HG3	1:109:A:LEU:H	2	0.22
(1,1288)	1:107:A:ARG:HG2	1:109:A:LEU:H	10	0.22
(1,1288)	1:107:A:ARG:HG3	1:109:A:LEU:H	10	0.22
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB2	5	0.22
(1,1111)	1:94:A:PHE:H	1:128:A:GLN:HB3	5	0.22
(1,1105)	1:93:A:ILE:HG12	1:142:A:VAL:HG11	6	0.22
(1,1105)	1:93:A:ILE:HG12	1:142:A:VAL:HG12	6	0.22
(1,1105)	1:93:A:ILE:HG12	1:142:A:VAL:HG13	6	0.22
(1,1105)	1:93:A:ILE:HG12	1:142:A:VAL:HG21	6	0.22
(1,1105)	1:93:A:ILE:HG12	1:142:A:VAL:HG22	6	0.22
(1,1105)	1:93:A:ILE:HG12	1:142:A:VAL:HG23	6	0.22
(1,1105)	1:93:A:ILE:HG13	1:142:A:VAL:HG11	6	0.22
(1,1105)	1:93:A:ILE:HG13	1:142:A:VAL:HG12	6	0.22
(1,1105)	1:93:A:ILE:HG13	1:142:A:VAL:HG13	6	0.22
(1,1105)	1:93:A:ILE:HG13	1:142:A:VAL:HG21	6	0.22
(1,1105)	1:93:A:ILE:HG13	1:142:A:VAL:HG22	6	0.22
(1,1105)	1:93:A:ILE:HG13	1:142:A:VAL:HG23	6	0.22
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD11	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD12	2	0.22
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD13	2	0.22
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD21	2	0.22
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD22	2	0.22
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD23	2	0.22
(1,1065)	1:91:A:LYS:HE3	1:150:A:GLN:H	8	0.22
(1,1048)	1:89:A:LEU:HG	1:90:A:ASN:H	8	0.22
(1,985)	1:80:A:ARG:H	1:80:A:ARG:HG2	6	0.22
(1,985)	1:80:A:ARG:H	1:80:A:ARG:HG3	6	0.22
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG21	9	0.22
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG22	9	0.22
(1,976)	1:79:A:GLN:HB3	1:86:A:THR:HG23	9	0.22
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG2	2	0.22
(1,910)	1:76:A:VAL:HA	1:147:A:MET:HG3	2	0.22
(1,905)	1:76:A:VAL:H	1:77:A:THR:H	1	0.22
(1,896)	1:75:A:GLU:HG3	1:88:A:THR:HG21	9	0.22
(1,896)	1:75:A:GLU:HG3	1:88:A:THR:HG22	9	0.22
(1,896)	1:75:A:GLU:HG3	1:88:A:THR:HG23	9	0.22
(1,887)	1:75:A:GLU:HB3	1:89:A:LEU:H	6	0.22
(1,884)	1:75:A:GLU:HB3	1:88:A:THR:HA	8	0.22
(1,790)	1:61:A:VAL:HG11	1:66:A:GLU:HG2	2	0.22
(1,790)	1:61:A:VAL:HG11	1:66:A:GLU:HG3	2	0.22
(1,790)	1:61:A:VAL:HG12	1:66:A:GLU:HG2	2	0.22
(1,790)	1:61:A:VAL:HG12	1:66:A:GLU:HG3	2	0.22
(1,790)	1:61:A:VAL:HG13	1:66:A:GLU:HG2	2	0.22
(1,790)	1:61:A:VAL:HG13	1:66:A:GLU:HG3	2	0.22
(1,790)	1:61:A:VAL:HG21	1:66:A:GLU:HG2	2	0.22
(1,790)	1:61:A:VAL:HG21	1:66:A:GLU:HG3	2	0.22
(1,790)	1:61:A:VAL:HG22	1:66:A:GLU:HG2	2	0.22
(1,790)	1:61:A:VAL:HG22	1:66:A:GLU:HG3	2	0.22
(1,790)	1:61:A:VAL:HG23	1:66:A:GLU:HG2	2	0.22
(1,790)	1:61:A:VAL:HG23	1:66:A:GLU:HG3	2	0.22
(1,756)	1:58:A:LYS:HD3	1:59:A:LYS:H	1	0.22
(1,730)	1:57:A:MET:HA	1:60:A:LEU:H	6	0.22
(1,725)	1:56:A:GLU:HG3	1:57:A:MET:H	4	0.22
(1,677)	1:54:A:VAL:HB	1:58:A:LYS:H	9	0.22
(1,675)	1:54:A:VAL:HB	1:56:A:GLU:H	10	0.22
(1,650)	1:52:A:GLU:HB2	1:55:A:GLU:H	6	0.22
(1,650)	1:52:A:GLU:HB3	1:55:A:GLU:H	6	0.22
(1,616)	1:50:A:TYR:HA	1:52:A:GLU:H	1	0.22
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB1	3	0.22
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB2	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB3	3	0.22
(1,518)	1:32:A:ASP:HB3	1:37:A:ALA:H	8	0.22
(1,460)	1:29:A:PHE:HA	1:40:A:VAL:HB	4	0.22
(1,294)	1:17:A:LEU:HA	1:21:A:LYS:HD2	4	0.22
(1,294)	1:17:A:LEU:HA	1:21:A:LYS:HD3	4	0.22
(1,280)	1:16:A:ASP:HB3	1:18:A:LEU:H	10	0.22
(1,226)	1:13:A:ASN:HB2	1:14:A:ALA:H	4	0.22
(1,161)	1:10:A:SER:HB2	1:12:A:LYS:H	3	0.22
(1,161)	1:10:A:SER:HB3	1:12:A:LYS:H	3	0.22
(1,159)	1:10:A:SER:HB3	1:13:A:ASN:H	6	0.22
(1,31)	1:5:A:VAL:HB	1:36:A:THR:HB	3	0.22
(1,18)	1:3:A:SER:HB2	1:4:A:GLY:H	7	0.22
(1,18)	1:3:A:SER:HB3	1:4:A:GLY:H	7	0.22
(1,4)	1:1:A:MET:HA	1:114:A:VAL:HB	3	0.22
(3,60)	1:143:A:LYS:O	1:147:A:MET:N	2	0.21
(3,37)	1:74:A:VAL:H	1:91:A:LYS:O	9	0.21
(3,9)	1:26:A:TYR:H	1:44:A:GLY:O	7	0.21
(3,4)	1:8:A:ASP:N	1:38:A:ILE:O	8	0.21
(2,35)	1:118:A:LYS:HE3	1:128:A:GLN:HA	7	0.21
(2,27)	1:78:A:VAL:HB	1:87:A:SER:HA	7	0.21
(1,1769)	1:149:A:ASN:H	1:150:A:GLN:H	3	0.21
(1,1727)	1:144:A:SER:HB3	1:147:A:MET:H	10	0.21
(1,1717)	1:144:A:SER:H	1:145:A:ASP:H	8	0.21
(1,1700)	1:143:A:LYS:H	1:145:A:ASP:H	2	0.21
(1,1627)	1:139:A:GLU:HA	1:143:A:LYS:HE2	8	0.21
(1,1627)	1:139:A:GLU:HA	1:143:A:LYS:HE3	8	0.21
(1,1587)	1:135:A:SER:HA	1:138:A:ASP:H	2	0.21
(1,1426)	1:117:A:LEU:HB2	1:119:A:ALA:H	7	0.21
(1,1396)	1:115:A:ARG:HA	1:118:A:LYS:H	5	0.21
(1,1316)	1:109:A:LEU:HA	1:113:A:SER:H	5	0.21
(1,1313)	1:109:A:LEU:HA	1:111:A:ALA:H	9	0.21
(1,1180)	1:99:A:PRO:HB2	1:132:A:SER:HB2	3	0.21
(1,1180)	1:99:A:PRO:HB2	1:132:A:SER:HB3	3	0.21
(1,1135)	1:95:A:VAL:HG11	1:131:A:ALA:HA	5	0.21
(1,1135)	1:95:A:VAL:HG12	1:131:A:ALA:HA	5	0.21
(1,1135)	1:95:A:VAL:HG13	1:131:A:ALA:HA	5	0.21
(1,1092)	1:93:A:ILE:HG12	1:127:A:PHE:H	4	0.21
(1,1082)	1:93:A:ILE:HA	1:127:A:PHE:HA	9	0.21
(1,1061)	1:91:A:LYS:HA	1:150:A:GLN:HG2	1	0.21
(1,1061)	1:91:A:LYS:HA	1:150:A:GLN:HG3	1	0.21
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG21	7	0.21
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG22	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:78:A:VAL:HA	1:88:A:THR:HG23	7	0.21
(1,944)	1:78:A:VAL:H	1:79:A:GLN:H	6	0.21
(1,751)	1:58:A:LYS:HB2	1:60:A:LEU:H	3	0.21
(1,749)	1:58:A:LYS:HA	1:62:A:GLU:H	4	0.21
(1,723)	1:56:A:GLU:HG2	1:57:A:MET:H	6	0.21
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD2	4	0.21
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD3	4	0.21
(1,677)	1:54:A:VAL:HB	1:58:A:LYS:H	1	0.21
(1,677)	1:54:A:VAL:HB	1:58:A:LYS:H	3	0.21
(1,677)	1:54:A:VAL:HB	1:58:A:LYS:H	4	0.21
(1,677)	1:54:A:VAL:HB	1:58:A:LYS:H	6	0.21
(1,590)	1:45:A:GLU:HB2	1:48:A:ALA:HA	5	0.21
(1,575)	1:42:A:LYS:HB2	1:43:A:VAL:H	2	0.21
(1,575)	1:42:A:LYS:HB3	1:43:A:VAL:H	2	0.21
(1,501)	1:31:A:ILE:HD11	1:109:A:LEU:H	2	0.21
(1,501)	1:31:A:ILE:HD12	1:109:A:LEU:H	2	0.21
(1,501)	1:31:A:ILE:HD13	1:109:A:LEU:H	2	0.21
(1,494)	1:31:A:ILE:HG12	1:38:A:ILE:HA	7	0.21
(1,426)	1:28:A:ILE:H	1:42:A:LYS:HA	8	0.21
(1,402)	1:27:A:ILE:HB	1:43:A:VAL:HA	4	0.21
(1,370)	1:25:A:SER:HB2	1:73:A:ASP:HB2	8	0.21
(1,370)	1:25:A:SER:HB2	1:73:A:ASP:HB3	8	0.21
(1,370)	1:25:A:SER:HB3	1:73:A:ASP:HB2	8	0.21
(1,370)	1:25:A:SER:HB3	1:73:A:ASP:HB3	8	0.21
(1,310)	1:18:A:LEU:HA	1:20:A:ASN:H	9	0.21
(1,283)	1:16:A:ASP:HB2	1:18:A:LEU:H	10	0.21
(1,283)	1:16:A:ASP:HB3	1:18:A:LEU:H	10	0.21
(1,280)	1:16:A:ASP:HB3	1:18:A:LEU:H	7	0.21
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD11	6	0.21
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD12	6	0.21
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD13	6	0.21
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD21	6	0.21
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD22	6	0.21
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD23	6	0.21
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD11	6	0.21
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD12	6	0.21
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD13	6	0.21
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD21	6	0.21
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD22	6	0.21
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD23	6	0.21
(1,218)	1:12:A:LYS:HG2	1:121:A:LEU:HA	2	0.21
(1,218)	1:12:A:LYS:HG3	1:121:A:LEU:HA	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,213)	1:12:A:LYS:HG3	1:14:A:ALA:H	8	0.21
(1,161)	1:10:A:SER:HB2	1:12:A:LYS:H	9	0.21
(1,161)	1:10:A:SER:HB3	1:12:A:LYS:H	9	0.21
(1,156)	1:10:A:SER:HB2	1:13:A:ASN:H	9	0.21
(1,136)	1:8:A:ASP:HB2	1:39:A:VAL:HG11	5	0.21
(1,136)	1:8:A:ASP:HB2	1:39:A:VAL:HG12	5	0.21
(1,136)	1:8:A:ASP:HB2	1:39:A:VAL:HG13	5	0.21
(1,136)	1:8:A:ASP:HB2	1:39:A:VAL:HG21	5	0.21
(1,136)	1:8:A:ASP:HB2	1:39:A:VAL:HG22	5	0.21
(1,136)	1:8:A:ASP:HB2	1:39:A:VAL:HG23	5	0.21
(1,136)	1:8:A:ASP:HB3	1:39:A:VAL:HG11	5	0.21
(1,136)	1:8:A:ASP:HB3	1:39:A:VAL:HG12	5	0.21
(1,136)	1:8:A:ASP:HB3	1:39:A:VAL:HG13	5	0.21
(1,136)	1:8:A:ASP:HB3	1:39:A:VAL:HG21	5	0.21
(1,136)	1:8:A:ASP:HB3	1:39:A:VAL:HG22	5	0.21
(1,136)	1:8:A:ASP:HB3	1:39:A:VAL:HG23	5	0.21
(1,45)	1:6:A:LYS:H	1:37:A:ALA:HB1	6	0.21
(1,45)	1:6:A:LYS:H	1:37:A:ALA:HB2	6	0.21
(1,45)	1:6:A:LYS:H	1:37:A:ALA:HB3	6	0.21
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG11	4	0.21
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG12	4	0.21
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG13	4	0.21
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG21	4	0.21
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG22	4	0.21
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG23	4	0.21
(3,59)	1:143:A:LYS:O	1:147:A:MET:H	4	0.2
(2,27)	1:78:A:VAL:HB	1:87:A:SER:HA	5	0.2
(1,1775)	1:149:A:ASN:HB3	1:152:A:ILE:HG21	6	0.2
(1,1775)	1:149:A:ASN:HB3	1:152:A:ILE:HG22	6	0.2
(1,1775)	1:149:A:ASN:HB3	1:152:A:ILE:HG23	6	0.2
(1,1770)	1:149:A:ASN:HA	1:150:A:GLN:H	4	0.2
(1,1769)	1:149:A:ASN:H	1:150:A:GLN:H	9	0.2
(1,1747)	1:146:A:LEU:HB2	1:147:A:MET:H	7	0.2
(1,1747)	1:146:A:LEU:HB3	1:147:A:MET:H	7	0.2
(1,1712)	1:143:A:LYS:HB3	1:147:A:MET:H	9	0.2
(1,1709)	1:143:A:LYS:HB2	1:147:A:MET:H	8	0.2
(1,1665)	1:141:A:SER:HA	1:144:A:SER:H	7	0.2
(1,1659)	1:140:A:LYS:HB2	1:143:A:LYS:H	5	0.2
(1,1659)	1:140:A:LYS:HB3	1:143:A:LYS:H	5	0.2
(1,1652)	1:140:A:LYS:HE2	1:141:A:SER:H	1	0.2
(1,1627)	1:139:A:GLU:HA	1:143:A:LYS:HE2	1	0.2
(1,1627)	1:139:A:GLU:HA	1:143:A:LYS:HE3	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1588)	1:135:A:SER:HA	1:138:A:ASP:HB2	1	0.2
(1,1588)	1:135:A:SER:HA	1:138:A:ASP:HB3	1	0.2
(1,1574)	1:134:A:MET:HA	1:136:A:ASP:H	10	0.2
(1,1498)	1:123:A:LEU:H	1:125:A:SER:H	1	0.2
(1,1488)	1:121:A:LEU:HD21	1:122:A:GLY:H	2	0.2
(1,1488)	1:121:A:LEU:HD22	1:122:A:GLY:H	2	0.2
(1,1488)	1:121:A:LEU:HD23	1:122:A:GLY:H	2	0.2
(1,1429)	1:117:A:LEU:HB3	1:119:A:ALA:H	3	0.2
(1,1405)	1:116:A:ALA:H	1:117:A:LEU:H	2	0.2
(1,1358)	1:113:A:SER:H	1:115:A:ARG:H	2	0.2
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD11	8	0.2
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD12	8	0.2
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD13	8	0.2
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD21	8	0.2
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD22	8	0.2
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD23	8	0.2
(1,1236)	1:104:A:VAL:HG21	1:108:A:MET:HB2	10	0.2
(1,1236)	1:104:A:VAL:HG22	1:108:A:MET:HB2	10	0.2
(1,1236)	1:104:A:VAL:HG23	1:108:A:MET:HB2	10	0.2
(1,1236)	1:104:A:VAL:HG21	1:108:A:MET:HB3	10	0.2
(1,1236)	1:104:A:VAL:HG22	1:108:A:MET:HB3	10	0.2
(1,1236)	1:104:A:VAL:HG23	1:108:A:MET:HB3	10	0.2
(1,1233)	1:104:A:VAL:HG21	1:106:A:ARG:H	8	0.2
(1,1233)	1:104:A:VAL:HG22	1:106:A:ARG:H	8	0.2
(1,1233)	1:104:A:VAL:HG23	1:106:A:ARG:H	8	0.2
(1,1233)	1:104:A:VAL:HG21	1:106:A:ARG:H	10	0.2
(1,1233)	1:104:A:VAL:HG22	1:106:A:ARG:H	10	0.2
(1,1233)	1:104:A:VAL:HG23	1:106:A:ARG:H	10	0.2
(1,1203)	1:102:A:ALA:HB1	1:103:A:PRO:HA	3	0.2
(1,1203)	1:102:A:ALA:HB2	1:103:A:PRO:HA	3	0.2
(1,1203)	1:102:A:ALA:HB3	1:103:A:PRO:HA	3	0.2
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB1	1	0.2
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB2	1	0.2
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB3	1	0.2
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB1	1	0.2
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB2	1	0.2
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB3	1	0.2
(1,1030)	1:87:A:SER:H	1:88:A:THR:H	2	0.2
(1,1027)	1:86:A:THR:HB	1:87:A:SER:H	7	0.2
(1,1024)	1:86:A:THR:H	1:86:A:THR:HB	2	0.2
(1,1016)	1:84:A:GLU:HA	1:85:A:GLY:H	8	0.2
(1,980)	1:79:A:GLN:HG3	1:85:A:GLY:H	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,905)	1:76:A:VAL:H	1:77:A:THR:H	9	0.2
(1,730)	1:57:A:MET:HA	1:60:A:LEU:H	4	0.2
(1,723)	1:56:A:GLU:HG2	1:57:A:MET:H	7	0.2
(1,689)	1:54:A:VAL:HG11	1:57:A:MET:H	7	0.2
(1,689)	1:54:A:VAL:HG12	1:57:A:MET:H	7	0.2
(1,689)	1:54:A:VAL:HG13	1:57:A:MET:H	7	0.2
(1,689)	1:54:A:VAL:HG21	1:57:A:MET:H	7	0.2
(1,689)	1:54:A:VAL:HG22	1:57:A:MET:H	7	0.2
(1,689)	1:54:A:VAL:HG23	1:57:A:MET:H	7	0.2
(1,677)	1:54:A:VAL:HB	1:58:A:LYS:H	7	0.2
(1,676)	1:54:A:VAL:HB	1:57:A:MET:H	7	0.2
(1,615)	1:50:A:TYR:HA	1:51:A:ALA:H	5	0.2
(1,607)	1:49:A:PRO:HG2	1:51:A:ALA:HB1	1	0.2
(1,607)	1:49:A:PRO:HG2	1:51:A:ALA:HB2	1	0.2
(1,607)	1:49:A:PRO:HG2	1:51:A:ALA:HB3	1	0.2
(1,607)	1:49:A:PRO:HG3	1:51:A:ALA:HB1	1	0.2
(1,607)	1:49:A:PRO:HG3	1:51:A:ALA:HB2	1	0.2
(1,607)	1:49:A:PRO:HG3	1:51:A:ALA:HB3	1	0.2
(1,599)	1:49:A:PRO:HA	1:52:A:GLU:H	6	0.2
(1,599)	1:49:A:PRO:HA	1:52:A:GLU:H	7	0.2
(1,598)	1:49:A:PRO:HA	1:51:A:ALA:HB1	10	0.2
(1,598)	1:49:A:PRO:HA	1:51:A:ALA:HB2	10	0.2
(1,598)	1:49:A:PRO:HA	1:51:A:ALA:HB3	10	0.2
(1,580)	1:42:A:LYS:HG2	1:56:A:GLU:HG2	9	0.2
(1,580)	1:42:A:LYS:HG2	1:56:A:GLU:HG3	9	0.2
(1,580)	1:42:A:LYS:HG3	1:56:A:GLU:HG2	9	0.2
(1,580)	1:42:A:LYS:HG3	1:56:A:GLU:HG3	9	0.2
(1,515)	1:31:A:ILE:HG21	1:37:A:ALA:H	8	0.2
(1,515)	1:31:A:ILE:HG22	1:37:A:ALA:H	8	0.2
(1,515)	1:31:A:ILE:HG23	1:37:A:ALA:H	8	0.2
(1,466)	1:29:A:PHE:HB3	1:41:A:GLU:H	5	0.2
(1,437)	1:28:A:ILE:HB	1:42:A:LYS:HA	7	0.2
(1,437)	1:28:A:ILE:HB	1:42:A:LYS:HA	8	0.2
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB1	8	0.2
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB2	8	0.2
(1,314)	1:18:A:LEU:HB2	1:71:A:ALA:HB3	8	0.2
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB1	8	0.2
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB2	8	0.2
(1,314)	1:18:A:LEU:HB3	1:71:A:ALA:HB3	8	0.2
(1,264)	1:15:A:TYR:HB3	1:27:A:ILE:HD11	1	0.2
(1,264)	1:15:A:TYR:HB3	1:27:A:ILE:HD12	1	0.2
(1,264)	1:15:A:TYR:HB3	1:27:A:ILE:HD13	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,261)	1:15:A:TYR:HB3	1:121:A:LEU:HD11	1	0.2
(1,261)	1:15:A:TYR:HB3	1:121:A:LEU:HD12	1	0.2
(1,261)	1:15:A:TYR:HB3	1:121:A:LEU:HD13	1	0.2
(1,261)	1:15:A:TYR:HB3	1:121:A:LEU:HD21	1	0.2
(1,261)	1:15:A:TYR:HB3	1:121:A:LEU:HD22	1	0.2
(1,261)	1:15:A:TYR:HB3	1:121:A:LEU:HD23	1	0.2
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG11	7	0.2
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG12	7	0.2
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG13	7	0.2
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG21	7	0.2
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG22	7	0.2
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG23	7	0.2
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG11	7	0.2
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG12	7	0.2
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG13	7	0.2
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG21	7	0.2
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG22	7	0.2
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG23	7	0.2
(1,213)	1:12:A:LYS:HG3	1:14:A:ALA:H	7	0.2
(1,213)	1:12:A:LYS:HG3	1:14:A:ALA:H	9	0.2
(1,184)	1:11:A:CYS:HB2	1:13:A:ASN:H	7	0.2
(1,184)	1:11:A:CYS:HB3	1:13:A:ASN:H	7	0.2
(1,124)	1:8:A:ASP:HB2	1:39:A:VAL:HB	6	0.2
(1,124)	1:8:A:ASP:HB2	1:39:A:VAL:HB	8	0.2
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD11	8	0.2
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD12	8	0.2
(1,59)	1:6:A:LYS:HB2	1:38:A:ILE:HD13	8	0.2
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD11	8	0.2
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD12	8	0.2
(1,59)	1:6:A:LYS:HB3	1:38:A:ILE:HD13	8	0.2
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG11	1	0.2
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG12	1	0.2
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG13	1	0.2
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG21	1	0.2
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG22	1	0.2
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG23	1	0.2
(1,4)	1:1:A:MET:HA	1:114:A:VAL:HB	7	0.2
(2,6)	1:12:A:LYS:HG2	1:15:A:TYR:H	6	0.19
(2,5)	1:12:A:LYS:HG2	1:121:A:LEU:HD21	1	0.19
(2,5)	1:12:A:LYS:HG2	1:121:A:LEU:HD22	1	0.19
(2,5)	1:12:A:LYS:HG2	1:121:A:LEU:HD23	1	0.19
(1,1794)	1:151:A:ARG:H	1:151:A:ARG:HA	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1730)	1:145:A:ASP:H	1:147:A:MET:H	1	0.19
(1,1704)	1:143:A:LYS:HA	1:146:A:LEU:HB2	4	0.19
(1,1704)	1:143:A:LYS:HA	1:146:A:LEU:HB3	4	0.19
(1,1703)	1:143:A:LYS:HA	1:146:A:LEU:HA	5	0.19
(1,1627)	1:139:A:GLU:HA	1:143:A:LYS:HE2	7	0.19
(1,1627)	1:139:A:GLU:HA	1:143:A:LYS:HE3	7	0.19
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG2	4	0.19
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG3	4	0.19
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG2	4	0.19
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG3	4	0.19
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG2	4	0.19
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG3	4	0.19
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG2	4	0.19
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG3	4	0.19
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG2	4	0.19
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG3	4	0.19
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG2	4	0.19
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG3	4	0.19
(1,1514)	1:124:A:GLU:HB2	1:126:A:LEU:H	6	0.19
(1,1514)	1:124:A:GLU:HB3	1:126:A:LEU:H	6	0.19
(1,1429)	1:117:A:LEU:HB3	1:119:A:ALA:H	2	0.19
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB2	10	0.19
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB2	10	0.19
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB2	10	0.19
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB3	10	0.19
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB3	10	0.19
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB3	10	0.19
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB2	10	0.19
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB3	10	0.19
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB2	10	0.19
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB3	10	0.19
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB2	10	0.19
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB3	10	0.19
(1,1324)	1:109:A:LEU:HD11	1:112:A:SER:H	2	0.19
(1,1324)	1:109:A:LEU:HD12	1:112:A:SER:H	2	0.19
(1,1324)	1:109:A:LEU:HD13	1:112:A:SER:H	2	0.19
(1,1324)	1:109:A:LEU:HD21	1:112:A:SER:H	2	0.19
(1,1324)	1:109:A:LEU:HD22	1:112:A:SER:H	2	0.19
(1,1324)	1:109:A:LEU:HD23	1:112:A:SER:H	2	0.19
(1,1207)	1:103:A:PRO:HA	1:106:A:ARG:H	9	0.19
(1,1186)	1:99:A:PRO:HG2	1:132:A:SER:HA	5	0.19
(1,1114)	1:94:A:PHE:H	1:129:A:VAL:H	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1097)	1:93:A:ILE:HD11	1:129:A:VAL:HA	1	0.19
(1,1097)	1:93:A:ILE:HD12	1:129:A:VAL:HA	1	0.19
(1,1097)	1:93:A:ILE:HD13	1:129:A:VAL:HA	1	0.19
(1,1048)	1:89:A:LEU:HG	1:90:A:ASN:H	6	0.19
(1,1033)	1:88:A:THR:H	1:88:A:THR:HB	9	0.19
(1,953)	1:78:A:VAL:HB	1:87:A:SER:HB2	4	0.19
(1,953)	1:78:A:VAL:HB	1:87:A:SER:HB3	4	0.19
(1,948)	1:78:A:VAL:HA	1:79:A:GLN:H	9	0.19
(1,944)	1:78:A:VAL:H	1:79:A:GLN:H	8	0.19
(1,932)	1:77:A:THR:HA	1:88:A:THR:HA	9	0.19
(1,921)	1:76:A:VAL:HG11	1:143:A:LYS:HG2	2	0.19
(1,921)	1:76:A:VAL:HG11	1:143:A:LYS:HG3	2	0.19
(1,921)	1:76:A:VAL:HG12	1:143:A:LYS:HG2	2	0.19
(1,921)	1:76:A:VAL:HG12	1:143:A:LYS:HG3	2	0.19
(1,921)	1:76:A:VAL:HG13	1:143:A:LYS:HG2	2	0.19
(1,921)	1:76:A:VAL:HG13	1:143:A:LYS:HG3	2	0.19
(1,921)	1:76:A:VAL:HG21	1:143:A:LYS:HG2	2	0.19
(1,921)	1:76:A:VAL:HG21	1:143:A:LYS:HG3	2	0.19
(1,921)	1:76:A:VAL:HG22	1:143:A:LYS:HG2	2	0.19
(1,921)	1:76:A:VAL:HG22	1:143:A:LYS:HG3	2	0.19
(1,921)	1:76:A:VAL:HG23	1:143:A:LYS:HG2	2	0.19
(1,921)	1:76:A:VAL:HG23	1:143:A:LYS:HG3	2	0.19
(1,888)	1:75:A:GLU:HG2	1:76:A:VAL:H	3	0.19
(1,875)	1:75:A:GLU:HA	1:89:A:LEU:H	5	0.19
(1,857)	1:74:A:VAL:H	1:146:A:LEU:HD11	10	0.19
(1,857)	1:74:A:VAL:H	1:146:A:LEU:HD12	10	0.19
(1,857)	1:74:A:VAL:H	1:146:A:LEU:HD13	10	0.19
(1,857)	1:74:A:VAL:H	1:146:A:LEU:HD21	10	0.19
(1,857)	1:74:A:VAL:H	1:146:A:LEU:HD22	10	0.19
(1,857)	1:74:A:VAL:H	1:146:A:LEU:HD23	10	0.19
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD2	6	0.19
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD3	6	0.19
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD2	10	0.19
(1,706)	1:55:A:GLU:HA	1:59:A:LYS:HD3	10	0.19
(1,677)	1:54:A:VAL:HB	1:58:A:LYS:H	2	0.19
(1,659)	1:53:A:PHE:HB2	1:56:A:GLU:H	3	0.19
(1,494)	1:31:A:ILE:HG12	1:38:A:ILE:HA	1	0.19
(1,480)	1:30:A:LYS:HB2	1:41:A:GLU:HA	1	0.19
(1,480)	1:30:A:LYS:HB3	1:41:A:GLU:HA	1	0.19
(1,464)	1:29:A:PHE:HB2	1:41:A:GLU:H	5	0.19
(1,453)	1:28:A:ILE:HG12	1:41:A:GLU:HB2	7	0.19
(1,453)	1:28:A:ILE:HG12	1:41:A:GLU:HB3	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:28:A:ILE:HG13	1:41:A:GLU:HB2	7	0.19
(1,453)	1:28:A:ILE:HG13	1:41:A:GLU:HB3	7	0.19
(1,426)	1:28:A:ILE:H	1:42:A:LYS:HA	10	0.19
(1,283)	1:16:A:ASP:HB2	1:18:A:LEU:H	3	0.19
(1,283)	1:16:A:ASP:HB3	1:18:A:LEU:H	3	0.19
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD11	8	0.19
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD12	8	0.19
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD13	8	0.19
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD21	8	0.19
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD22	8	0.19
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD23	8	0.19
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD11	8	0.19
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD12	8	0.19
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD13	8	0.19
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD21	8	0.19
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD22	8	0.19
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD23	8	0.19
(1,213)	1:12:A:LYS:HG3	1:14:A:ALA:H	3	0.19
(1,181)	1:11:A:CYS:HB3	1:13:A:ASN:H	10	0.19
(1,178)	1:11:A:CYS:HB2	1:13:A:ASN:H	1	0.19
(1,162)	1:10:A:SER:HB2	1:13:A:ASN:H	5	0.19
(1,162)	1:10:A:SER:HB3	1:13:A:ASN:H	5	0.19
(1,147)	1:10:A:SER:H	1:13:A:ASN:H	10	0.19
(1,131)	1:8:A:ASP:HB2	1:10:A:SER:H	1	0.19
(1,131)	1:8:A:ASP:HB3	1:10:A:SER:H	1	0.19
(1,48)	1:6:A:LYS:H	1:6:A:LYS:HE2	6	0.19
(1,48)	1:6:A:LYS:H	1:6:A:LYS:HE3	6	0.19
(1,33)	1:5:A:VAL:HB	1:7:A:VAL:HA	1	0.19
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG11	10	0.19
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG12	10	0.19
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG13	10	0.19
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG21	10	0.19
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG22	10	0.19
(1,5)	1:1:A:MET:HA	1:114:A:VAL:HG23	10	0.19
(2,31)	1:97:A:TYR:HB2	1:131:A:ALA:HA	1	0.18
(2,31)	1:97:A:TYR:HB3	1:131:A:ALA:HA	1	0.18
(2,27)	1:78:A:VAL:HB	1:87:A:SER:HA	4	0.18
(2,11)	1:18:A:LEU:HD11	1:71:A:ALA:HA	4	0.18
(2,11)	1:18:A:LEU:HD12	1:71:A:ALA:HA	4	0.18
(2,11)	1:18:A:LEU:HD13	1:71:A:ALA:HA	4	0.18
(1,1808)	1:152:A:ILE:H	1:152:A:ILE:HG12	2	0.18
(1,1808)	1:152:A:ILE:H	1:152:A:ILE:HG13	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1794)	1:151:A:ARG:H	1:151:A:ARG:HA	8	0.18
(1,1769)	1:149:A:ASN:H	1:150:A:GLN:H	5	0.18
(1,1757)	1:147:A:MET:HA	1:150:A:GLN:H	5	0.18
(1,1717)	1:144:A:SER:H	1:145:A:ASP:H	2	0.18
(1,1703)	1:143:A:LYS:HA	1:146:A:LEU:HA	2	0.18
(1,1652)	1:140:A:LYS:HE2	1:141:A:SER:H	6	0.18
(1,1652)	1:140:A:LYS:HE2	1:141:A:SER:H	7	0.18
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG11	9	0.18
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG12	9	0.18
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG13	9	0.18
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG21	9	0.18
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG22	9	0.18
(1,1636)	1:139:A:GLU:HG2	1:142:A:VAL:HG23	9	0.18
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG11	9	0.18
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG12	9	0.18
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG13	9	0.18
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG21	9	0.18
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG22	9	0.18
(1,1636)	1:139:A:GLU:HG3	1:142:A:VAL:HG23	9	0.18
(1,1555)	1:132:A:SER:H	1:136:A:ASP:HA	4	0.18
(1,1466)	1:120:A:SER:HB3	1:122:A:GLY:H	4	0.18
(1,1453)	1:119:A:ALA:HA	1:122:A:GLY:H	1	0.18
(1,1441)	1:118:A:LYS:HE2	1:119:A:ALA:H	6	0.18
(1,1426)	1:117:A:LEU:HB2	1:119:A:ALA:H	5	0.18
(1,1325)	1:109:A:LEU:HD11	1:112:A:SER:HB2	1	0.18
(1,1325)	1:109:A:LEU:HD11	1:112:A:SER:HB3	1	0.18
(1,1325)	1:109:A:LEU:HD12	1:112:A:SER:HB2	1	0.18
(1,1325)	1:109:A:LEU:HD12	1:112:A:SER:HB3	1	0.18
(1,1325)	1:109:A:LEU:HD13	1:112:A:SER:HB2	1	0.18
(1,1325)	1:109:A:LEU:HD13	1:112:A:SER:HB3	1	0.18
(1,1325)	1:109:A:LEU:HD21	1:112:A:SER:HB2	1	0.18
(1,1325)	1:109:A:LEU:HD21	1:112:A:SER:HB3	1	0.18
(1,1325)	1:109:A:LEU:HD22	1:112:A:SER:HB2	1	0.18
(1,1325)	1:109:A:LEU:HD22	1:112:A:SER:HB3	1	0.18
(1,1325)	1:109:A:LEU:HD23	1:112:A:SER:HB2	1	0.18
(1,1325)	1:109:A:LEU:HD23	1:112:A:SER:HB3	1	0.18
(1,1324)	1:109:A:LEU:HD11	1:112:A:SER:H	9	0.18
(1,1324)	1:109:A:LEU:HD12	1:112:A:SER:H	9	0.18
(1,1324)	1:109:A:LEU:HD13	1:112:A:SER:H	9	0.18
(1,1324)	1:109:A:LEU:HD21	1:112:A:SER:H	9	0.18
(1,1324)	1:109:A:LEU:HD22	1:112:A:SER:H	9	0.18
(1,1324)	1:109:A:LEU:HD23	1:112:A:SER:H	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1314)	1:109:A:LEU:HA	1:112:A:SER:H	9	0.18
(1,1313)	1:109:A:LEU:HA	1:111:A:ALA:H	1	0.18
(1,1313)	1:109:A:LEU:HA	1:111:A:ALA:H	6	0.18
(1,1218)	1:104:A:VAL:HA	1:106:A:ARG:H	4	0.18
(1,1204)	1:102:A:ALA:HB1	1:103:A:PRO:HG2	8	0.18
(1,1204)	1:102:A:ALA:HB1	1:103:A:PRO:HG3	8	0.18
(1,1204)	1:102:A:ALA:HB2	1:103:A:PRO:HG2	8	0.18
(1,1204)	1:102:A:ALA:HB2	1:103:A:PRO:HG3	8	0.18
(1,1204)	1:102:A:ALA:HB3	1:103:A:PRO:HG2	8	0.18
(1,1204)	1:102:A:ALA:HB3	1:103:A:PRO:HG3	8	0.18
(1,1190)	1:99:A:PRO:HG3	1:132:A:SER:HA	10	0.18
(1,1173)	1:98:A:CYS:HB2	1:107:A:ARG:HD2	7	0.18
(1,1173)	1:98:A:CYS:HB2	1:107:A:ARG:HD3	7	0.18
(1,1173)	1:98:A:CYS:HB3	1:107:A:ARG:HD2	7	0.18
(1,1173)	1:98:A:CYS:HB3	1:107:A:ARG:HD3	7	0.18
(1,1114)	1:94:A:PHE:H	1:129:A:VAL:H	3	0.18
(1,1109)	1:94:A:PHE:H	1:127:A:PHE:H	6	0.18
(1,1030)	1:87:A:SER:H	1:88:A:THR:H	3	0.18
(1,1030)	1:87:A:SER:H	1:88:A:THR:H	5	0.18
(1,1027)	1:86:A:THR:HB	1:87:A:SER:H	1	0.18
(1,963)	1:79:A:GLN:H	1:79:A:GLN:HA	1	0.18
(1,963)	1:79:A:GLN:H	1:79:A:GLN:HA	3	0.18
(1,963)	1:79:A:GLN:H	1:79:A:GLN:HA	10	0.18
(1,892)	1:75:A:GLU:HG2	1:90:A:ASN:HA	6	0.18
(1,874)	1:75:A:GLU:HA	1:88:A:THR:HG21	8	0.18
(1,874)	1:75:A:GLU:HA	1:88:A:THR:HG22	8	0.18
(1,874)	1:75:A:GLU:HA	1:88:A:THR:HG23	8	0.18
(1,822)	1:70:A:ALA:H	1:94:A:PHE:HA	8	0.18
(1,800)	1:64:A:GLY:H	1:65:A:LYS:H	6	0.18
(1,761)	1:59:A:LYS:H	1:59:A:LYS:HE2	5	0.18
(1,761)	1:59:A:LYS:H	1:59:A:LYS:HE3	5	0.18
(1,750)	1:58:A:LYS:HB2	1:59:A:LYS:H	8	0.18
(1,725)	1:56:A:GLU:HG3	1:57:A:MET:H	2	0.18
(1,723)	1:56:A:GLU:HG2	1:57:A:MET:H	1	0.18
(1,682)	1:54:A:VAL:HG21	1:57:A:MET:H	2	0.18
(1,682)	1:54:A:VAL:HG22	1:57:A:MET:H	2	0.18
(1,682)	1:54:A:VAL:HG23	1:57:A:MET:H	2	0.18
(1,664)	1:53:A:PHE:HB2	1:57:A:MET:H	1	0.18
(1,664)	1:53:A:PHE:HB3	1:57:A:MET:H	1	0.18
(1,664)	1:53:A:PHE:HB2	1:57:A:MET:H	3	0.18
(1,664)	1:53:A:PHE:HB3	1:57:A:MET:H	3	0.18
(1,615)	1:50:A:TYR:HA	1:51:A:ALA:H	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,606)	1:49:A:PRO:HB3	1:52:A:GLU:H	4	0.18
(1,590)	1:45:A:GLU:HB2	1:48:A:ALA:HA	3	0.18
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB2	9	0.18
(1,574)	1:42:A:LYS:HA	1:56:A:GLU:HB3	9	0.18
(1,518)	1:32:A:ASP:HB3	1:37:A:ALA:H	4	0.18
(1,499)	1:31:A:ILE:HG13	1:38:A:ILE:HB	1	0.18
(1,437)	1:28:A:ILE:HB	1:42:A:LYS:HA	3	0.18
(1,437)	1:28:A:ILE:HB	1:42:A:LYS:HA	4	0.18
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG11	6	0.18
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG12	6	0.18
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG13	6	0.18
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG21	6	0.18
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG22	6	0.18
(1,386)	1:26:A:TYR:HB2	1:72:A:VAL:HG23	6	0.18
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG11	6	0.18
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG12	6	0.18
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG13	6	0.18
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG21	6	0.18
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG22	6	0.18
(1,386)	1:26:A:TYR:HB3	1:72:A:VAL:HG23	6	0.18
(1,302)	1:17:A:LEU:HD21	1:19:A:HIS:H	6	0.18
(1,302)	1:17:A:LEU:HD22	1:19:A:HIS:H	6	0.18
(1,302)	1:17:A:LEU:HD23	1:19:A:HIS:H	6	0.18
(1,294)	1:17:A:LEU:HA	1:21:A:LYS:HD2	8	0.18
(1,294)	1:17:A:LEU:HA	1:21:A:LYS:HD3	8	0.18
(1,289)	1:17:A:LEU:H	1:23:A:GLN:HB2	2	0.18
(1,289)	1:17:A:LEU:H	1:23:A:GLN:HB3	2	0.18
(1,277)	1:16:A:ASP:HB2	1:18:A:LEU:H	1	0.18
(1,243)	1:14:A:ALA:HB1	1:27:A:ILE:HB	6	0.18
(1,243)	1:14:A:ALA:HB2	1:27:A:ILE:HB	6	0.18
(1,243)	1:14:A:ALA:HB3	1:27:A:ILE:HB	6	0.18
(1,227)	1:13:A:ASN:HB2	1:15:A:TYR:H	4	0.18
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD11	4	0.18
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD12	4	0.18
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD13	4	0.18
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD21	4	0.18
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD22	4	0.18
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD23	4	0.18
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD11	4	0.18
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD12	4	0.18
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD13	4	0.18
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD21	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD22	4	0.18
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD23	4	0.18
(1,181)	1:11:A:CYS:HB3	1:13:A:ASN:H	8	0.18
(1,135)	1:8:A:ASP:HB2	1:39:A:VAL:HB	8	0.18
(1,135)	1:8:A:ASP:HB3	1:39:A:VAL:HB	8	0.18
(1,131)	1:8:A:ASP:HB2	1:10:A:SER:H	5	0.18
(1,131)	1:8:A:ASP:HB3	1:10:A:SER:H	5	0.18
(1,65)	1:7:A:VAL:HA	1:37:A:ALA:HA	1	0.18
(1,40)	1:5:A:VAL:HG11	1:37:A:ALA:HA	5	0.18
(1,40)	1:5:A:VAL:HG12	1:37:A:ALA:HA	5	0.18
(1,40)	1:5:A:VAL:HG13	1:37:A:ALA:HA	5	0.18
(1,40)	1:5:A:VAL:HG21	1:37:A:ALA:HA	5	0.18
(1,40)	1:5:A:VAL:HG22	1:37:A:ALA:HA	5	0.18
(1,40)	1:5:A:VAL:HG23	1:37:A:ALA:HA	5	0.18
(3,60)	1:143:A:LYS:O	1:147:A:MET:N	7	0.17
(2,31)	1:97:A:TYR:HB2	1:131:A:ALA:HA	10	0.17
(2,31)	1:97:A:TYR:HB3	1:131:A:ALA:HA	10	0.17
(2,29)	1:86:A:THR:HG21	1:88:A:THR:HA	10	0.17
(2,29)	1:86:A:THR:HG22	1:88:A:THR:HA	10	0.17
(2,29)	1:86:A:THR:HG23	1:88:A:THR:HA	10	0.17
(2,27)	1:78:A:VAL:HB	1:87:A:SER:HA	8	0.17
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG11	7	0.17
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG12	7	0.17
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG13	7	0.17
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG21	7	0.17
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG22	7	0.17
(2,19)	1:53:A:PHE:HA	1:72:A:VAL:HG23	7	0.17
(2,16)	1:27:A:ILE:HG21	1:43:A:VAL:H	4	0.17
(2,16)	1:27:A:ILE:HG22	1:43:A:VAL:H	4	0.17
(2,16)	1:27:A:ILE:HG23	1:43:A:VAL:H	4	0.17
(2,16)	1:27:A:ILE:HG21	1:43:A:VAL:H	6	0.17
(2,16)	1:27:A:ILE:HG22	1:43:A:VAL:H	6	0.17
(2,16)	1:27:A:ILE:HG23	1:43:A:VAL:H	6	0.17
(2,16)	1:27:A:ILE:HG21	1:43:A:VAL:H	9	0.17
(2,16)	1:27:A:ILE:HG22	1:43:A:VAL:H	9	0.17
(2,16)	1:27:A:ILE:HG23	1:43:A:VAL:H	9	0.17
(1,1756)	1:147:A:MET:HA	1:149:A:ASN:H	2	0.17
(1,1747)	1:146:A:LEU:HB2	1:147:A:MET:H	4	0.17
(1,1747)	1:146:A:LEU:HB3	1:147:A:MET:H	4	0.17
(1,1727)	1:144:A:SER:HB3	1:147:A:MET:H	9	0.17
(1,1701)	1:143:A:LYS:HA	1:145:A:ASP:H	1	0.17
(1,1659)	1:140:A:LYS:HB2	1:143:A:LYS:H	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1659)	1:140:A:LYS:HB3	1:143:A:LYS:H	7	0.17
(1,1635)	1:139:A:GLU:HG2	1:142:A:VAL:H	7	0.17
(1,1635)	1:139:A:GLU:HG3	1:142:A:VAL:H	7	0.17
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG2	9	0.17
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG3	9	0.17
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG2	9	0.17
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG3	9	0.17
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG2	9	0.17
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG3	9	0.17
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG2	9	0.17
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG3	9	0.17
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG2	9	0.17
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG3	9	0.17
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG2	9	0.17
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG3	9	0.17
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG2	10	0.17
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG3	10	0.17
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG2	10	0.17
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG3	10	0.17
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG2	10	0.17
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG3	10	0.17
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG2	10	0.17
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG3	10	0.17
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG2	10	0.17
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG3	10	0.17
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG2	10	0.17
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG3	10	0.17
(1,1585)	1:135:A:SER:HA	1:136:A:ASP:HA	3	0.17
(1,1469)	1:120:A:SER:HB2	1:122:A:GLY:H	10	0.17
(1,1469)	1:120:A:SER:HB3	1:122:A:GLY:H	10	0.17
(1,1444)	1:118:A:LYS:HG2	1:119:A:ALA:H	2	0.17
(1,1444)	1:118:A:LYS:HG2	1:119:A:ALA:H	4	0.17
(1,1414)	1:116:A:ALA:HB1	1:120:A:SER:H	8	0.17
(1,1414)	1:116:A:ALA:HB2	1:120:A:SER:H	8	0.17
(1,1414)	1:116:A:ALA:HB3	1:120:A:SER:H	8	0.17
(1,1405)	1:116:A:ALA:H	1:117:A:LEU:H	3	0.17
(1,1366)	1:113:A:SER:HB3	1:116:A:ALA:H	3	0.17
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD11	8	0.17
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD12	8	0.17
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD13	8	0.17
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD21	8	0.17
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD22	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1362)	1:113:A:SER:HA	1:117:A:LEU:HD23	8	0.17
(1,1358)	1:113:A:SER:H	1:115:A:ARG:H	5	0.17
(1,1298)	1:108:A:MET:HB2	1:110:A:TYR:H	2	0.17
(1,1298)	1:108:A:MET:HB2	1:110:A:TYR:H	6	0.17
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG2	4	0.17
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG3	4	0.17
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG2	4	0.17
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG3	4	0.17
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG2	4	0.17
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG3	4	0.17
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG2	4	0.17
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG3	4	0.17
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG2	4	0.17
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG3	4	0.17
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG2	4	0.17
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG3	4	0.17
(1,1224)	1:104:A:VAL:HB	1:106:A:ARG:H	3	0.17
(1,1052)	1:89:A:LEU:HD21	1:90:A:ASN:H	10	0.17
(1,1052)	1:89:A:LEU:HD22	1:90:A:ASN:H	10	0.17
(1,1052)	1:89:A:LEU:HD23	1:90:A:ASN:H	10	0.17
(1,1033)	1:88:A:THR:H	1:88:A:THR:HB	8	0.17
(1,1030)	1:87:A:SER:H	1:88:A:THR:H	9	0.17
(1,963)	1:79:A:GLN:H	1:79:A:GLN:HA	6	0.17
(1,930)	1:77:A:THR:HA	1:78:A:VAL:HB	3	0.17
(1,898)	1:75:A:GLU:HG3	1:90:A:ASN:HA	6	0.17
(1,862)	1:74:A:VAL:H	1:90:A:ASN:HB2	7	0.17
(1,862)	1:74:A:VAL:H	1:90:A:ASN:HB3	7	0.17
(1,705)	1:55:A:GLU:HA	1:59:A:LYS:HB3	7	0.17
(1,689)	1:54:A:VAL:HG11	1:57:A:MET:H	6	0.17
(1,689)	1:54:A:VAL:HG12	1:57:A:MET:H	6	0.17
(1,689)	1:54:A:VAL:HG13	1:57:A:MET:H	6	0.17
(1,689)	1:54:A:VAL:HG21	1:57:A:MET:H	6	0.17
(1,689)	1:54:A:VAL:HG22	1:57:A:MET:H	6	0.17
(1,689)	1:54:A:VAL:HG23	1:57:A:MET:H	6	0.17
(1,683)	1:54:A:VAL:HG21	1:58:A:LYS:H	9	0.17
(1,683)	1:54:A:VAL:HG22	1:58:A:LYS:H	9	0.17
(1,683)	1:54:A:VAL:HG23	1:58:A:LYS:H	9	0.17
(1,682)	1:54:A:VAL:HG21	1:57:A:MET:H	5	0.17
(1,682)	1:54:A:VAL:HG22	1:57:A:MET:H	5	0.17
(1,682)	1:54:A:VAL:HG23	1:57:A:MET:H	5	0.17
(1,675)	1:54:A:VAL:HB	1:56:A:GLU:H	3	0.17
(1,656)	1:53:A:PHE:HA	1:56:A:GLU:HB2	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,656)	1:53:A:PHE:HA	1:56:A:GLU:HB3	5	0.17
(1,627)	1:51:A:ALA:HA	1:53:A:PHE:H	7	0.17
(1,616)	1:50:A:TYR:HA	1:52:A:GLU:H	4	0.17
(1,577)	1:42:A:LYS:HB2	1:53:A:PHE:HA	2	0.17
(1,577)	1:42:A:LYS:HB3	1:53:A:PHE:HA	2	0.17
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG21	2	0.17
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG22	2	0.17
(1,525)	1:33:A:LYS:HG2	1:36:A:THR:HG23	2	0.17
(1,521)	1:33:A:LYS:HE2	1:35:A:ASP:H	5	0.17
(1,521)	1:33:A:LYS:HE3	1:35:A:ASP:H	5	0.17
(1,331)	1:18:A:LEU:HD11	1:92:A:VAL:HA	2	0.17
(1,331)	1:18:A:LEU:HD12	1:92:A:VAL:HA	2	0.17
(1,331)	1:18:A:LEU:HD13	1:92:A:VAL:HA	2	0.17
(1,331)	1:18:A:LEU:HD21	1:92:A:VAL:HA	2	0.17
(1,331)	1:18:A:LEU:HD22	1:92:A:VAL:HA	2	0.17
(1,331)	1:18:A:LEU:HD23	1:92:A:VAL:HA	2	0.17
(1,294)	1:17:A:LEU:HA	1:21:A:LYS:HD2	9	0.17
(1,294)	1:17:A:LEU:HA	1:21:A:LYS:HD3	9	0.17
(1,280)	1:16:A:ASP:HB3	1:18:A:LEU:H	2	0.17
(1,273)	1:16:A:ASP:HA	1:19:A:HIS:H	6	0.17
(1,273)	1:16:A:ASP:HA	1:19:A:HIS:H	9	0.17
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD11	3	0.17
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD12	3	0.17
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD13	3	0.17
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD21	3	0.17
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD22	3	0.17
(1,266)	1:15:A:TYR:HB2	1:123:A:LEU:HD23	3	0.17
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD11	3	0.17
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD12	3	0.17
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD13	3	0.17
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD21	3	0.17
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD22	3	0.17
(1,266)	1:15:A:TYR:HB3	1:123:A:LEU:HD23	3	0.17
(1,227)	1:13:A:ASN:HB2	1:15:A:TYR:H	2	0.17
(1,217)	1:12:A:LYS:HD2	1:15:A:TYR:HB2	5	0.17
(1,217)	1:12:A:LYS:HD2	1:15:A:TYR:HB3	5	0.17
(1,217)	1:12:A:LYS:HD3	1:15:A:TYR:HB2	5	0.17
(1,217)	1:12:A:LYS:HD3	1:15:A:TYR:HB3	5	0.17
(1,213)	1:12:A:LYS:HG3	1:14:A:ALA:H	4	0.17
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD11	8	0.17
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD12	8	0.17
(1,211)	1:12:A:LYS:HG3	1:121:A:LEU:HD13	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:8:A:ASP:HB2	1:10:A:SER:H	6	0.17
(1,107)	1:7:A:VAL:HG11	1:38:A:ILE:H	3	0.17
(1,107)	1:7:A:VAL:HG12	1:38:A:ILE:H	3	0.17
(1,107)	1:7:A:VAL:HG13	1:38:A:ILE:H	3	0.17
(1,107)	1:7:A:VAL:HG21	1:38:A:ILE:H	3	0.17
(1,107)	1:7:A:VAL:HG22	1:38:A:ILE:H	3	0.17
(1,107)	1:7:A:VAL:HG23	1:38:A:ILE:H	3	0.17
(3,59)	1:143:A:LYS:O	1:147:A:MET:H	5	0.16
(3,19)	1:29:A:PHE:O	1:69:A:TYR:H	4	0.16
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG21	3	0.16
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG22	3	0.16
(1,1772)	1:149:A:ASN:HB2	1:152:A:ILE:HG23	3	0.16
(1,1764)	1:148:A:SER:HB2	1:149:A:ASN:H	8	0.16
(1,1729)	1:145:A:ASP:H	1:146:A:LEU:H	3	0.16
(1,1723)	1:144:A:SER:HB2	1:146:A:LEU:H	2	0.16
(1,1665)	1:141:A:SER:HA	1:144:A:SER:H	5	0.16
(1,1665)	1:141:A:SER:HA	1:144:A:SER:H	10	0.16
(1,1657)	1:140:A:LYS:HB2	1:141:A:SER:H	7	0.16
(1,1657)	1:140:A:LYS:HB3	1:141:A:SER:H	7	0.16
(1,1657)	1:140:A:LYS:HB2	1:141:A:SER:H	8	0.16
(1,1657)	1:140:A:LYS:HB3	1:141:A:SER:H	8	0.16
(1,1633)	1:139:A:GLU:HG2	1:140:A:LYS:HG2	8	0.16
(1,1633)	1:139:A:GLU:HG2	1:140:A:LYS:HG3	8	0.16
(1,1633)	1:139:A:GLU:HG3	1:140:A:LYS:HG2	8	0.16
(1,1633)	1:139:A:GLU:HG3	1:140:A:LYS:HG3	8	0.16
(1,1628)	1:139:A:GLU:HB2	1:140:A:LYS:H	8	0.16
(1,1627)	1:139:A:GLU:HA	1:143:A:LYS:HE2	10	0.16
(1,1627)	1:139:A:GLU:HA	1:143:A:LYS:HE3	10	0.16
(1,1549)	1:131:A:ALA:H	1:136:A:ASP:HB2	3	0.16
(1,1549)	1:131:A:ALA:H	1:136:A:ASP:HB3	3	0.16
(1,1536)	1:128:A:GLN:HB2	1:129:A:VAL:H	1	0.16
(1,1536)	1:128:A:GLN:HB3	1:129:A:VAL:H	1	0.16
(1,1536)	1:128:A:GLN:HB2	1:129:A:VAL:H	2	0.16
(1,1536)	1:128:A:GLN:HB3	1:129:A:VAL:H	2	0.16
(1,1433)	1:117:A:LEU:HD11	1:120:A:SER:H	9	0.16
(1,1433)	1:117:A:LEU:HD12	1:120:A:SER:H	9	0.16
(1,1433)	1:117:A:LEU:HD13	1:120:A:SER:H	9	0.16
(1,1433)	1:117:A:LEU:HD21	1:120:A:SER:H	9	0.16
(1,1433)	1:117:A:LEU:HD22	1:120:A:SER:H	9	0.16
(1,1433)	1:117:A:LEU:HD23	1:120:A:SER:H	9	0.16
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB2	4	0.16
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB2	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB2	4	0.16
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB3	4	0.16
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB3	4	0.16
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB3	4	0.16
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB2	4	0.16
(1,1415)	1:116:A:ALA:HB1	1:120:A:SER:HB3	4	0.16
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB2	4	0.16
(1,1415)	1:116:A:ALA:HB2	1:120:A:SER:HB3	4	0.16
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB2	4	0.16
(1,1415)	1:116:A:ALA:HB3	1:120:A:SER:HB3	4	0.16
(1,1358)	1:113:A:SER:H	1:115:A:ARG:H	6	0.16
(1,1294)	1:108:A:MET:HA	1:111:A:ALA:H	8	0.16
(1,1288)	1:107:A:ARG:HG2	1:109:A:LEU:H	4	0.16
(1,1288)	1:107:A:ARG:HG3	1:109:A:LEU:H	4	0.16
(1,1204)	1:102:A:ALA:HB1	1:103:A:PRO:HG2	6	0.16
(1,1204)	1:102:A:ALA:HB1	1:103:A:PRO:HG3	6	0.16
(1,1204)	1:102:A:ALA:HB2	1:103:A:PRO:HG2	6	0.16
(1,1204)	1:102:A:ALA:HB2	1:103:A:PRO:HG3	6	0.16
(1,1204)	1:102:A:ALA:HB3	1:103:A:PRO:HG2	6	0.16
(1,1204)	1:102:A:ALA:HB3	1:103:A:PRO:HG3	6	0.16
(1,1174)	1:99:A:PRO:HA	1:102:A:ALA:H	3	0.16
(1,1147)	1:95:A:VAL:HG11	1:97:A:TYR:HB2	1	0.16
(1,1147)	1:95:A:VAL:HG11	1:97:A:TYR:HB3	1	0.16
(1,1147)	1:95:A:VAL:HG12	1:97:A:TYR:HB2	1	0.16
(1,1147)	1:95:A:VAL:HG12	1:97:A:TYR:HB3	1	0.16
(1,1147)	1:95:A:VAL:HG13	1:97:A:TYR:HB2	1	0.16
(1,1147)	1:95:A:VAL:HG13	1:97:A:TYR:HB3	1	0.16
(1,1147)	1:95:A:VAL:HG21	1:97:A:TYR:HB2	1	0.16
(1,1147)	1:95:A:VAL:HG21	1:97:A:TYR:HB3	1	0.16
(1,1147)	1:95:A:VAL:HG22	1:97:A:TYR:HB2	1	0.16
(1,1147)	1:95:A:VAL:HG22	1:97:A:TYR:HB3	1	0.16
(1,1147)	1:95:A:VAL:HG23	1:97:A:TYR:HB2	1	0.16
(1,1147)	1:95:A:VAL:HG23	1:97:A:TYR:HB3	1	0.16
(1,1114)	1:94:A:PHE:H	1:129:A:VAL:H	5	0.16
(1,1092)	1:93:A:ILE:HG12	1:127:A:PHE:H	7	0.16
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD11	9	0.16
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD12	9	0.16
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD13	9	0.16
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD21	9	0.16
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD22	9	0.16
(1,1085)	1:93:A:ILE:HA	1:146:A:LEU:HD23	9	0.16
(1,1038)	1:88:A:THR:HG21	1:89:A:LEU:H	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1038)	1:88:A:THR:HG22	1:89:A:LEU:H	7	0.16
(1,1038)	1:88:A:THR:HG23	1:89:A:LEU:H	7	0.16
(1,1028)	1:86:A:THR:HG21	1:87:A:SER:H	2	0.16
(1,1028)	1:86:A:THR:HG22	1:87:A:SER:H	2	0.16
(1,1028)	1:86:A:THR:HG23	1:87:A:SER:H	2	0.16
(1,1024)	1:86:A:THR:H	1:86:A:THR:HB	1	0.16
(1,1021)	1:85:A:GLY:H	1:86:A:THR:H	2	0.16
(1,1014)	1:84:A:GLU:H	1:84:A:GLU:HB2	7	0.16
(1,1014)	1:84:A:GLU:H	1:84:A:GLU:HB3	7	0.16
(1,985)	1:80:A:ARG:H	1:80:A:ARG:HG2	2	0.16
(1,985)	1:80:A:ARG:H	1:80:A:ARG:HG3	2	0.16
(1,913)	1:76:A:VAL:HB	1:147:A:MET:HG2	6	0.16
(1,913)	1:76:A:VAL:HB	1:147:A:MET:HG3	6	0.16
(1,909)	1:76:A:VAL:H	1:89:A:LEU:H	8	0.16
(1,905)	1:76:A:VAL:H	1:77:A:THR:H	2	0.16
(1,833)	1:71:A:ALA:HB1	1:93:A:ILE:H	10	0.16
(1,833)	1:71:A:ALA:HB2	1:93:A:ILE:H	10	0.16
(1,833)	1:71:A:ALA:HB3	1:93:A:ILE:H	10	0.16
(1,708)	1:55:A:GLU:HB2	1:57:A:MET:H	3	0.16
(1,708)	1:55:A:GLU:HB2	1:57:A:MET:H	7	0.16
(1,689)	1:54:A:VAL:HG11	1:57:A:MET:H	2	0.16
(1,689)	1:54:A:VAL:HG12	1:57:A:MET:H	2	0.16
(1,689)	1:54:A:VAL:HG13	1:57:A:MET:H	2	0.16
(1,689)	1:54:A:VAL:HG21	1:57:A:MET:H	2	0.16
(1,689)	1:54:A:VAL:HG22	1:57:A:MET:H	2	0.16
(1,689)	1:54:A:VAL:HG23	1:57:A:MET:H	2	0.16
(1,683)	1:54:A:VAL:HG21	1:58:A:LYS:H	7	0.16
(1,683)	1:54:A:VAL:HG22	1:58:A:LYS:H	7	0.16
(1,683)	1:54:A:VAL:HG23	1:58:A:LYS:H	7	0.16
(1,675)	1:54:A:VAL:HB	1:56:A:GLU:H	9	0.16
(1,628)	1:51:A:ALA:HA	1:54:A:VAL:H	9	0.16
(1,615)	1:50:A:TYR:HA	1:51:A:ALA:H	7	0.16
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB1	7	0.16
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB2	7	0.16
(1,610)	1:49:A:PRO:HG2	1:51:A:ALA:HB3	7	0.16
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB1	7	0.16
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB2	7	0.16
(1,610)	1:49:A:PRO:HG3	1:51:A:ALA:HB3	7	0.16
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB1	4	0.16
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB2	4	0.16
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB3	4	0.16
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB1	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB2	4	0.16
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB3	4	0.16
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB1	4	0.16
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB2	4	0.16
(1,594)	1:45:A:GLU:HG2	1:48:A:ALA:HB3	4	0.16
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB1	4	0.16
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB2	4	0.16
(1,594)	1:45:A:GLU:HG3	1:48:A:ALA:HB3	4	0.16
(1,590)	1:45:A:GLU:HB2	1:48:A:ALA:HA	10	0.16
(1,577)	1:42:A:LYS:HB2	1:53:A:PHE:HA	8	0.16
(1,577)	1:42:A:LYS:HB3	1:53:A:PHE:HA	8	0.16
(1,511)	1:31:A:ILE:HG21	1:109:A:LEU:HG	5	0.16
(1,511)	1:31:A:ILE:HG22	1:109:A:LEU:HG	5	0.16
(1,511)	1:31:A:ILE:HG23	1:109:A:LEU:HG	5	0.16
(1,485)	1:30:A:LYS:HG2	1:41:A:GLU:HB2	3	0.16
(1,485)	1:30:A:LYS:HG2	1:41:A:GLU:HB3	3	0.16
(1,485)	1:30:A:LYS:HG3	1:41:A:GLU:HB2	3	0.16
(1,485)	1:30:A:LYS:HG3	1:41:A:GLU:HB3	3	0.16
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG11	3	0.16
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG12	3	0.16
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG13	3	0.16
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG21	3	0.16
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG22	3	0.16
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG23	3	0.16
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG11	3	0.16
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG12	3	0.16
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG13	3	0.16
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG21	3	0.16
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG22	3	0.16
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG23	3	0.16
(1,391)	1:27:A:ILE:H	1:28:A:ILE:H	6	0.16
(1,380)	1:26:A:TYR:HB2	1:72:A:VAL:HG11	5	0.16
(1,380)	1:26:A:TYR:HB2	1:72:A:VAL:HG12	5	0.16
(1,380)	1:26:A:TYR:HB2	1:72:A:VAL:HG13	5	0.16
(1,380)	1:26:A:TYR:HB2	1:72:A:VAL:HG21	5	0.16
(1,380)	1:26:A:TYR:HB2	1:72:A:VAL:HG22	5	0.16
(1,380)	1:26:A:TYR:HB2	1:72:A:VAL:HG23	5	0.16
(1,366)	1:25:A:SER:H	1:73:A:ASP:H	3	0.16
(1,334)	1:19:A:HIS:H	1:21:A:LYS:H	3	0.16
(1,327)	1:18:A:LEU:HD21	1:73:A:ASP:HA	9	0.16
(1,327)	1:18:A:LEU:HD22	1:73:A:ASP:HA	9	0.16
(1,327)	1:18:A:LEU:HD23	1:73:A:ASP:HA	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:17:A:LEU:HD21	1:19:A:HIS:H	2	0.16
(1,302)	1:17:A:LEU:HD22	1:19:A:HIS:H	2	0.16
(1,302)	1:17:A:LEU:HD23	1:19:A:HIS:H	2	0.16
(1,296)	1:17:A:LEU:HA	1:23:A:GLN:HB2	2	0.16
(1,296)	1:17:A:LEU:HA	1:23:A:GLN:HB3	2	0.16
(1,256)	1:15:A:TYR:HB2	1:121:A:LEU:HG	7	0.16
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG11	6	0.16
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG12	6	0.16
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG13	6	0.16
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG21	6	0.16
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG22	6	0.16
(1,216)	1:12:A:LYS:HB2	1:40:A:VAL:HG23	6	0.16
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG11	6	0.16
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG12	6	0.16
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG13	6	0.16
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG21	6	0.16
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG22	6	0.16
(1,216)	1:12:A:LYS:HB3	1:40:A:VAL:HG23	6	0.16
(1,213)	1:12:A:LYS:HG3	1:14:A:ALA:H	1	0.16
(1,213)	1:12:A:LYS:HG3	1:14:A:ALA:H	5	0.16
(1,213)	1:12:A:LYS:HG3	1:14:A:ALA:H	10	0.16
(1,162)	1:10:A:SER:HB2	1:13:A:ASN:H	6	0.16
(1,162)	1:10:A:SER:HB3	1:13:A:ASN:H	6	0.16
(1,161)	1:10:A:SER:HB2	1:12:A:LYS:H	2	0.16
(1,161)	1:10:A:SER:HB3	1:12:A:LYS:H	2	0.16
(1,156)	1:10:A:SER:HB2	1:13:A:ASN:H	1	0.16
(1,124)	1:8:A:ASP:HB2	1:39:A:VAL:HB	7	0.16
(1,121)	1:8:A:ASP:HB2	1:10:A:SER:H	9	0.16
(1,111)	1:7:A:VAL:HG11	1:9:A:PRO:HA	1	0.16
(1,111)	1:7:A:VAL:HG12	1:9:A:PRO:HA	1	0.16
(1,111)	1:7:A:VAL:HG13	1:9:A:PRO:HA	1	0.16
(1,111)	1:7:A:VAL:HG21	1:9:A:PRO:HA	1	0.16
(1,111)	1:7:A:VAL:HG22	1:9:A:PRO:HA	1	0.16
(1,111)	1:7:A:VAL:HG23	1:9:A:PRO:HA	1	0.16
(1,105)	1:7:A:VAL:HG11	1:37:A:ALA:HA	9	0.16
(1,105)	1:7:A:VAL:HG12	1:37:A:ALA:HA	9	0.16
(1,105)	1:7:A:VAL:HG13	1:37:A:ALA:HA	9	0.16
(1,105)	1:7:A:VAL:HG21	1:37:A:ALA:HA	9	0.16
(1,105)	1:7:A:VAL:HG22	1:37:A:ALA:HA	9	0.16
(1,105)	1:7:A:VAL:HG23	1:37:A:ALA:HA	9	0.16
(1,90)	1:7:A:VAL:HG21	1:117:A:LEU:HA	1	0.16
(1,90)	1:7:A:VAL:HG22	1:117:A:LEU:HA	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:7:A:VAL:HG23	1:117:A:LEU:HA	1	0.16
(1,87)	1:7:A:VAL:HG11	1:38:A:ILE:HG21	8	0.16
(1,87)	1:7:A:VAL:HG11	1:38:A:ILE:HG22	8	0.16
(1,87)	1:7:A:VAL:HG11	1:38:A:ILE:HG23	8	0.16
(1,87)	1:7:A:VAL:HG12	1:38:A:ILE:HG21	8	0.16
(1,87)	1:7:A:VAL:HG12	1:38:A:ILE:HG22	8	0.16
(1,87)	1:7:A:VAL:HG12	1:38:A:ILE:HG23	8	0.16
(1,87)	1:7:A:VAL:HG13	1:38:A:ILE:HG21	8	0.16
(1,87)	1:7:A:VAL:HG13	1:38:A:ILE:HG22	8	0.16
(1,87)	1:7:A:VAL:HG13	1:38:A:ILE:HG23	8	0.16
(1,83)	1:7:A:VAL:HG11	1:120:A:SER:HA	7	0.16
(1,83)	1:7:A:VAL:HG12	1:120:A:SER:HA	7	0.16
(1,83)	1:7:A:VAL:HG13	1:120:A:SER:HA	7	0.16
(3,38)	1:74:A:VAL:N	1:91:A:LYS:O	9	0.15
(2,35)	1:118:A:LYS:HE3	1:128:A:GLN:HA	8	0.15
(2,16)	1:27:A:ILE:HG21	1:43:A:VAL:H	5	0.15
(2,16)	1:27:A:ILE:HG22	1:43:A:VAL:H	5	0.15
(2,16)	1:27:A:ILE:HG23	1:43:A:VAL:H	5	0.15
(2,16)	1:27:A:ILE:HG21	1:43:A:VAL:H	8	0.15
(2,16)	1:27:A:ILE:HG22	1:43:A:VAL:H	8	0.15
(2,16)	1:27:A:ILE:HG23	1:43:A:VAL:H	8	0.15
(1,1794)	1:151:A:ARG:H	1:151:A:ARG:HA	4	0.15
(1,1794)	1:151:A:ARG:H	1:151:A:ARG:HA	10	0.15
(1,1764)	1:148:A:SER:HB2	1:149:A:ASN:H	6	0.15
(1,1762)	1:148:A:SER:H	1:150:A:GLN:H	3	0.15
(1,1659)	1:140:A:LYS:HB2	1:143:A:LYS:H	10	0.15
(1,1659)	1:140:A:LYS:HB3	1:143:A:LYS:H	10	0.15
(1,1645)	1:140:A:LYS:HA	1:142:A:VAL:H	6	0.15
(1,1555)	1:132:A:SER:H	1:136:A:ASP:HA	6	0.15
(1,1488)	1:121:A:LEU:HD21	1:122:A:GLY:H	1	0.15
(1,1488)	1:121:A:LEU:HD22	1:122:A:GLY:H	1	0.15
(1,1488)	1:121:A:LEU:HD23	1:122:A:GLY:H	1	0.15
(1,1421)	1:117:A:LEU:HA	1:120:A:SER:H	10	0.15
(1,1419)	1:117:A:LEU:H	1:119:A:ALA:H	6	0.15
(1,1394)	1:115:A:ARG:HA	1:117:A:LEU:H	9	0.15
(1,1296)	1:108:A:MET:HA	1:112:A:SER:H	10	0.15
(1,1293)	1:108:A:MET:HA	1:110:A:TYR:H	4	0.15
(1,1293)	1:108:A:MET:HA	1:110:A:TYR:H	7	0.15
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG2	3	0.15
(1,1245)	1:104:A:VAL:HG11	1:108:A:MET:HG3	3	0.15
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG2	3	0.15
(1,1245)	1:104:A:VAL:HG12	1:108:A:MET:HG3	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG2	3	0.15
(1,1245)	1:104:A:VAL:HG13	1:108:A:MET:HG3	3	0.15
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG2	3	0.15
(1,1245)	1:104:A:VAL:HG21	1:108:A:MET:HG3	3	0.15
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG2	3	0.15
(1,1245)	1:104:A:VAL:HG22	1:108:A:MET:HG3	3	0.15
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG2	3	0.15
(1,1245)	1:104:A:VAL:HG23	1:108:A:MET:HG3	3	0.15
(1,1228)	1:104:A:VAL:HG11	1:107:A:ARG:H	4	0.15
(1,1228)	1:104:A:VAL:HG12	1:107:A:ARG:H	4	0.15
(1,1228)	1:104:A:VAL:HG13	1:107:A:ARG:H	4	0.15
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB1	6	0.15
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB2	6	0.15
(1,1167)	1:97:A:TYR:HB2	1:131:A:ALA:HB3	6	0.15
(1,1145)	1:95:A:VAL:HG11	1:131:A:ALA:HA	3	0.15
(1,1145)	1:95:A:VAL:HG12	1:131:A:ALA:HA	3	0.15
(1,1145)	1:95:A:VAL:HG13	1:131:A:ALA:HA	3	0.15
(1,1145)	1:95:A:VAL:HG21	1:131:A:ALA:HA	3	0.15
(1,1145)	1:95:A:VAL:HG22	1:131:A:ALA:HA	3	0.15
(1,1145)	1:95:A:VAL:HG23	1:131:A:ALA:HA	3	0.15
(1,1119)	1:94:A:PHE:HA	1:128:A:GLN:HG2	1	0.15
(1,1119)	1:94:A:PHE:HA	1:128:A:GLN:HG3	1	0.15
(1,1119)	1:94:A:PHE:HA	1:128:A:GLN:HG2	10	0.15
(1,1119)	1:94:A:PHE:HA	1:128:A:GLN:HG3	10	0.15
(1,1107)	1:93:A:ILE:HG21	1:146:A:LEU:HA	8	0.15
(1,1107)	1:93:A:ILE:HG22	1:146:A:LEU:HA	8	0.15
(1,1107)	1:93:A:ILE:HG23	1:146:A:LEU:HA	8	0.15
(1,1018)	1:84:A:GLU:HG2	1:85:A:GLY:H	1	0.15
(1,1018)	1:84:A:GLU:HG3	1:85:A:GLY:H	1	0.15
(1,1014)	1:84:A:GLU:H	1:84:A:GLU:HB2	8	0.15
(1,1014)	1:84:A:GLU:H	1:84:A:GLU:HB3	8	0.15
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD11	7	0.15
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD12	7	0.15
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD13	7	0.15
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD21	7	0.15
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD22	7	0.15
(1,1001)	1:81:A:GLN:HB2	1:89:A:LEU:HD23	7	0.15
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD11	7	0.15
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD12	7	0.15
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD13	7	0.15
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD21	7	0.15
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD22	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1001)	1:81:A:GLN:HB3	1:89:A:LEU:HD23	7	0.15
(1,978)	1:79:A:GLN:HG2	1:85:A:GLY:H	10	0.15
(1,963)	1:79:A:GLN:H	1:79:A:GLN:HA	5	0.15
(1,963)	1:79:A:GLN:H	1:79:A:GLN:HA	9	0.15
(1,944)	1:78:A:VAL:H	1:79:A:GLN:H	2	0.15
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	9	0.15
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	9	0.15
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	9	0.15
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG11	9	0.15
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG12	9	0.15
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG13	9	0.15
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG21	9	0.15
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG22	9	0.15
(1,934)	1:77:A:THR:HB	1:78:A:VAL:HG23	9	0.15
(1,874)	1:75:A:GLU:HA	1:88:A:THR:HG21	9	0.15
(1,874)	1:75:A:GLU:HA	1:88:A:THR:HG22	9	0.15
(1,874)	1:75:A:GLU:HA	1:88:A:THR:HG23	9	0.15
(1,751)	1:58:A:LYS:HB2	1:60:A:LEU:H	7	0.15
(1,742)	1:58:A:LYS:H	1:58:A:LYS:HE2	7	0.15
(1,742)	1:58:A:LYS:H	1:58:A:LYS:HE3	7	0.15
(1,733)	1:57:A:MET:HA	1:61:A:VAL:H	1	0.15
(1,724)	1:56:A:GLU:HG2	1:58:A:LYS:H	1	0.15
(1,723)	1:56:A:GLU:HG2	1:57:A:MET:H	4	0.15
(1,709)	1:55:A:GLU:HB2	1:58:A:LYS:H	10	0.15
(1,655)	1:53:A:PHE:HA	1:56:A:GLU:H	7	0.15
(1,636)	1:51:A:ALA:HB1	1:54:A:VAL:H	1	0.15
(1,636)	1:51:A:ALA:HB2	1:54:A:VAL:H	1	0.15
(1,636)	1:51:A:ALA:HB3	1:54:A:VAL:H	1	0.15
(1,615)	1:50:A:TYR:HA	1:51:A:ALA:H	1	0.15
(1,599)	1:49:A:PRO:HA	1:52:A:GLU:H	4	0.15
(1,575)	1:42:A:LYS:HB2	1:43:A:VAL:H	10	0.15
(1,575)	1:42:A:LYS:HB3	1:43:A:VAL:H	10	0.15
(1,509)	1:31:A:ILE:HG21	1:109:A:LEU:H	4	0.15
(1,509)	1:31:A:ILE:HG22	1:109:A:LEU:H	4	0.15
(1,509)	1:31:A:ILE:HG23	1:109:A:LEU:H	4	0.15
(1,494)	1:31:A:ILE:HG12	1:38:A:ILE:HA	5	0.15
(1,440)	1:28:A:ILE:HB	1:70:A:ALA:HB1	3	0.15
(1,440)	1:28:A:ILE:HB	1:70:A:ALA:HB2	3	0.15
(1,440)	1:28:A:ILE:HB	1:70:A:ALA:HB3	3	0.15
(1,404)	1:27:A:ILE:HB	1:71:A:ALA:HB1	8	0.15
(1,404)	1:27:A:ILE:HB	1:71:A:ALA:HB2	8	0.15
(1,404)	1:27:A:ILE:HB	1:71:A:ALA:HB3	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,325)	1:18:A:LEU:HD21	1:72:A:VAL:H	4	0.15
(1,325)	1:18:A:LEU:HD22	1:72:A:VAL:H	4	0.15
(1,325)	1:18:A:LEU:HD23	1:72:A:VAL:H	4	0.15
(1,297)	1:17:A:LEU:HB2	1:18:A:LEU:H	9	0.15
(1,296)	1:17:A:LEU:HA	1:23:A:GLN:HB2	4	0.15
(1,296)	1:17:A:LEU:HA	1:23:A:GLN:HB3	4	0.15
(1,283)	1:16:A:ASP:HB2	1:18:A:LEU:H	1	0.15
(1,283)	1:16:A:ASP:HB3	1:18:A:LEU:H	1	0.15
(1,283)	1:16:A:ASP:HB2	1:18:A:LEU:H	8	0.15
(1,283)	1:16:A:ASP:HB3	1:18:A:LEU:H	8	0.15
(1,277)	1:16:A:ASP:HB2	1:18:A:LEU:H	7	0.15
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG11	10	0.15
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG12	10	0.15
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG13	10	0.15
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG21	10	0.15
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG22	10	0.15
(1,234)	1:14:A:ALA:H	1:43:A:VAL:HG23	10	0.15
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG11	1	0.15
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG12	1	0.15
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG13	1	0.15
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG21	1	0.15
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG22	1	0.15
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG23	1	0.15
(1,129)	1:8:A:ASP:HB3	1:39:A:VAL:HB	9	0.15
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG11	8	0.15
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG12	8	0.15
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG13	8	0.15
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG21	8	0.15
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG22	8	0.15
(1,118)	1:8:A:ASP:H	1:39:A:VAL:HG23	8	0.15
(1,116)	1:8:A:ASP:H	1:39:A:VAL:HA	8	0.15
(1,108)	1:7:A:VAL:HG11	1:38:A:ILE:HB	1	0.15
(1,108)	1:7:A:VAL:HG12	1:38:A:ILE:HB	1	0.15
(1,108)	1:7:A:VAL:HG13	1:38:A:ILE:HB	1	0.15
(1,108)	1:7:A:VAL:HG21	1:38:A:ILE:HB	1	0.15
(1,108)	1:7:A:VAL:HG22	1:38:A:ILE:HB	1	0.15
(1,108)	1:7:A:VAL:HG23	1:38:A:ILE:HB	1	0.15
(1,91)	1:7:A:VAL:HG21	1:120:A:SER:HA	8	0.15
(1,91)	1:7:A:VAL:HG22	1:120:A:SER:HA	8	0.15
(1,91)	1:7:A:VAL:HG23	1:120:A:SER:HA	8	0.15
(1,64)	1:7:A:VAL:HA	1:117:A:LEU:HA	2	0.15
(1,6)	1:1:A:MET:HA	1:2:A:ALA:H	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,15)	1:27:A:ILE:O	1:71:A:ALA:H	6	0.14
(3,4)	1:8:A:ASP:N	1:38:A:ILE:O	9	0.14
(2,31)	1:97:A:TYR:HB2	1:131:A:ALA:HA	5	0.14
(2,31)	1:97:A:TYR:HB3	1:131:A:ALA:HA	5	0.14
(2,27)	1:78:A:VAL:HB	1:87:A:SER:HA	6	0.14
(2,16)	1:27:A:ILE:HG21	1:43:A:VAL:H	2	0.14
(2,16)	1:27:A:ILE:HG22	1:43:A:VAL:H	2	0.14
(2,16)	1:27:A:ILE:HG23	1:43:A:VAL:H	2	0.14
(2,11)	1:18:A:LEU:HD11	1:71:A:ALA:HA	7	0.14
(2,11)	1:18:A:LEU:HD12	1:71:A:ALA:HA	7	0.14
(2,11)	1:18:A:LEU:HD13	1:71:A:ALA:HA	7	0.14
(2,11)	1:18:A:LEU:HD11	1:71:A:ALA:HA	8	0.14
(2,11)	1:18:A:LEU:HD12	1:71:A:ALA:HA	8	0.14
(2,11)	1:18:A:LEU:HD13	1:71:A:ALA:HA	8	0.14
(1,1794)	1:151:A:ARG:H	1:151:A:ARG:HA	3	0.14
(1,1794)	1:151:A:ARG:H	1:151:A:ARG:HA	5	0.14
(1,1788)	1:150:A:GLN:HB2	1:152:A:ILE:H	8	0.14
(1,1782)	1:150:A:GLN:H	1:150:A:GLN:HA	2	0.14
(1,1782)	1:150:A:GLN:H	1:150:A:GLN:HA	3	0.14
(1,1779)	1:149:A:ASN:HB2	1:152:A:ILE:H	2	0.14
(1,1779)	1:149:A:ASN:HB3	1:152:A:ILE:H	2	0.14
(1,1747)	1:146:A:LEU:HB2	1:147:A:MET:H	2	0.14
(1,1747)	1:146:A:LEU:HB3	1:147:A:MET:H	2	0.14
(1,1747)	1:146:A:LEU:HB2	1:147:A:MET:H	9	0.14
(1,1747)	1:146:A:LEU:HB3	1:147:A:MET:H	9	0.14
(1,1745)	1:146:A:LEU:HG	1:147:A:MET:H	8	0.14
(1,1717)	1:144:A:SER:H	1:145:A:ASP:H	9	0.14
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD2	8	0.14
(1,1696)	1:143:A:LYS:H	1:143:A:LYS:HD3	8	0.14
(1,1655)	1:140:A:LYS:HE3	1:142:A:VAL:H	3	0.14
(1,1652)	1:140:A:LYS:HE2	1:141:A:SER:H	9	0.14
(1,1627)	1:139:A:GLU:HA	1:143:A:LYS:HE2	9	0.14
(1,1627)	1:139:A:GLU:HA	1:143:A:LYS:HE3	9	0.14
(1,1555)	1:132:A:SER:H	1:136:A:ASP:HA	10	0.14
(1,1514)	1:124:A:GLU:HB2	1:126:A:LEU:H	10	0.14
(1,1514)	1:124:A:GLU:HB3	1:126:A:LEU:H	10	0.14
(1,1453)	1:119:A:ALA:HA	1:122:A:GLY:H	3	0.14
(1,1410)	1:116:A:ALA:HA	1:120:A:SER:H	8	0.14
(1,1322)	1:109:A:LEU:HD21	1:113:A:SER:H	8	0.14
(1,1322)	1:109:A:LEU:HD22	1:113:A:SER:H	8	0.14
(1,1322)	1:109:A:LEU:HD23	1:113:A:SER:H	8	0.14
(1,1299)	1:108:A:MET:HB2	1:112:A:SER:H	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1298)	1:108:A:MET:HB2	1:110:A:TYR:H	10	0.14
(1,1273)	1:106:A:ARG:HB2	1:108:A:MET:H	8	0.14
(1,1273)	1:106:A:ARG:HB3	1:108:A:MET:H	8	0.14
(1,1233)	1:104:A:VAL:HG21	1:106:A:ARG:H	7	0.14
(1,1233)	1:104:A:VAL:HG22	1:106:A:ARG:H	7	0.14
(1,1233)	1:104:A:VAL:HG23	1:106:A:ARG:H	7	0.14
(1,1178)	1:99:A:PRO:HB2	1:102:A:ALA:HA	10	0.14
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB1	6	0.14
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB2	6	0.14
(1,1171)	1:97:A:TYR:HB2	1:131:A:ALA:HB3	6	0.14
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB1	6	0.14
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB2	6	0.14
(1,1171)	1:97:A:TYR:HB3	1:131:A:ALA:HB3	6	0.14
(1,1145)	1:95:A:VAL:HG11	1:131:A:ALA:HA	4	0.14
(1,1145)	1:95:A:VAL:HG12	1:131:A:ALA:HA	4	0.14
(1,1145)	1:95:A:VAL:HG13	1:131:A:ALA:HA	4	0.14
(1,1145)	1:95:A:VAL:HG21	1:131:A:ALA:HA	4	0.14
(1,1145)	1:95:A:VAL:HG22	1:131:A:ALA:HA	4	0.14
(1,1145)	1:95:A:VAL:HG23	1:131:A:ALA:HA	4	0.14
(1,1135)	1:95:A:VAL:HG11	1:131:A:ALA:HA	7	0.14
(1,1135)	1:95:A:VAL:HG12	1:131:A:ALA:HA	7	0.14
(1,1135)	1:95:A:VAL:HG13	1:131:A:ALA:HA	7	0.14
(1,1114)	1:94:A:PHE:H	1:129:A:VAL:H	8	0.14
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB2	7	0.14
(1,1113)	1:94:A:PHE:H	1:128:A:GLN:HB3	7	0.14
(1,1094)	1:93:A:ILE:HG13	1:127:A:PHE:H	3	0.14
(1,1037)	1:88:A:THR:HB	1:89:A:LEU:H	10	0.14
(1,1033)	1:88:A:THR:H	1:88:A:THR:HB	2	0.14
(1,1024)	1:86:A:THR:H	1:86:A:THR:HB	3	0.14
(1,1024)	1:86:A:THR:H	1:86:A:THR:HB	4	0.14
(1,1024)	1:86:A:THR:H	1:86:A:THR:HB	10	0.14
(1,1014)	1:84:A:GLU:H	1:84:A:GLU:HB2	3	0.14
(1,1014)	1:84:A:GLU:H	1:84:A:GLU:HB3	3	0.14
(1,986)	1:80:A:ARG:H	1:81:A:GLN:H	5	0.14
(1,985)	1:80:A:ARG:H	1:80:A:ARG:HG2	10	0.14
(1,985)	1:80:A:ARG:H	1:80:A:ARG:HG3	10	0.14
(1,906)	1:76:A:VAL:H	1:88:A:THR:HA	6	0.14
(1,905)	1:76:A:VAL:H	1:77:A:THR:H	6	0.14
(1,883)	1:75:A:GLU:HB3	1:76:A:VAL:H	3	0.14
(1,875)	1:75:A:GLU:HA	1:89:A:LEU:H	4	0.14
(1,742)	1:58:A:LYS:H	1:58:A:LYS:HE2	3	0.14
(1,742)	1:58:A:LYS:H	1:58:A:LYS:HE3	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,683)	1:54:A:VAL:HG21	1:58:A:LYS:H	3	0.14
(1,683)	1:54:A:VAL:HG22	1:58:A:LYS:H	3	0.14
(1,683)	1:54:A:VAL:HG23	1:58:A:LYS:H	3	0.14
(1,615)	1:50:A:TYR:HA	1:51:A:ALA:H	9	0.14
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB1	9	0.14
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB2	9	0.14
(1,533)	1:35:A:ASP:H	1:37:A:ALA:HB3	9	0.14
(1,499)	1:31:A:ILE:HG13	1:38:A:ILE:HB	10	0.14
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG11	1	0.14
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG12	1	0.14
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG13	1	0.14
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG21	1	0.14
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG22	1	0.14
(1,479)	1:30:A:LYS:HB2	1:39:A:VAL:HG23	1	0.14
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG11	1	0.14
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG12	1	0.14
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG13	1	0.14
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG21	1	0.14
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG22	1	0.14
(1,479)	1:30:A:LYS:HB3	1:39:A:VAL:HG23	1	0.14
(1,437)	1:28:A:ILE:HB	1:42:A:LYS:HA	10	0.14
(1,426)	1:28:A:ILE:H	1:42:A:LYS:HA	5	0.14
(1,327)	1:18:A:LEU:HD21	1:73:A:ASP:HA	5	0.14
(1,327)	1:18:A:LEU:HD22	1:73:A:ASP:HA	5	0.14
(1,327)	1:18:A:LEU:HD23	1:73:A:ASP:HA	5	0.14
(1,294)	1:17:A:LEU:HA	1:21:A:LYS:HD2	7	0.14
(1,294)	1:17:A:LEU:HA	1:21:A:LYS:HD3	7	0.14
(1,281)	1:16:A:ASP:HB3	1:19:A:HIS:H	8	0.14
(1,256)	1:15:A:TYR:HB2	1:121:A:LEU:HG	4	0.14
(1,255)	1:15:A:TYR:HA	1:19:A:HIS:H	2	0.14
(1,227)	1:13:A:ASN:HB2	1:15:A:TYR:H	6	0.14
(1,210)	1:12:A:LYS:HG2	1:13:A:ASN:H	6	0.14
(1,208)	1:12:A:LYS:HE2	1:122:A:GLY:H	4	0.14
(1,208)	1:12:A:LYS:HE3	1:122:A:GLY:H	4	0.14
(1,178)	1:11:A:CYS:HB2	1:13:A:ASN:H	10	0.14
(1,159)	1:10:A:SER:HB3	1:13:A:ASN:H	4	0.14
(1,156)	1:10:A:SER:HB2	1:13:A:ASN:H	2	0.14
(1,147)	1:10:A:SER:H	1:13:A:ASN:H	8	0.14
(1,127)	1:8:A:ASP:HB3	1:37:A:ALA:HB1	5	0.14
(1,127)	1:8:A:ASP:HB3	1:37:A:ALA:HB2	5	0.14
(1,127)	1:8:A:ASP:HB3	1:37:A:ALA:HB3	5	0.14
(1,112)	1:8:A:ASP:H	1:11:A:CYS:HB2	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,112)	1:8:A:ASP:H	1:11:A:CYS:HB3	10	0.14
(1,83)	1:7:A:VAL:HG11	1:120:A:SER:HA	4	0.14
(1,83)	1:7:A:VAL:HG12	1:120:A:SER:HA	4	0.14
(1,83)	1:7:A:VAL:HG13	1:120:A:SER:HA	4	0.14
(1,83)	1:7:A:VAL:HG11	1:120:A:SER:HA	8	0.14
(1,83)	1:7:A:VAL:HG12	1:120:A:SER:HA	8	0.14
(1,83)	1:7:A:VAL:HG13	1:120:A:SER:HA	8	0.14
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB2	9	0.14
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB3	9	0.14
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB2	9	0.14
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB3	9	0.14
(1,63)	1:7:A:VAL:H	1:8:A:ASP:H	7	0.14
(1,57)	1:6:A:LYS:HB2	1:37:A:ALA:HA	7	0.14
(1,57)	1:6:A:LYS:HB3	1:37:A:ALA:HA	7	0.14
(1,57)	1:6:A:LYS:HB2	1:37:A:ALA:HA	8	0.14
(1,57)	1:6:A:LYS:HB3	1:37:A:ALA:HA	8	0.14
(1,16)	1:3:A:SER:H	1:4:A:GLY:H	2	0.14
(3,27)	1:68:A:ARG:O	1:97:A:TYR:H	7	0.13
(3,4)	1:8:A:ASP:N	1:38:A:ILE:O	7	0.13
(2,39)	1:135:A:SER:HA	1:140:A:LYS:HE3	6	0.13
(2,13)	1:21:A:LYS:HD2	1:22:A:HIS:H	4	0.13
(1,1757)	1:147:A:MET:HA	1:150:A:GLN:H	8	0.13
(1,1756)	1:147:A:MET:HA	1:149:A:ASN:H	9	0.13
(1,1747)	1:146:A:LEU:HB2	1:147:A:MET:H	10	0.13
(1,1747)	1:146:A:LEU:HB3	1:147:A:MET:H	10	0.13
(1,1703)	1:143:A:LYS:HA	1:146:A:LEU:HA	1	0.13
(1,1660)	1:140:A:LYS:HG2	1:142:A:VAL:H	3	0.13
(1,1660)	1:140:A:LYS:HG3	1:142:A:VAL:H	3	0.13
(1,1660)	1:140:A:LYS:HG2	1:142:A:VAL:H	5	0.13
(1,1660)	1:140:A:LYS:HG3	1:142:A:VAL:H	5	0.13
(1,1645)	1:140:A:LYS:HA	1:142:A:VAL:H	5	0.13
(1,1637)	1:139:A:GLU:HG2	1:143:A:LYS:H	7	0.13
(1,1637)	1:139:A:GLU:HG3	1:143:A:LYS:H	7	0.13
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG2	3	0.13
(1,1612)	1:137:A:LEU:HD11	1:139:A:GLU:HG3	3	0.13
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG2	3	0.13
(1,1612)	1:137:A:LEU:HD12	1:139:A:GLU:HG3	3	0.13
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG2	3	0.13
(1,1612)	1:137:A:LEU:HD13	1:139:A:GLU:HG3	3	0.13
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG2	3	0.13
(1,1612)	1:137:A:LEU:HD21	1:139:A:GLU:HG3	3	0.13
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG2	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1612)	1:137:A:LEU:HD22	1:139:A:GLU:HG3	3	0.13
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG2	3	0.13
(1,1612)	1:137:A:LEU:HD23	1:139:A:GLU:HG3	3	0.13
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD2	3	0.13
(1,1593)	1:135:A:SER:HB2	1:140:A:LYS:HD3	3	0.13
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD2	3	0.13
(1,1593)	1:135:A:SER:HB3	1:140:A:LYS:HD3	3	0.13
(1,1587)	1:135:A:SER:HA	1:138:A:ASP:H	7	0.13
(1,1585)	1:135:A:SER:HA	1:136:A:ASP:HA	9	0.13
(1,1536)	1:128:A:GLN:HB2	1:129:A:VAL:H	3	0.13
(1,1536)	1:128:A:GLN:HB3	1:129:A:VAL:H	3	0.13
(1,1536)	1:128:A:GLN:HB2	1:129:A:VAL:H	6	0.13
(1,1536)	1:128:A:GLN:HB3	1:129:A:VAL:H	6	0.13
(1,1514)	1:124:A:GLU:HB2	1:126:A:LEU:H	2	0.13
(1,1514)	1:124:A:GLU:HB3	1:126:A:LEU:H	2	0.13
(1,1475)	1:121:A:LEU:HA	1:122:A:GLY:H	10	0.13
(1,1464)	1:120:A:SER:HB2	1:122:A:GLY:H	6	0.13
(1,1429)	1:117:A:LEU:HB3	1:119:A:ALA:H	8	0.13
(1,1358)	1:113:A:SER:H	1:115:A:ARG:H	1	0.13
(1,1358)	1:113:A:SER:H	1:115:A:ARG:H	3	0.13
(1,1329)	1:110:A:TYR:H	1:112:A:SER:H	5	0.13
(1,1273)	1:106:A:ARG:HB2	1:108:A:MET:H	2	0.13
(1,1273)	1:106:A:ARG:HB3	1:108:A:MET:H	2	0.13
(1,1233)	1:104:A:VAL:HG21	1:106:A:ARG:H	2	0.13
(1,1233)	1:104:A:VAL:HG22	1:106:A:ARG:H	2	0.13
(1,1233)	1:104:A:VAL:HG23	1:106:A:ARG:H	2	0.13
(1,1224)	1:104:A:VAL:HB	1:106:A:ARG:H	9	0.13
(1,1203)	1:102:A:ALA:HB1	1:103:A:PRO:HA	4	0.13
(1,1203)	1:102:A:ALA:HB2	1:103:A:PRO:HA	4	0.13
(1,1203)	1:102:A:ALA:HB3	1:103:A:PRO:HA	4	0.13
(1,1186)	1:99:A:PRO:HG2	1:132:A:SER:HA	1	0.13
(1,1147)	1:95:A:VAL:HG11	1:97:A:TYR:HB2	7	0.13
(1,1147)	1:95:A:VAL:HG11	1:97:A:TYR:HB3	7	0.13
(1,1147)	1:95:A:VAL:HG12	1:97:A:TYR:HB2	7	0.13
(1,1147)	1:95:A:VAL:HG12	1:97:A:TYR:HB3	7	0.13
(1,1147)	1:95:A:VAL:HG13	1:97:A:TYR:HB2	7	0.13
(1,1147)	1:95:A:VAL:HG13	1:97:A:TYR:HB3	7	0.13
(1,1147)	1:95:A:VAL:HG21	1:97:A:TYR:HB2	7	0.13
(1,1147)	1:95:A:VAL:HG21	1:97:A:TYR:HB3	7	0.13
(1,1147)	1:95:A:VAL:HG22	1:97:A:TYR:HB2	7	0.13
(1,1147)	1:95:A:VAL:HG22	1:97:A:TYR:HB3	7	0.13
(1,1147)	1:95:A:VAL:HG23	1:97:A:TYR:HB2	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1147)	1:95:A:VAL:HG23	1:97:A:TYR:HB3	7	0.13
(1,1145)	1:95:A:VAL:HG11	1:131:A:ALA:HA	2	0.13
(1,1145)	1:95:A:VAL:HG12	1:131:A:ALA:HA	2	0.13
(1,1145)	1:95:A:VAL:HG13	1:131:A:ALA:HA	2	0.13
(1,1145)	1:95:A:VAL:HG21	1:131:A:ALA:HA	2	0.13
(1,1145)	1:95:A:VAL:HG22	1:131:A:ALA:HA	2	0.13
(1,1145)	1:95:A:VAL:HG23	1:131:A:ALA:HA	2	0.13
(1,1131)	1:95:A:VAL:HB	1:129:A:VAL:HG11	7	0.13
(1,1131)	1:95:A:VAL:HB	1:129:A:VAL:HG12	7	0.13
(1,1131)	1:95:A:VAL:HB	1:129:A:VAL:HG13	7	0.13
(1,1131)	1:95:A:VAL:HB	1:129:A:VAL:HG21	7	0.13
(1,1131)	1:95:A:VAL:HB	1:129:A:VAL:HG22	7	0.13
(1,1131)	1:95:A:VAL:HB	1:129:A:VAL:HG23	7	0.13
(1,1094)	1:93:A:ILE:HG13	1:127:A:PHE:H	8	0.13
(1,963)	1:79:A:GLN:H	1:79:A:GLN:HA	4	0.13
(1,940)	1:77:A:THR:HG21	1:87:A:SER:H	8	0.13
(1,940)	1:77:A:THR:HG22	1:87:A:SER:H	8	0.13
(1,940)	1:77:A:THR:HG23	1:87:A:SER:H	8	0.13
(1,875)	1:75:A:GLU:HA	1:89:A:LEU:H	3	0.13
(1,814)	1:68:A:ARG:H	1:69:A:TYR:H	2	0.13
(1,753)	1:58:A:LYS:HB3	1:60:A:LEU:H	10	0.13
(1,724)	1:56:A:GLU:HG2	1:58:A:LYS:H	2	0.13
(1,689)	1:54:A:VAL:HG11	1:57:A:MET:H	9	0.13
(1,689)	1:54:A:VAL:HG12	1:57:A:MET:H	9	0.13
(1,689)	1:54:A:VAL:HG13	1:57:A:MET:H	9	0.13
(1,689)	1:54:A:VAL:HG21	1:57:A:MET:H	9	0.13
(1,689)	1:54:A:VAL:HG22	1:57:A:MET:H	9	0.13
(1,689)	1:54:A:VAL:HG23	1:57:A:MET:H	9	0.13
(1,682)	1:54:A:VAL:HG21	1:57:A:MET:H	9	0.13
(1,682)	1:54:A:VAL:HG22	1:57:A:MET:H	9	0.13
(1,682)	1:54:A:VAL:HG23	1:57:A:MET:H	9	0.13
(1,676)	1:54:A:VAL:HB	1:57:A:MET:H	2	0.13
(1,655)	1:53:A:PHE:HA	1:56:A:GLU:H	4	0.13
(1,636)	1:51:A:ALA:HB1	1:54:A:VAL:H	7	0.13
(1,636)	1:51:A:ALA:HB2	1:54:A:VAL:H	7	0.13
(1,636)	1:51:A:ALA:HB3	1:54:A:VAL:H	7	0.13
(1,615)	1:50:A:TYR:HA	1:51:A:ALA:H	2	0.13
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG21	6	0.13
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG22	6	0.13
(1,531)	1:34:A:ASN:H	1:36:A:THR:HG23	6	0.13
(1,480)	1:30:A:LYS:HB2	1:41:A:GLU:HA	5	0.13
(1,480)	1:30:A:LYS:HB3	1:41:A:GLU:HA	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,464)	1:29:A:PHE:HB2	1:41:A:GLU:H	10	0.13
(1,449)	1:28:A:ILE:HD11	1:42:A:LYS:HD2	10	0.13
(1,449)	1:28:A:ILE:HD12	1:42:A:LYS:HD2	10	0.13
(1,449)	1:28:A:ILE:HD13	1:42:A:LYS:HD2	10	0.13
(1,449)	1:28:A:ILE:HD11	1:42:A:LYS:HD3	10	0.13
(1,449)	1:28:A:ILE:HD12	1:42:A:LYS:HD3	10	0.13
(1,449)	1:28:A:ILE:HD13	1:42:A:LYS:HD3	10	0.13
(1,439)	1:28:A:ILE:HB	1:42:A:LYS:HD2	6	0.13
(1,439)	1:28:A:ILE:HB	1:42:A:LYS:HD3	6	0.13
(1,404)	1:27:A:ILE:HB	1:71:A:ALA:HB1	7	0.13
(1,404)	1:27:A:ILE:HB	1:71:A:ALA:HB2	7	0.13
(1,404)	1:27:A:ILE:HB	1:71:A:ALA:HB3	7	0.13
(1,402)	1:27:A:ILE:HB	1:43:A:VAL:HA	8	0.13
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB1	5	0.13
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB2	5	0.13
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB3	5	0.13
(1,350)	1:21:A:LYS:HD3	1:22:A:HIS:H	4	0.13
(1,277)	1:16:A:ASP:HB2	1:18:A:LEU:H	8	0.13
(1,255)	1:15:A:TYR:HA	1:19:A:HIS:H	7	0.13
(1,224)	1:13:A:ASN:HA	1:16:A:ASP:H	2	0.13
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD11	2	0.13
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD12	2	0.13
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD13	2	0.13
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD21	2	0.13
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD22	2	0.13
(1,219)	1:12:A:LYS:HG2	1:121:A:LEU:HD23	2	0.13
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD11	2	0.13
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD12	2	0.13
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD13	2	0.13
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD21	2	0.13
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD22	2	0.13
(1,219)	1:12:A:LYS:HG3	1:121:A:LEU:HD23	2	0.13
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD11	2	0.13
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD12	2	0.13
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD13	2	0.13
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD21	2	0.13
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD22	2	0.13
(1,215)	1:12:A:LYS:HB2	1:121:A:LEU:HD23	2	0.13
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD11	2	0.13
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD12	2	0.13
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD13	2	0.13
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD21	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD22	2	0.13
(1,215)	1:12:A:LYS:HB3	1:121:A:LEU:HD23	2	0.13
(1,209)	1:12:A:LYS:HG2	1:121:A:LEU:HD11	4	0.13
(1,209)	1:12:A:LYS:HG2	1:121:A:LEU:HD12	4	0.13
(1,209)	1:12:A:LYS:HG2	1:121:A:LEU:HD13	4	0.13
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG11	6	0.13
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG12	6	0.13
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG13	6	0.13
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG21	6	0.13
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG22	6	0.13
(1,153)	1:10:A:SER:HA	1:40:A:VAL:HG23	6	0.13
(1,115)	1:8:A:ASP:H	1:38:A:ILE:H	5	0.13
(1,63)	1:7:A:VAL:H	1:8:A:ASP:H	8	0.13
(3,8)	1:13:A:ASN:O	1:17:A:LEU:N	9	0.12
(2,34)	1:114:A:VAL:HA	1:117:A:LEU:HA	7	0.12
(1,1794)	1:151:A:ARG:H	1:151:A:ARG:HA	6	0.12
(1,1782)	1:150:A:GLN:H	1:150:A:GLN:HA	7	0.12
(1,1775)	1:149:A:ASN:HB3	1:152:A:ILE:HG21	2	0.12
(1,1775)	1:149:A:ASN:HB3	1:152:A:ILE:HG22	2	0.12
(1,1775)	1:149:A:ASN:HB3	1:152:A:ILE:HG23	2	0.12
(1,1757)	1:147:A:MET:HA	1:150:A:GLN:H	3	0.12
(1,1740)	1:146:A:LEU:H	1:148:A:SER:H	9	0.12
(1,1736)	1:146:A:LEU:H	1:146:A:LEU:HG	1	0.12
(1,1717)	1:144:A:SER:H	1:145:A:ASP:H	3	0.12
(1,1712)	1:143:A:LYS:HB3	1:147:A:MET:H	3	0.12
(1,1706)	1:143:A:LYS:HA	1:147:A:MET:H	7	0.12
(1,1665)	1:141:A:SER:HA	1:144:A:SER:H	9	0.12
(1,1646)	1:140:A:LYS:HA	1:143:A:LYS:H	2	0.12
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE2	6	0.12
(1,1606)	1:137:A:LEU:HA	1:140:A:LYS:HE3	6	0.12
(1,1547)	1:130:A:GLN:HG2	1:131:A:ALA:H	3	0.12
(1,1547)	1:130:A:GLN:HG3	1:131:A:ALA:H	3	0.12
(1,1536)	1:128:A:GLN:HB2	1:129:A:VAL:H	8	0.12
(1,1536)	1:128:A:GLN:HB3	1:129:A:VAL:H	8	0.12
(1,1514)	1:124:A:GLU:HB2	1:126:A:LEU:H	1	0.12
(1,1514)	1:124:A:GLU:HB3	1:126:A:LEU:H	1	0.12
(1,1469)	1:120:A:SER:HB2	1:122:A:GLY:H	9	0.12
(1,1469)	1:120:A:SER:HB3	1:122:A:GLY:H	9	0.12
(1,1466)	1:120:A:SER:HB3	1:122:A:GLY:H	3	0.12
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB2	3	0.12
(1,1447)	1:118:A:LYS:HG3	1:128:A:GLN:HB3	3	0.12
(1,1429)	1:117:A:LEU:HB3	1:119:A:ALA:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1426)	1:117:A:LEU:HB2	1:119:A:ALA:H	4	0.12
(1,1420)	1:117:A:LEU:HA	1:119:A:ALA:H	10	0.12
(1,1385)	1:114:A:VAL:HG11	1:116:A:ALA:H	9	0.12
(1,1385)	1:114:A:VAL:HG12	1:116:A:ALA:H	9	0.12
(1,1385)	1:114:A:VAL:HG13	1:116:A:ALA:H	9	0.12
(1,1385)	1:114:A:VAL:HG21	1:116:A:ALA:H	9	0.12
(1,1385)	1:114:A:VAL:HG22	1:116:A:ALA:H	9	0.12
(1,1385)	1:114:A:VAL:HG23	1:116:A:ALA:H	9	0.12
(1,1382)	1:114:A:VAL:HG21	1:116:A:ALA:H	4	0.12
(1,1382)	1:114:A:VAL:HG22	1:116:A:ALA:H	4	0.12
(1,1382)	1:114:A:VAL:HG23	1:116:A:ALA:H	4	0.12
(1,1323)	1:109:A:LEU:HD11	1:111:A:ALA:H	2	0.12
(1,1323)	1:109:A:LEU:HD12	1:111:A:ALA:H	2	0.12
(1,1323)	1:109:A:LEU:HD13	1:111:A:ALA:H	2	0.12
(1,1323)	1:109:A:LEU:HD21	1:111:A:ALA:H	2	0.12
(1,1323)	1:109:A:LEU:HD22	1:111:A:ALA:H	2	0.12
(1,1323)	1:109:A:LEU:HD23	1:111:A:ALA:H	2	0.12
(1,1298)	1:108:A:MET:HB2	1:110:A:TYR:H	7	0.12
(1,1293)	1:108:A:MET:HA	1:110:A:TYR:H	10	0.12
(1,1239)	1:104:A:VAL:HG11	1:107:A:ARG:H	5	0.12
(1,1239)	1:104:A:VAL:HG12	1:107:A:ARG:H	5	0.12
(1,1239)	1:104:A:VAL:HG13	1:107:A:ARG:H	5	0.12
(1,1239)	1:104:A:VAL:HG21	1:107:A:ARG:H	5	0.12
(1,1239)	1:104:A:VAL:HG22	1:107:A:ARG:H	5	0.12
(1,1239)	1:104:A:VAL:HG23	1:107:A:ARG:H	5	0.12
(1,1218)	1:104:A:VAL:HA	1:106:A:ARG:H	2	0.12
(1,1208)	1:103:A:PRO:HA	1:107:A:ARG:H	6	0.12
(1,1203)	1:102:A:ALA:HB1	1:103:A:PRO:HA	7	0.12
(1,1203)	1:102:A:ALA:HB2	1:103:A:PRO:HA	7	0.12
(1,1203)	1:102:A:ALA:HB3	1:103:A:PRO:HA	7	0.12
(1,1065)	1:91:A:LYS:HE3	1:150:A:GLN:H	1	0.12
(1,1037)	1:88:A:THR:HB	1:89:A:LEU:H	3	0.12
(1,1035)	1:88:A:THR:H	1:89:A:LEU:H	8	0.12
(1,1030)	1:87:A:SER:H	1:88:A:THR:H	1	0.12
(1,1014)	1:84:A:GLU:H	1:84:A:GLU:HB2	1	0.12
(1,1014)	1:84:A:GLU:H	1:84:A:GLU:HB3	1	0.12
(1,993)	1:80:A:ARG:HG2	1:81:A:GLN:H	4	0.12
(1,993)	1:80:A:ARG:HG3	1:81:A:GLN:H	4	0.12
(1,947)	1:78:A:VAL:H	1:87:A:SER:H	7	0.12
(1,930)	1:77:A:THR:HA	1:78:A:VAL:HB	10	0.12
(1,905)	1:76:A:VAL:H	1:77:A:THR:H	8	0.12
(1,887)	1:75:A:GLU:HB3	1:89:A:LEU:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:70:A:ALA:H	1:94:A:PHE:HA	6	0.12
(1,784)	1:61:A:VAL:HG11	1:66:A:GLU:HG2	3	0.12
(1,784)	1:61:A:VAL:HG12	1:66:A:GLU:HG2	3	0.12
(1,784)	1:61:A:VAL:HG13	1:66:A:GLU:HG2	3	0.12
(1,784)	1:61:A:VAL:HG11	1:66:A:GLU:HG3	3	0.12
(1,784)	1:61:A:VAL:HG12	1:66:A:GLU:HG3	3	0.12
(1,784)	1:61:A:VAL:HG13	1:66:A:GLU:HG3	3	0.12
(1,725)	1:56:A:GLU:HG3	1:57:A:MET:H	7	0.12
(1,690)	1:54:A:VAL:HG11	1:57:A:MET:HB2	3	0.12
(1,690)	1:54:A:VAL:HG11	1:57:A:MET:HB3	3	0.12
(1,690)	1:54:A:VAL:HG12	1:57:A:MET:HB2	3	0.12
(1,690)	1:54:A:VAL:HG12	1:57:A:MET:HB3	3	0.12
(1,690)	1:54:A:VAL:HG13	1:57:A:MET:HB2	3	0.12
(1,690)	1:54:A:VAL:HG13	1:57:A:MET:HB3	3	0.12
(1,690)	1:54:A:VAL:HG21	1:57:A:MET:HB2	3	0.12
(1,690)	1:54:A:VAL:HG21	1:57:A:MET:HB3	3	0.12
(1,690)	1:54:A:VAL:HG22	1:57:A:MET:HB2	3	0.12
(1,690)	1:54:A:VAL:HG22	1:57:A:MET:HB3	3	0.12
(1,690)	1:54:A:VAL:HG23	1:57:A:MET:HB2	3	0.12
(1,690)	1:54:A:VAL:HG23	1:57:A:MET:HB3	3	0.12
(1,676)	1:54:A:VAL:HB	1:57:A:MET:H	5	0.12
(1,657)	1:53:A:PHE:HA	1:57:A:MET:H	7	0.12
(1,646)	1:52:A:GLU:HA	1:56:A:GLU:H	6	0.12
(1,636)	1:51:A:ALA:HB1	1:54:A:VAL:H	10	0.12
(1,636)	1:51:A:ALA:HB2	1:54:A:VAL:H	10	0.12
(1,636)	1:51:A:ALA:HB3	1:54:A:VAL:H	10	0.12
(1,528)	1:33:A:LYS:HG3	1:36:A:THR:HB	8	0.12
(1,466)	1:29:A:PHE:HB3	1:41:A:GLU:H	10	0.12
(1,429)	1:28:A:ILE:H	1:42:A:LYS:HG2	3	0.12
(1,429)	1:28:A:ILE:H	1:42:A:LYS:HG3	3	0.12
(1,402)	1:27:A:ILE:HB	1:43:A:VAL:HA	1	0.12
(1,402)	1:27:A:ILE:HB	1:43:A:VAL:HA	9	0.12
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB1	2	0.12
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB2	2	0.12
(1,400)	1:27:A:ILE:HA	1:71:A:ALA:HB3	2	0.12
(1,398)	1:27:A:ILE:HA	1:43:A:VAL:HB	3	0.12
(1,382)	1:26:A:TYR:HB3	1:72:A:VAL:HA	10	0.12
(1,366)	1:25:A:SER:H	1:73:A:ASP:H	10	0.12
(1,323)	1:18:A:LEU:HD21	1:71:A:ALA:HA	4	0.12
(1,323)	1:18:A:LEU:HD22	1:71:A:ALA:HA	4	0.12
(1,323)	1:18:A:LEU:HD23	1:71:A:ALA:HA	4	0.12
(1,291)	1:17:A:LEU:HA	1:20:A:ASN:H	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,277)	1:16:A:ASP:HB2	1:18:A:LEU:H	4	0.12
(1,277)	1:16:A:ASP:HB2	1:18:A:LEU:H	6	0.12
(1,272)	1:16:A:ASP:HA	1:18:A:LEU:H	4	0.12
(1,210)	1:12:A:LYS:HG2	1:13:A:ASN:H	2	0.12
(1,184)	1:11:A:CYS:HB2	1:13:A:ASN:H	3	0.12
(1,184)	1:11:A:CYS:HB3	1:13:A:ASN:H	3	0.12
(1,161)	1:10:A:SER:HB2	1:12:A:LYS:H	4	0.12
(1,161)	1:10:A:SER:HB3	1:12:A:LYS:H	4	0.12
(1,156)	1:10:A:SER:HB2	1:13:A:ASN:H	5	0.12
(1,121)	1:8:A:ASP:HB2	1:10:A:SER:H	5	0.12
(1,107)	1:7:A:VAL:HG11	1:38:A:ILE:H	7	0.12
(1,107)	1:7:A:VAL:HG12	1:38:A:ILE:H	7	0.12
(1,107)	1:7:A:VAL:HG13	1:38:A:ILE:H	7	0.12
(1,107)	1:7:A:VAL:HG21	1:38:A:ILE:H	7	0.12
(1,107)	1:7:A:VAL:HG22	1:38:A:ILE:H	7	0.12
(1,107)	1:7:A:VAL:HG23	1:38:A:ILE:H	7	0.12
(1,89)	1:7:A:VAL:HG21	1:116:A:ALA:HB1	10	0.12
(1,89)	1:7:A:VAL:HG21	1:116:A:ALA:HB2	10	0.12
(1,89)	1:7:A:VAL:HG21	1:116:A:ALA:HB3	10	0.12
(1,89)	1:7:A:VAL:HG22	1:116:A:ALA:HB1	10	0.12
(1,89)	1:7:A:VAL:HG22	1:116:A:ALA:HB2	10	0.12
(1,89)	1:7:A:VAL:HG22	1:116:A:ALA:HB3	10	0.12
(1,89)	1:7:A:VAL:HG23	1:116:A:ALA:HB1	10	0.12
(1,89)	1:7:A:VAL:HG23	1:116:A:ALA:HB2	10	0.12
(1,89)	1:7:A:VAL:HG23	1:116:A:ALA:HB3	10	0.12
(1,72)	1:7:A:VAL:HB	1:117:A:LEU:HA	8	0.12
(1,65)	1:7:A:VAL:HA	1:37:A:ALA:HA	4	0.12
(1,26)	1:5:A:VAL:HA	1:116:A:ALA:HB1	6	0.12
(1,26)	1:5:A:VAL:HA	1:116:A:ALA:HB2	6	0.12
(1,26)	1:5:A:VAL:HA	1:116:A:ALA:HB3	6	0.12
(1,25)	1:5:A:VAL:H	1:6:A:LYS:H	2	0.12
(3,4)	1:8:A:ASP:N	1:38:A:ILE:O	2	0.11
(1,1806)	1:152:A:ILE:H	1:152:A:ILE:HG12	9	0.11
(1,1806)	1:152:A:ILE:H	1:152:A:ILE:HG13	9	0.11
(1,1782)	1:150:A:GLN:H	1:150:A:GLN:HA	1	0.11
(1,1765)	1:148:A:SER:HB2	1:150:A:GLN:H	8	0.11
(1,1764)	1:148:A:SER:HB2	1:149:A:ASN:H	2	0.11
(1,1764)	1:148:A:SER:HB2	1:149:A:ASN:H	10	0.11
(1,1740)	1:146:A:LEU:H	1:148:A:SER:H	1	0.11
(1,1736)	1:146:A:LEU:H	1:146:A:LEU:HG	8	0.11
(1,1729)	1:145:A:ASP:H	1:146:A:LEU:H	9	0.11
(1,1729)	1:145:A:ASP:H	1:146:A:LEU:H	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1721)	1:144:A:SER:HA	1:148:A:SER:H	6	0.11
(1,1704)	1:143:A:LYS:HA	1:146:A:LEU:HB2	5	0.11
(1,1704)	1:143:A:LYS:HA	1:146:A:LEU:HB3	5	0.11
(1,1657)	1:140:A:LYS:HB2	1:141:A:SER:H	3	0.11
(1,1657)	1:140:A:LYS:HB3	1:141:A:SER:H	3	0.11
(1,1657)	1:140:A:LYS:HB2	1:141:A:SER:H	5	0.11
(1,1657)	1:140:A:LYS:HB3	1:141:A:SER:H	5	0.11
(1,1550)	1:131:A:ALA:HA	1:136:A:ASP:HA	5	0.11
(1,1444)	1:118:A:LYS:HG2	1:119:A:ALA:H	1	0.11
(1,1402)	1:115:A:ARG:HB2	1:118:A:LYS:H	8	0.11
(1,1402)	1:115:A:ARG:HB3	1:118:A:LYS:H	8	0.11
(1,1385)	1:114:A:VAL:HG11	1:116:A:ALA:H	7	0.11
(1,1385)	1:114:A:VAL:HG12	1:116:A:ALA:H	7	0.11
(1,1385)	1:114:A:VAL:HG13	1:116:A:ALA:H	7	0.11
(1,1385)	1:114:A:VAL:HG21	1:116:A:ALA:H	7	0.11
(1,1385)	1:114:A:VAL:HG22	1:116:A:ALA:H	7	0.11
(1,1385)	1:114:A:VAL:HG23	1:116:A:ALA:H	7	0.11
(1,1366)	1:113:A:SER:HB3	1:116:A:ALA:H	2	0.11
(1,1333)	1:110:A:TYR:HA	1:114:A:VAL:H	9	0.11
(1,1330)	1:110:A:TYR:HA	1:111:A:ALA:H	2	0.11
(1,1305)	1:108:A:MET:HG2	1:112:A:SER:H	4	0.11
(1,1305)	1:108:A:MET:HG3	1:112:A:SER:H	4	0.11
(1,1296)	1:108:A:MET:HA	1:112:A:SER:H	7	0.11
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD11	6	0.11
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD12	6	0.11
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD13	6	0.11
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD21	6	0.11
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD22	6	0.11
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD23	6	0.11
(1,1288)	1:107:A:ARG:HG2	1:109:A:LEU:H	6	0.11
(1,1288)	1:107:A:ARG:HG3	1:109:A:LEU:H	6	0.11
(1,1273)	1:106:A:ARG:HB2	1:108:A:MET:H	1	0.11
(1,1273)	1:106:A:ARG:HB3	1:108:A:MET:H	1	0.11
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	9	0.11
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	9	0.11
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG2	9	0.11
(1,1254)	1:105:A:ARG:HA	1:108:A:MET:HG3	9	0.11
(1,1244)	1:104:A:VAL:HG11	1:108:A:MET:HB2	10	0.11
(1,1244)	1:104:A:VAL:HG11	1:108:A:MET:HB3	10	0.11
(1,1244)	1:104:A:VAL:HG12	1:108:A:MET:HB2	10	0.11
(1,1244)	1:104:A:VAL:HG12	1:108:A:MET:HB3	10	0.11
(1,1244)	1:104:A:VAL:HG13	1:108:A:MET:HB2	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1244)	1:104:A:VAL:HG13	1:108:A:MET:HB3	10	0.11
(1,1244)	1:104:A:VAL:HG21	1:108:A:MET:HB2	10	0.11
(1,1244)	1:104:A:VAL:HG21	1:108:A:MET:HB3	10	0.11
(1,1244)	1:104:A:VAL:HG22	1:108:A:MET:HB2	10	0.11
(1,1244)	1:104:A:VAL:HG22	1:108:A:MET:HB3	10	0.11
(1,1244)	1:104:A:VAL:HG23	1:108:A:MET:HB2	10	0.11
(1,1244)	1:104:A:VAL:HG23	1:108:A:MET:HB3	10	0.11
(1,1234)	1:104:A:VAL:HG21	1:107:A:ARG:H	6	0.11
(1,1234)	1:104:A:VAL:HG22	1:107:A:ARG:H	6	0.11
(1,1234)	1:104:A:VAL:HG23	1:107:A:ARG:H	6	0.11
(1,1178)	1:99:A:PRO:HB2	1:102:A:ALA:HA	1	0.11
(1,1160)	1:96:A:GLN:HB2	1:130:A:GLN:HA	1	0.11
(1,1160)	1:96:A:GLN:HB3	1:130:A:GLN:HA	1	0.11
(1,1114)	1:94:A:PHE:H	1:129:A:VAL:H	10	0.11
(1,1092)	1:93:A:ILE:HG12	1:127:A:PHE:H	10	0.11
(1,905)	1:76:A:VAL:H	1:77:A:THR:H	7	0.11
(1,902)	1:75:A:GLU:HG2	1:90:A:ASN:HB2	1	0.11
(1,902)	1:75:A:GLU:HG2	1:90:A:ASN:HB3	1	0.11
(1,902)	1:75:A:GLU:HG3	1:90:A:ASN:HB2	1	0.11
(1,902)	1:75:A:GLU:HG3	1:90:A:ASN:HB3	1	0.11
(1,902)	1:75:A:GLU:HG2	1:90:A:ASN:HB2	6	0.11
(1,902)	1:75:A:GLU:HG2	1:90:A:ASN:HB3	6	0.11
(1,902)	1:75:A:GLU:HG3	1:90:A:ASN:HB2	6	0.11
(1,902)	1:75:A:GLU:HG3	1:90:A:ASN:HB3	6	0.11
(1,879)	1:75:A:GLU:HB2	1:88:A:THR:HA	1	0.11
(1,833)	1:71:A:ALA:HB1	1:93:A:ILE:H	1	0.11
(1,833)	1:71:A:ALA:HB2	1:93:A:ILE:H	1	0.11
(1,833)	1:71:A:ALA:HB3	1:93:A:ILE:H	1	0.11
(1,800)	1:64:A:GLY:H	1:65:A:LYS:H	8	0.11
(1,755)	1:58:A:LYS:HD2	1:60:A:LEU:H	2	0.11
(1,683)	1:54:A:VAL:HG21	1:58:A:LYS:H	1	0.11
(1,683)	1:54:A:VAL:HG22	1:58:A:LYS:H	1	0.11
(1,683)	1:54:A:VAL:HG23	1:58:A:LYS:H	1	0.11
(1,615)	1:50:A:TYR:HA	1:51:A:ALA:H	10	0.11
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD11	5	0.11
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD12	5	0.11
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD13	5	0.11
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD21	5	0.11
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD22	5	0.11
(1,496)	1:31:A:ILE:HG13	1:109:A:LEU:HD23	5	0.11
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD11	4	0.11
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD12	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD13	4	0.11
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD21	4	0.11
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD22	4	0.11
(1,492)	1:31:A:ILE:HG12	1:109:A:LEU:HD23	4	0.11
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD11	5	0.11
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD12	5	0.11
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD13	5	0.11
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD21	5	0.11
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD22	5	0.11
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD23	5	0.11
(1,426)	1:28:A:ILE:H	1:42:A:LYS:HA	3	0.11
(1,404)	1:27:A:ILE:HB	1:71:A:ALA:HB1	9	0.11
(1,404)	1:27:A:ILE:HB	1:71:A:ALA:HB2	9	0.11
(1,404)	1:27:A:ILE:HB	1:71:A:ALA:HB3	9	0.11
(1,292)	1:17:A:LEU:HA	1:21:A:LYS:H	7	0.11
(1,283)	1:16:A:ASP:HB2	1:18:A:LEU:H	4	0.11
(1,283)	1:16:A:ASP:HB3	1:18:A:LEU:H	4	0.11
(1,283)	1:16:A:ASP:HB2	1:18:A:LEU:H	6	0.11
(1,283)	1:16:A:ASP:HB3	1:18:A:LEU:H	6	0.11
(1,278)	1:16:A:ASP:HB2	1:19:A:HIS:H	9	0.11
(1,272)	1:16:A:ASP:HA	1:18:A:LEU:H	1	0.11
(1,259)	1:15:A:TYR:HB2	1:27:A:ILE:HD11	4	0.11
(1,259)	1:15:A:TYR:HB2	1:27:A:ILE:HD12	4	0.11
(1,259)	1:15:A:TYR:HB2	1:27:A:ILE:HD13	4	0.11
(1,128)	1:8:A:ASP:HB3	1:39:A:VAL:HA	3	0.11
(1,111)	1:7:A:VAL:HG11	1:9:A:PRO:HA	5	0.11
(1,111)	1:7:A:VAL:HG12	1:9:A:PRO:HA	5	0.11
(1,111)	1:7:A:VAL:HG13	1:9:A:PRO:HA	5	0.11
(1,111)	1:7:A:VAL:HG21	1:9:A:PRO:HA	5	0.11
(1,111)	1:7:A:VAL:HG22	1:9:A:PRO:HA	5	0.11
(1,111)	1:7:A:VAL:HG23	1:9:A:PRO:HA	5	0.11
(1,105)	1:7:A:VAL:HG11	1:37:A:ALA:HA	2	0.11
(1,105)	1:7:A:VAL:HG12	1:37:A:ALA:HA	2	0.11
(1,105)	1:7:A:VAL:HG13	1:37:A:ALA:HA	2	0.11
(1,105)	1:7:A:VAL:HG21	1:37:A:ALA:HA	2	0.11
(1,105)	1:7:A:VAL:HG22	1:37:A:ALA:HA	2	0.11
(1,105)	1:7:A:VAL:HG23	1:37:A:ALA:HA	2	0.11
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB2	7	0.11
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB3	7	0.11
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB2	7	0.11
(1,74)	1:7:A:VAL:HB	1:120:A:SER:HB3	7	0.11
(1,51)	1:6:A:LYS:HA	1:37:A:ALA:HA	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,57)	1:139:A:GLU:O	1:143:A:LYS:H	2	0.1
(3,43)	1:76:A:VAL:O	1:89:A:LEU:H	2	0.1
(3,9)	1:26:A:TYR:H	1:44:A:GLY:O	9	0.1
(1,1748)	1:146:A:LEU:HB2	1:148:A:SER:H	3	0.1
(1,1748)	1:146:A:LEU:HB3	1:148:A:SER:H	3	0.1
(1,1730)	1:145:A:ASP:H	1:147:A:MET:H	10	0.1
(1,1729)	1:145:A:ASP:H	1:146:A:LEU:H	2	0.1
(1,1463)	1:120:A:SER:HB2	1:121:A:LEU:H	9	0.1
(1,1444)	1:118:A:LYS:HG2	1:119:A:ALA:H	6	0.1
(1,1433)	1:117:A:LEU:HD11	1:120:A:SER:H	10	0.1
(1,1433)	1:117:A:LEU:HD12	1:120:A:SER:H	10	0.1
(1,1433)	1:117:A:LEU:HD13	1:120:A:SER:H	10	0.1
(1,1433)	1:117:A:LEU:HD21	1:120:A:SER:H	10	0.1
(1,1433)	1:117:A:LEU:HD22	1:120:A:SER:H	10	0.1
(1,1433)	1:117:A:LEU:HD23	1:120:A:SER:H	10	0.1
(1,1429)	1:117:A:LEU:HB3	1:119:A:ALA:H	4	0.1
(1,1373)	1:114:A:VAL:HA	1:117:A:LEU:HB2	4	0.1
(1,1373)	1:114:A:VAL:HA	1:117:A:LEU:HB3	4	0.1
(1,1366)	1:113:A:SER:HB3	1:116:A:ALA:H	5	0.1
(1,1330)	1:110:A:TYR:HA	1:111:A:ALA:H	1	0.1
(1,1330)	1:110:A:TYR:HA	1:111:A:ALA:H	3	0.1
(1,1330)	1:110:A:TYR:HA	1:111:A:ALA:H	4	0.1
(1,1330)	1:110:A:TYR:HA	1:111:A:ALA:H	7	0.1
(1,1322)	1:109:A:LEU:HD21	1:113:A:SER:H	7	0.1
(1,1322)	1:109:A:LEU:HD22	1:113:A:SER:H	7	0.1
(1,1322)	1:109:A:LEU:HD23	1:113:A:SER:H	7	0.1
(1,1293)	1:108:A:MET:HA	1:110:A:TYR:H	6	0.1
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD11	3	0.1
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD12	3	0.1
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD13	3	0.1
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD21	3	0.1
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD22	3	0.1
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD23	3	0.1
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD11	10	0.1
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD12	10	0.1
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD13	10	0.1
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD21	10	0.1
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD22	10	0.1
(1,1292)	1:108:A:MET:HA	1:109:A:LEU:HD23	10	0.1
(1,1266)	1:106:A:ARG:HA	1:108:A:MET:H	6	0.1
(1,1259)	1:105:A:ARG:HB2	1:108:A:MET:H	3	0.1
(1,1259)	1:105:A:ARG:HB3	1:108:A:MET:H	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1240)	1:104:A:VAL:HG11	1:107:A:ARG:HA	3	0.1
(1,1240)	1:104:A:VAL:HG12	1:107:A:ARG:HA	3	0.1
(1,1240)	1:104:A:VAL:HG13	1:107:A:ARG:HA	3	0.1
(1,1240)	1:104:A:VAL:HG21	1:107:A:ARG:HA	3	0.1
(1,1240)	1:104:A:VAL:HG22	1:107:A:ARG:HA	3	0.1
(1,1240)	1:104:A:VAL:HG23	1:107:A:ARG:HA	3	0.1
(1,1208)	1:103:A:PRO:HA	1:107:A:ARG:H	3	0.1
(1,1208)	1:103:A:PRO:HA	1:107:A:ARG:H	10	0.1
(1,1203)	1:102:A:ALA:HB1	1:103:A:PRO:HA	10	0.1
(1,1203)	1:102:A:ALA:HB2	1:103:A:PRO:HA	10	0.1
(1,1203)	1:102:A:ALA:HB3	1:103:A:PRO:HA	10	0.1
(1,1179)	1:99:A:PRO:HB2	1:132:A:SER:HA	4	0.1
(1,1097)	1:93:A:ILE:HD11	1:129:A:VAL:HA	3	0.1
(1,1097)	1:93:A:ILE:HD12	1:129:A:VAL:HA	3	0.1
(1,1097)	1:93:A:ILE:HD13	1:129:A:VAL:HA	3	0.1
(1,1044)	1:89:A:LEU:HB2	1:90:A:ASN:H	7	0.1
(1,963)	1:79:A:GLN:H	1:79:A:GLN:HA	7	0.1
(1,958)	1:78:A:VAL:HG21	1:80:A:ARG:HG2	2	0.1
(1,958)	1:78:A:VAL:HG22	1:80:A:ARG:HG2	2	0.1
(1,958)	1:78:A:VAL:HG23	1:80:A:ARG:HG2	2	0.1
(1,958)	1:78:A:VAL:HG21	1:80:A:ARG:HG3	2	0.1
(1,958)	1:78:A:VAL:HG22	1:80:A:ARG:HG3	2	0.1
(1,958)	1:78:A:VAL:HG23	1:80:A:ARG:HG3	2	0.1
(1,751)	1:58:A:LYS:HB2	1:60:A:LEU:H	5	0.1
(1,737)	1:57:A:MET:HG2	1:60:A:LEU:HG	2	0.1
(1,737)	1:57:A:MET:HG3	1:60:A:LEU:HG	2	0.1
(1,725)	1:56:A:GLU:HG3	1:57:A:MET:H	3	0.1
(1,725)	1:56:A:GLU:HG3	1:57:A:MET:H	10	0.1
(1,709)	1:55:A:GLU:HB2	1:58:A:LYS:H	4	0.1
(1,699)	1:55:A:GLU:HA	1:58:A:LYS:HD2	4	0.1
(1,699)	1:55:A:GLU:HA	1:58:A:LYS:HD3	4	0.1
(1,676)	1:54:A:VAL:HB	1:57:A:MET:H	6	0.1
(1,675)	1:54:A:VAL:HB	1:56:A:GLU:H	7	0.1
(1,629)	1:51:A:ALA:HA	1:54:A:VAL:HA	7	0.1
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB1	9	0.1
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB2	9	0.1
(1,589)	1:45:A:GLU:HA	1:48:A:ALA:HB3	9	0.1
(1,579)	1:42:A:LYS:HG2	1:56:A:GLU:HB2	8	0.1
(1,579)	1:42:A:LYS:HG2	1:56:A:GLU:HB3	8	0.1
(1,579)	1:42:A:LYS:HG3	1:56:A:GLU:HB2	8	0.1
(1,579)	1:42:A:LYS:HG3	1:56:A:GLU:HB3	8	0.1
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD11	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD12	10	0.1
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD13	10	0.1
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD21	10	0.1
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD22	10	0.1
(1,490)	1:31:A:ILE:HB	1:109:A:LEU:HD23	10	0.1
(1,450)	1:28:A:ILE:HD11	1:70:A:ALA:HA	10	0.1
(1,450)	1:28:A:ILE:HD12	1:70:A:ALA:HA	10	0.1
(1,450)	1:28:A:ILE:HD13	1:70:A:ALA:HA	10	0.1
(1,426)	1:28:A:ILE:H	1:42:A:LYS:HA	2	0.1
(1,391)	1:27:A:ILE:H	1:28:A:ILE:H	2	0.1
(1,335)	1:19:A:HIS:HA	1:21:A:LYS:H	1	0.1
(1,218)	1:12:A:LYS:HG2	1:121:A:LEU:HA	4	0.1
(1,218)	1:12:A:LYS:HG3	1:121:A:LEU:HA	4	0.1
(1,193)	1:12:A:LYS:HA	1:121:A:LEU:HD11	1	0.1
(1,193)	1:12:A:LYS:HA	1:121:A:LEU:HD12	1	0.1
(1,193)	1:12:A:LYS:HA	1:121:A:LEU:HD13	1	0.1
(1,193)	1:12:A:LYS:HA	1:121:A:LEU:HD21	1	0.1
(1,193)	1:12:A:LYS:HA	1:121:A:LEU:HD22	1	0.1
(1,193)	1:12:A:LYS:HA	1:121:A:LEU:HD23	1	0.1
(1,125)	1:8:A:ASP:HB2	1:39:A:VAL:HG11	3	0.1
(1,125)	1:8:A:ASP:HB2	1:39:A:VAL:HG12	3	0.1
(1,125)	1:8:A:ASP:HB2	1:39:A:VAL:HG13	3	0.1
(1,125)	1:8:A:ASP:HB2	1:39:A:VAL:HG21	3	0.1
(1,125)	1:8:A:ASP:HB2	1:39:A:VAL:HG22	3	0.1
(1,125)	1:8:A:ASP:HB2	1:39:A:VAL:HG23	3	0.1
(1,102)	1:7:A:VAL:HG11	1:120:A:SER:HA	4	0.1
(1,102)	1:7:A:VAL:HG12	1:120:A:SER:HA	4	0.1
(1,102)	1:7:A:VAL:HG13	1:120:A:SER:HA	4	0.1
(1,102)	1:7:A:VAL:HG21	1:120:A:SER:HA	4	0.1
(1,102)	1:7:A:VAL:HG22	1:120:A:SER:HA	4	0.1
(1,102)	1:7:A:VAL:HG23	1:120:A:SER:HA	4	0.1
(1,50)	1:6:A:LYS:H	1:7:A:VAL:H	6	0.1

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

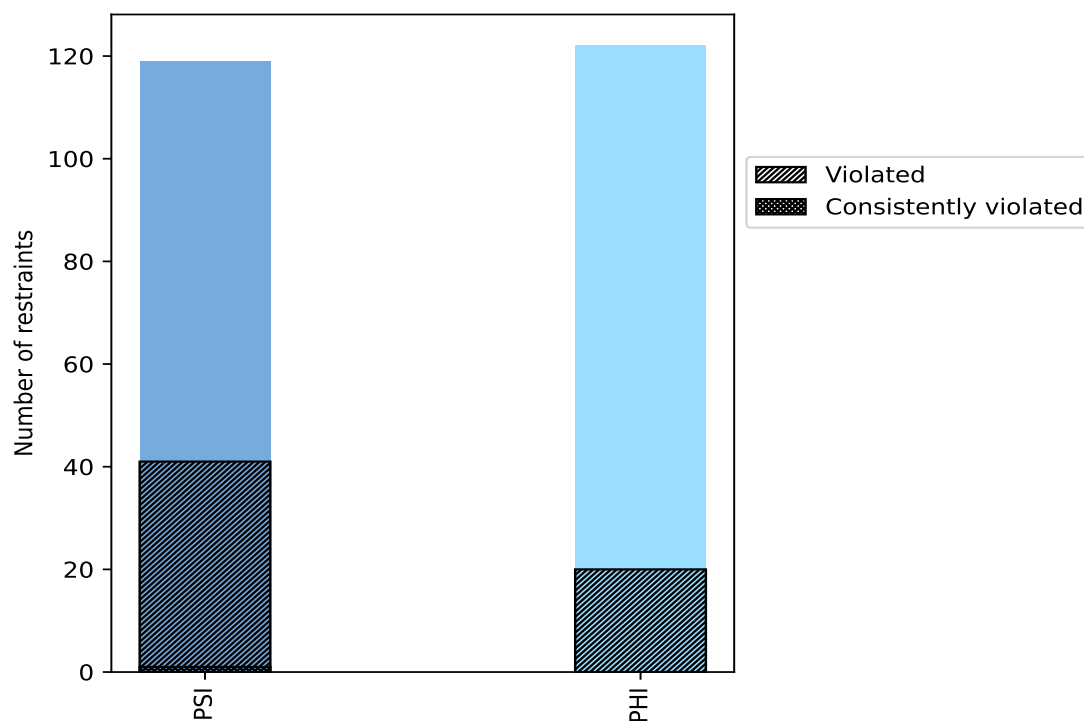
10.1 Summary of dihedral-angle violations [i](#)

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
PSI	119	49.4	41	34.5	17.0	1	0.8	0.4
PHI	122	50.6	20	16.4	8.3	0	0.0	0.0
Total	241	100.0	61	25.3	25.3	1	0.4	0.4

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](#)



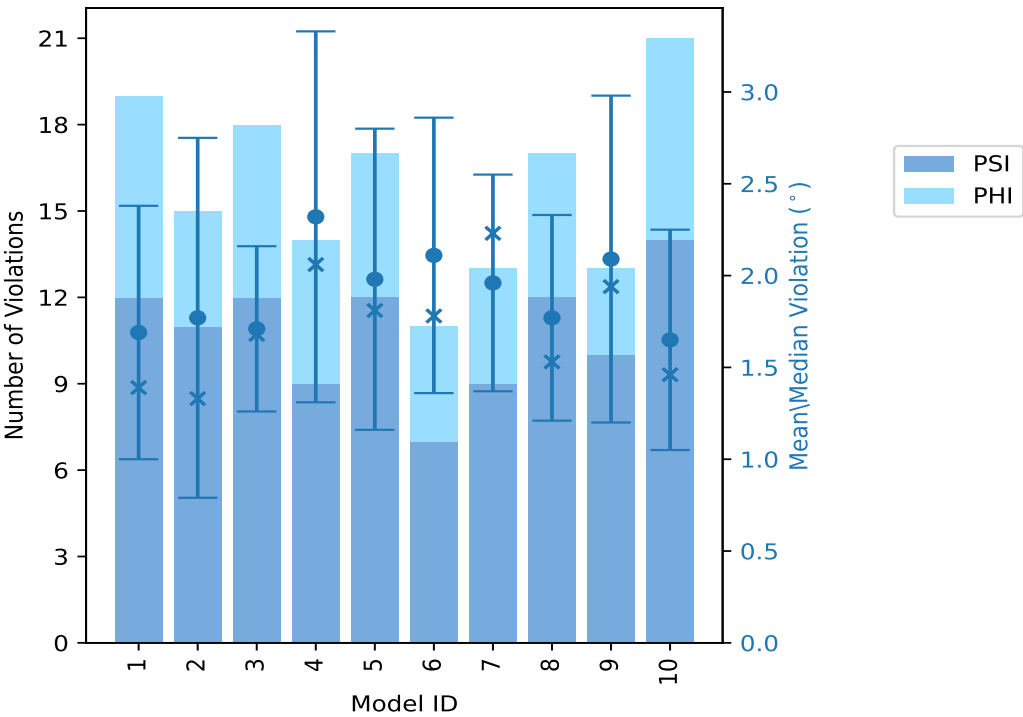
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	12	7	19	1.69	3.68	0.69	1.39
2	11	4	15	1.77	4.66	0.98	1.33
3	12	6	18	1.71	2.81	0.45	1.68
4	9	5	14	2.32	4.06	1.01	2.06
5	12	5	17	1.98	3.81	0.82	1.81
6	7	4	11	2.11	3.37	0.75	1.78
7	9	4	13	1.96	3.03	0.59	2.23
8	12	5	17	1.77	2.68	0.56	1.53
9	10	3	13	2.09	3.51	0.89	1.94
10	14	7	21	1.65	3.21	0.6	1.46

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

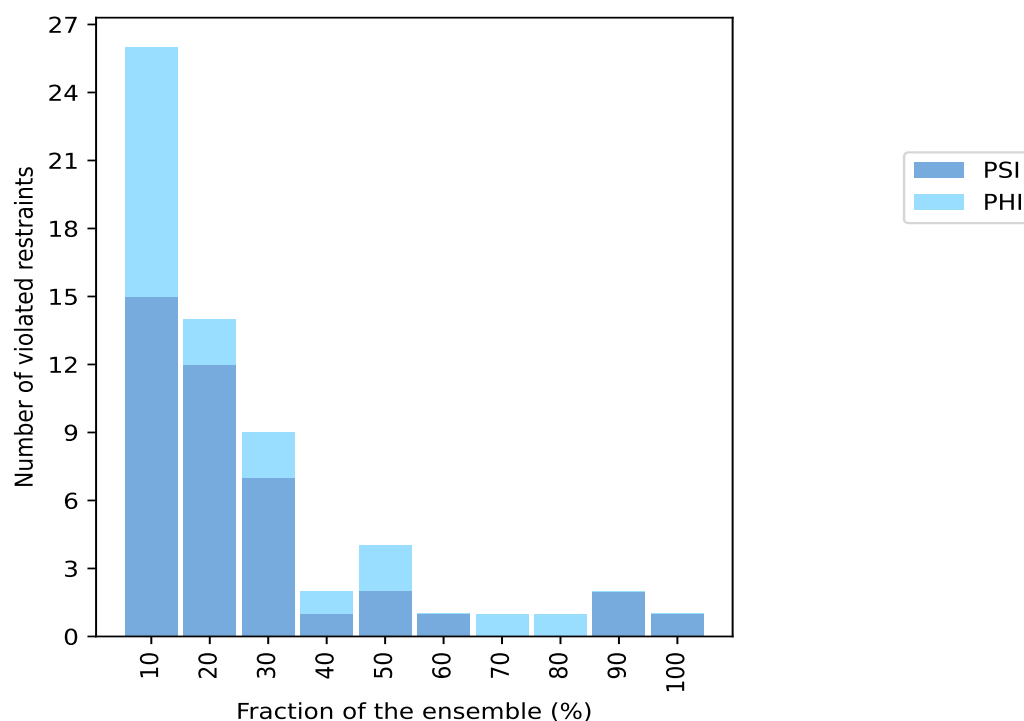
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	
PSI	PHI	Total	Count ¹	%
15	11	26	1	10.0
12	2	14	2	20.0
7	2	9	3	30.0
1	1	2	4	40.0
2	2	4	5	50.0
1	0	1	6	60.0
0	1	1	7	70.0
0	1	1	8	80.0
2	0	2	9	90.0
1	0	1	10	100.0

¹ Number of models with violations

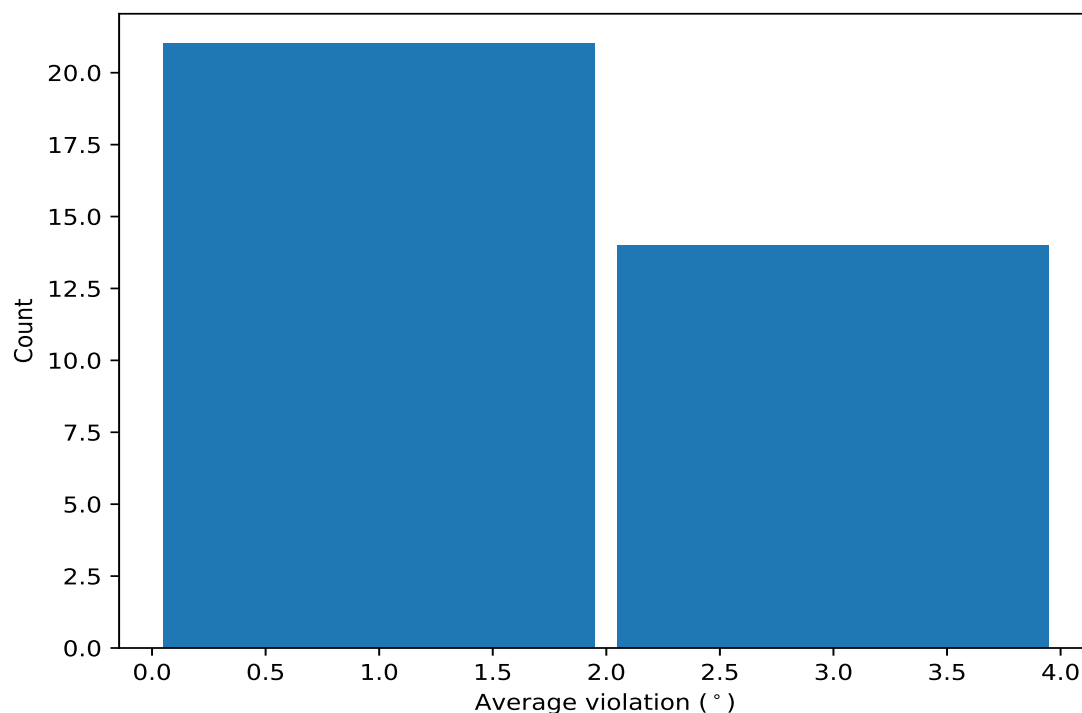
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,221)	1:139:A:GLU:N	1:139:A:GLU:CA	1:139:A:GLU:C	1:140:A:LYS:N	10	2.08	0.65	2.09
(1,219)	1:138:A:ASP:N	1:138:A:ASP:CA	1:138:A:ASP:C	1:139:A:GLU:N	9	2.93	1.1	3.37
(1,122)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:ARG:N	9	1.8	0.76	1.46
(1,147)	1:95:A:VAL:C	1:96:A:GLN:N	1:96:A:GLN:CA	1:96:A:GLN:C	8	1.62	0.73	1.29
(1,25)	1:17:A:LEU:C	1:18:A:LEU:N	1:18:A:LEU:CA	1:18:A:LEU:C	7	2.41	0.75	2.25
(1,56)	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	1:42:A:LYS:N	6	2.0	0.96	1.81
(1,35)	1:26:A:TYR:C	1:27:A:ILE:N	1:27:A:ILE:CA	1:27:A:ILE:C	5	2.62	0.76	2.14
(1,86)	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	1:60:A:LEU:N	5	2.09	0.21	2.09
(1,50)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:VAL:N	5	1.79	0.44	1.68
(1,87)	1:59:A:LYS:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	5	1.74	0.44	1.53
(1,95)	1:64:A:GLY:C	1:65:A:LYS:N	1:65:A:LYS:CA	1:65:A:LYS:C	4	2.12	0.58	2.03
(1,92)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASP:N	4	1.72	0.24	1.76
(1,58)	1:42:A:LYS:N	1:42:A:LYS:CA	1:42:A:LYS:C	1:43:A:VAL:N	3	2.25	0.44	2.42

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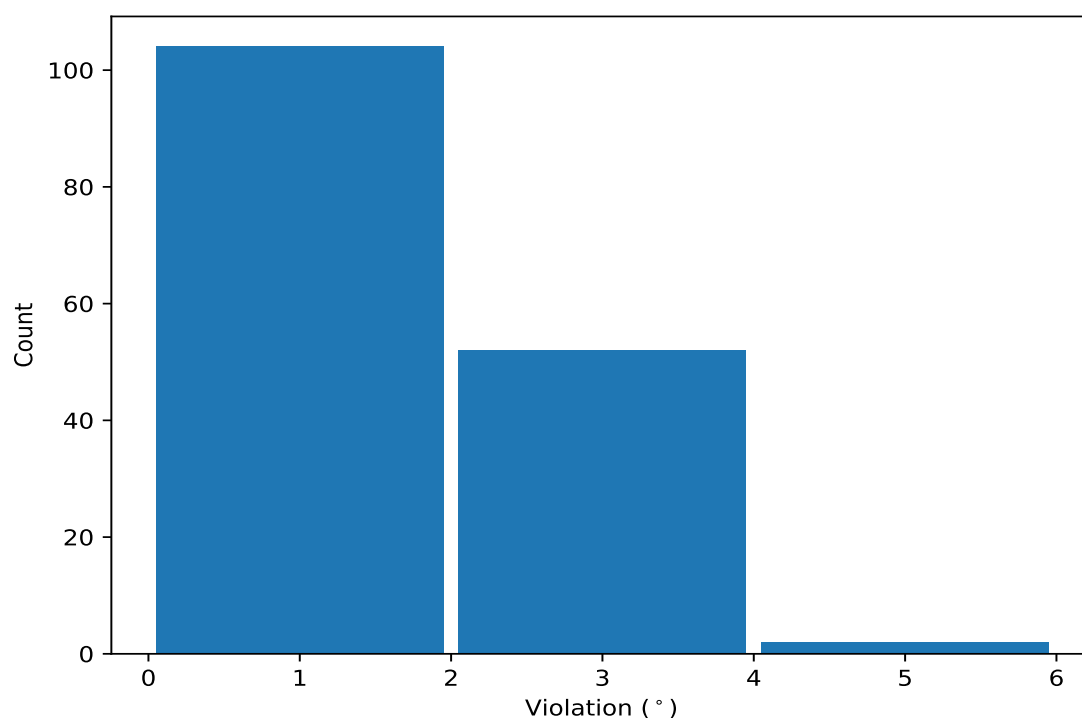
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,125)	1:81:A:GLN:N	1:81:A:GLN:CA	1:81:A:GLN:C	1:82:A:GLY:N	3	2.12	0.96	1.57
(1,97)	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	1:67:A:CYS:N	3	2.01	0.66	2.14
(1,100)	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	1:69:A:TYR:N	3	1.93	0.37	1.78
(1,68)	1:50:A:TYR:N	1:50:A:TYR:CA	1:50:A:TYR:C	1:51:A:ALA:N	3	1.55	0.62	1.17
(1,93)	1:62:A:GLU:C	1:63:A:ASP:N	1:63:A:ASP:CA	1:63:A:ASP:C	3	1.52	0.4	1.42
(1,133)	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	1:89:A:LEU:N	3	1.38	0.31	1.26
(1,179)	1:115:A:ARG:N	1:115:A:ARG:CA	1:115:A:ARG:C	1:116:A:ALA:N	3	1.35	0.14	1.35
(1,209)	1:132:A:SER:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	3	1.33	0.33	1.19
(1,163)	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	1:108:A:MET:N	2	2.81	0.54	2.81
(1,65)	1:47:A:ASN:C	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	2	2.78	0.2	2.78
(1,144)	1:93:A:ILE:C	1:94:A:PHE:N	1:94:A:PHE:CA	1:94:A:PHE:C	2	2.04	0.32	2.04
(1,240)	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	1:150:A:GLN:N	2	2.03	0.14	2.03
(1,94)	1:63:A:ASP:N	1:63:A:ASP:CA	1:63:A:ASP:C	1:64:A:GLY:N	2	1.9	0.31	1.9
(1,99)	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	1:68:A:ARG:N	2	1.88	0.74	1.88
(1,114)	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	1:76:A:VAL:N	2	1.82	0.49	1.82
(1,30)	1:24:A:HIS:N	1:24:A:HIS:CA	1:24:A:HIS:C	1:25:A:SER:N	2	1.67	0.63	1.67
(1,195)	1:124:A:GLU:N	1:124:A:GLU:CA	1:124:A:GLU:C	1:125:A:SER:N	2	1.52	0.23	1.52
(1,214)	1:135:A:SER:N	1:135:A:SER:CA	1:135:A:SER:C	1:136:A:ASP:N	2	1.44	0.22	1.44
(1,131)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:THR:N	2	1.22	0.06	1.22
(1,193)	1:123:A:LEU:N	1:123:A:LEU:CA	1:123:A:LEU:C	1:124:A:GLU:N	2	1.12	0.01	1.12
(1,120)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:GLN:N	2	1.12	0.04	1.12
(1,210)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:MET:N	2	1.06	0.01	1.06

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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 (°)
(1,219)	1:138:A:ASP:N	1:138:A:ASP:CA	1:138:A:ASP:C	1:139:A:GLU:N	2	4.66
(1,56)	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	1:42:A:LYS:N	4	4.06
(1,35)	1:26:A:TYR:C	1:27:A:ILE:N	1:27:A:ILE:CA	1:27:A:ILE:C	5	3.81
(1,90)	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	1:62:A:GLU:N	4	3.77
(1,219)	1:138:A:ASP:N	1:138:A:ASP:CA	1:138:A:ASP:C	1:139:A:GLU:N	5	3.68
(1,122)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:ARG:N	1	3.68
(1,219)	1:138:A:ASP:N	1:138:A:ASP:CA	1:138:A:ASP:C	1:139:A:GLU:N	4	3.53
(1,219)	1:138:A:ASP:N	1:138:A:ASP:CA	1:138:A:ASP:C	1:139:A:GLU:N	9	3.51
(1,125)	1:81:A:GLN:N	1:81:A:GLN:CA	1:81:A:GLN:C	1:82:A:GLY:N	9	3.47
(1,219)	1:138:A:ASP:N	1:138:A:ASP:CA	1:138:A:ASP:C	1:139:A:GLU:N	6	3.37
(1,163)	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	1:108:A:MET:N	4	3.35
(1,147)	1:95:A:VAL:C	1:96:A:GLN:N	1:96:A:GLN:CA	1:96:A:GLN:C	5	3.32
(1,25)	1:17:A:LEU:C	1:18:A:LEU:N	1:18:A:LEU:CA	1:18:A:LEU:C	9	3.32
(1,35)	1:26:A:TYR:C	1:27:A:ILE:N	1:27:A:ILE:CA	1:27:A:ILE:C	6	3.23
(1,25)	1:17:A:LEU:C	1:18:A:LEU:N	1:18:A:LEU:CA	1:18:A:LEU:C	10	3.21
(1,221)	1:139:A:GLU:N	1:139:A:GLU:CA	1:139:A:GLU:C	1:140:A:LYS:N	10	3.15
(1,221)	1:139:A:GLU:N	1:139:A:GLU:CA	1:139:A:GLU:C	1:140:A:LYS:N	7	3.03
(1,95)	1:64:A:GLY:C	1:65:A:LYS:N	1:65:A:LYS:CA	1:65:A:LYS:C	6	3.0
(1,65)	1:47:A:ASN:C	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	2	2.97
(1,39)	1:28:A:ILE:C	1:29:A:PHE:N	1:29:A:PHE:CA	1:29:A:PHE:C	4	2.95
(1,25)	1:17:A:LEU:C	1:18:A:LEU:N	1:18:A:LEU:CA	1:18:A:LEU:C	2	2.9

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,219)	1:138:A:ASP:N	1:138:A:ASP:CA	1:138:A:ASP:C	1:139:A:GLU:N	3	2.81
(1,97)	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	1:67:A:CYS:N	9	2.74
(1,58)	1:42:A:LYS:N	1:42:A:LYS:CA	1:42:A:LYS:C	1:43:A:VAL:N	8	2.68
(1,50)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:VAL:N	1	2.63
(1,99)	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	1:68:A:ARG:N	4	2.62
(1,65)	1:47:A:ASN:C	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	8	2.58
(1,219)	1:138:A:ASP:N	1:138:A:ASP:CA	1:138:A:ASP:C	1:139:A:GLU:N	1	2.51
(1,87)	1:59:A:LYS:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	8	2.5
(1,86)	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	1:60:A:LEU:N	9	2.46
(1,122)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:ARG:N	7	2.45
(1,100)	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	1:69:A:TYR:N	7	2.44
(1,68)	1:50:A:TYR:N	1:50:A:TYR:CA	1:50:A:TYR:C	1:51:A:ALA:N	8	2.43
(1,58)	1:42:A:LYS:N	1:42:A:LYS:CA	1:42:A:LYS:C	1:43:A:VAL:N	1	2.42
(1,221)	1:139:A:GLU:N	1:139:A:GLU:CA	1:139:A:GLU:C	1:140:A:LYS:N	6	2.37
(1,221)	1:139:A:GLU:N	1:139:A:GLU:CA	1:139:A:GLU:C	1:140:A:LYS:N	1	2.35
(1,144)	1:93:A:ILE:C	1:94:A:PHE:N	1:94:A:PHE:CA	1:94:A:PHE:C	7	2.35
(1,114)	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	1:76:A:VAL:N	7	2.31
(1,30)	1:24:A:HIS:N	1:24:A:HIS:CA	1:24:A:HIS:C	1:25:A:SER:N	5	2.3
(1,163)	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	1:108:A:MET:N	7	2.27
(1,221)	1:139:A:GLU:N	1:139:A:GLU:CA	1:139:A:GLU:C	1:140:A:LYS:N	8	2.25
(1,25)	1:17:A:LEU:C	1:18:A:LEU:N	1:18:A:LEU:CA	1:18:A:LEU:C	3	2.25
(1,147)	1:95:A:VAL:C	1:96:A:GLN:N	1:96:A:GLN:CA	1:96:A:GLN:C	10	2.24
(1,25)	1:17:A:LEU:C	1:18:A:LEU:N	1:18:A:LEU:CA	1:18:A:LEU:C	7	2.23
(1,95)	1:64:A:GLY:C	1:65:A:LYS:N	1:65:A:LYS:CA	1:65:A:LYS:C	8	2.22
(1,94)	1:63:A:ASP:N	1:63:A:ASP:CA	1:63:A:ASP:C	1:64:A:GLY:N	10	2.21
(1,240)	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	1:150:A:GLN:N	4	2.17
(1,86)	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	1:60:A:LEU:N	6	2.15
(1,97)	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	1:67:A:CYS:N	8	2.14
(1,35)	1:26:A:TYR:C	1:27:A:ILE:N	1:27:A:ILE:CA	1:27:A:ILE:C	3	2.14
(1,86)	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	1:60:A:LEU:N	2	2.09
(1,93)	1:62:A:GLU:C	1:63:A:ASP:N	1:63:A:ASP:CA	1:63:A:ASP:C	5	2.05
(1,29)	1:23:A:GLN:C	1:24:A:HIS:N	1:24:A:HIS:CA	1:24:A:HIS:C	3	2.03
(1,92)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASP:N	3	2.0
(1,64)	1:45:A:GLU:N	1:45:A:GLU:CA	1:45:A:GLU:C	1:46:A:LYS:N	9	1.99
(1,87)	1:59:A:LYS:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	3	1.97
(1,25)	1:17:A:LEU:C	1:18:A:LEU:N	1:18:A:LEU:CA	1:18:A:LEU:C	5	1.96
(1,35)	1:26:A:TYR:C	1:27:A:ILE:N	1:27:A:ILE:CA	1:27:A:ILE:C	4	1.95
(1,35)	1:26:A:TYR:C	1:27:A:ILE:N	1:27:A:ILE:CA	1:27:A:ILE:C	7	1.95
(1,221)	1:139:A:GLU:N	1:139:A:GLU:CA	1:139:A:GLU:C	1:140:A:LYS:N	9	1.94
(1,86)	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	1:60:A:LEU:N	10	1.92
(1,240)	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	1:150:A:GLN:N	1	1.89
(1,92)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASP:N	10	1.88
(1,56)	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	1:42:A:LYS:N	3	1.86
(1,86)	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:C	1:60:A:LEU:N	5	1.85
(1,56)	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	1:42:A:LYS:N	9	1.85
(1,95)	1:64:A:GLY:C	1:65:A:LYS:N	1:65:A:LYS:CA	1:65:A:LYS:C	5	1.83
(1,133)	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	1:89:A:LEU:N	5	1.81
(1,209)	1:132:A:SER:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	6	1.78
(1,100)	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	1:69:A:TYR:N	3	1.78
(1,56)	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	1:42:A:LYS:N	8	1.76
(1,195)	1:124:A:GLU:N	1:124:A:GLU:CA	1:124:A:GLU:C	1:125:A:SER:N	10	1.75

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,122)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:ARG:N	6	1.75
(1,221)	1:139:A:GLU:N	1:139:A:GLU:CA	1:139:A:GLU:C	1:140:A:LYS:N	4	1.72
(1,144)	1:93:A:ILE:C	1:94:A:PHE:N	1:94:A:PHE:CA	1:94:A:PHE:C	6	1.72
(1,50)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:VAL:N	7	1.71
(1,221)	1:139:A:GLU:N	1:139:A:GLU:CA	1:139:A:GLU:C	1:140:A:LYS:N	3	1.69
(1,122)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:ARG:N	3	1.68
(1,50)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:VAL:N	2	1.68
(1,214)	1:135:A:SER:N	1:135:A:SER:CA	1:135:A:SER:C	1:136:A:ASP:N	3	1.67
(1,58)	1:42:A:LYS:N	1:42:A:LYS:CA	1:42:A:LYS:C	1:43:A:VAL:N	5	1.65
(1,92)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASP:N	5	1.63
(1,94)	1:63:A:ASP:N	1:63:A:ASP:CA	1:63:A:ASP:C	1:64:A:GLY:N	1	1.59
(1,125)	1:81:A:GLN:N	1:81:A:GLN:CA	1:81:A:GLN:C	1:82:A:GLY:N	1	1.57
(1,100)	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	1:69:A:TYR:N	10	1.56
(1,147)	1:95:A:VAL:C	1:96:A:GLN:N	1:96:A:GLN:CA	1:96:A:GLN:C	1	1.54
(1,181)	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	1:117:A:LEU:N	8	1.53
(1,87)	1:59:A:LYS:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	4	1.53
(1,189)	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	1:121:A:LEU:N	3	1.52
(1,179)	1:115:A:ARG:N	1:115:A:ARG:CA	1:115:A:ARG:C	1:116:A:ALA:N	10	1.52
(1,135)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:90:A:ASN:N	2	1.52
(1,22)	1:16:A:ASP:N	1:16:A:ASP:CA	1:16:A:ASP:C	1:17:A:LEU:N	5	1.51
(1,103)	1:69:A:TYR:C	1:70:A:ALA:N	1:70:A:ALA:CA	1:70:A:ALA:C	2	1.47
(1,50)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:VAL:N	5	1.47
(1,17)	1:13:A:ASN:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	10	1.47
(1,122)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:ARG:N	10	1.46
(1,50)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:VAL:N	6	1.44
(1,95)	1:64:A:GLY:C	1:65:A:LYS:N	1:65:A:LYS:CA	1:65:A:LYS:C	10	1.43
(1,4)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:VAL:N	10	1.43
(1,93)	1:62:A:GLU:C	1:63:A:ASP:N	1:63:A:ASP:CA	1:63:A:ASP:C	3	1.42
(1,92)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASP:N	1	1.39
(1,147)	1:95:A:VAL:C	1:96:A:GLN:N	1:96:A:GLN:CA	1:96:A:GLN:C	9	1.37
(1,122)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:ARG:N	8	1.37
(1,87)	1:59:A:LYS:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	1	1.36
(1,41)	1:29:A:PHE:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	3	1.36
(1,201)	1:128:A:GLN:N	1:128:A:GLN:CA	1:128:A:GLN:C	1:129:A:VAL:N	6	1.35
(1,179)	1:115:A:ARG:N	1:115:A:ARG:CA	1:115:A:ARG:C	1:116:A:ALA:N	8	1.35
(1,56)	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	1:42:A:LYS:N	7	1.35
(1,186)	1:118:A:LYS:C	1:119:A:ALA:N	1:119:A:ALA:CA	1:119:A:ALA:C	1	1.34
(1,122)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:ARG:N	4	1.34
(1,125)	1:81:A:GLN:N	1:81:A:GLN:CA	1:81:A:GLN:C	1:82:A:GLY:N	10	1.33
(1,114)	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	1:76:A:VAL:N	8	1.33
(1,104)	1:70:A:ALA:N	1:70:A:ALA:CA	1:70:A:ALA:C	1:71:A:ALA:N	2	1.33
(1,87)	1:59:A:LYS:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	10	1.33
(1,111)	1:73:A:ASP:C	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	8	1.31
(1,195)	1:124:A:GLU:N	1:124:A:GLU:CA	1:124:A:GLU:C	1:125:A:SER:N	2	1.29
(1,32)	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	1:26:A:TYR:N	10	1.29
(1,131)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:THR:N	1	1.28
(1,133)	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	1:89:A:LEU:N	9	1.26
(1,122)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:ARG:N	9	1.25
(1,221)	1:139:A:GLU:N	1:139:A:GLU:CA	1:139:A:GLU:C	1:140:A:LYS:N	5	1.22
(1,214)	1:135:A:SER:N	1:135:A:SER:CA	1:135:A:SER:C	1:136:A:ASP:N	5	1.22
(1,148)	1:96:A:GLN:N	1:96:A:GLN:CA	1:96:A:GLN:C	1:97:A:TYR:N	8	1.22

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,147)	1:95:A:VAL:C	1:96:A:GLN:N	1:96:A:GLN:CA	1:96:A:GLN:C	8	1.21
(1,122)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:ARG:N	5	1.21
(1,219)	1:138:A:ASP:N	1:138:A:ASP:CA	1:138:A:ASP:C	1:139:A:GLU:N	10	1.2
(1,153)	1:101:A:ASN:N	1:101:A:ASN:CA	1:101:A:ASN:C	1:102:A:ALA:N	7	1.2
(1,209)	1:132:A:SER:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	4	1.19
(1,89)	1:60:A:LEU:C	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	1	1.18
(1,179)	1:115:A:ARG:N	1:115:A:ARG:CA	1:115:A:ARG:C	1:116:A:ALA:N	4	1.17
(1,68)	1:50:A:TYR:N	1:50:A:TYR:CA	1:50:A:TYR:C	1:51:A:ALA:N	10	1.17
(1,131)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:THR:N	3	1.16
(1,120)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:GLN:N	3	1.16
(1,224)	1:141:A:SER:N	1:141:A:SER:CA	1:141:A:SER:C	1:142:A:VAL:N	3	1.14
(1,215)	1:135:A:SER:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	1	1.14
(1,99)	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	1:68:A:ARG:N	5	1.14
(1,97)	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	1:67:A:CYS:N	2	1.14
(1,219)	1:138:A:ASP:N	1:138:A:ASP:CA	1:138:A:ASP:C	1:139:A:GLU:N	8	1.13
(1,193)	1:123:A:LEU:N	1:123:A:LEU:CA	1:123:A:LEU:C	1:124:A:GLU:N	2	1.13
(1,193)	1:123:A:LEU:N	1:123:A:LEU:CA	1:123:A:LEU:C	1:124:A:GLU:N	7	1.11
(1,147)	1:95:A:VAL:C	1:96:A:GLN:N	1:96:A:GLN:CA	1:96:A:GLN:C	4	1.11
(1,147)	1:95:A:VAL:C	1:96:A:GLN:N	1:96:A:GLN:CA	1:96:A:GLN:C	7	1.11
(1,139)	1:91:A:LYS:N	1:91:A:LYS:CA	1:91:A:LYS:C	1:92:A:VAL:N	1	1.11
(1,56)	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	1:42:A:LYS:N	2	1.11
(1,221)	1:139:A:GLU:N	1:139:A:GLU:CA	1:139:A:GLU:C	1:140:A:LYS:N	2	1.09
(1,147)	1:95:A:VAL:C	1:96:A:GLN:N	1:96:A:GLN:CA	1:96:A:GLN:C	2	1.09
(1,93)	1:62:A:GLU:C	1:63:A:ASP:N	1:63:A:ASP:CA	1:63:A:ASP:C	1	1.09
(1,133)	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	1:89:A:LEU:N	8	1.08
(1,81)	1:56:A:GLU:C	1:57:A:MET:N	1:57:A:MET:CA	1:57:A:MET:C	10	1.08
(1,120)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:GLN:N	10	1.07
(1,210)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:MET:N	6	1.06
(1,183)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:LYS:N	1	1.06
(1,68)	1:50:A:TYR:N	1:50:A:TYR:CA	1:50:A:TYR:C	1:51:A:ALA:N	3	1.06
(1,210)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:MET:N	9	1.05
(1,30)	1:24:A:HIS:N	1:24:A:HIS:CA	1:24:A:HIS:C	1:25:A:SER:N	2	1.04
(1,217)	1:136:A:ASP:C	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	9	1.02
(1,209)	1:132:A:SER:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	10	1.02
(1,25)	1:17:A:LEU:C	1:18:A:LEU:N	1:18:A:LEU:CA	1:18:A:LEU:C	1	1.02