



Full wwPDB NMR Structure Validation Report ⓘ

Feb 28, 2026 – 06:00 PM UTC

PDB ID : 2M5B / pdb_00002m5b
BMRB ID : 19045
Title : The NMR structure of the BID-BAK complex
Authors : Moldoveanu, T.; Grace, C.R.; Kriwacki, R.W.; Green, D.R.
Deposited on : 2013-02-19

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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

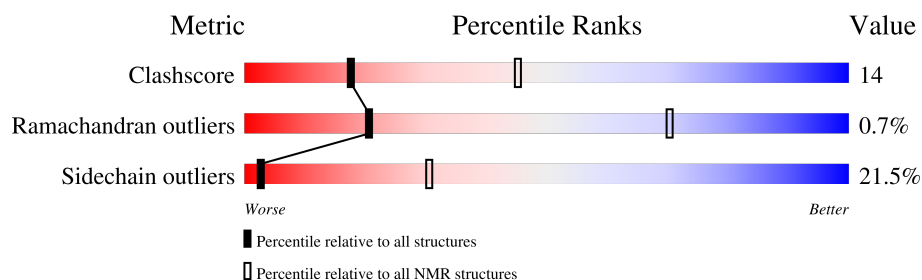
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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	169	
2	B	23	

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:22-A:45, A:66-A:184, B:81-B:91, B:93-B:95, B:98-B:101 (161)	0.62	13

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2783 atoms, of which 1268 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	Atoms						Trace
1	A	169	Total	C	H	N	O	S	0
			2440	850	1103	234	248	5	

- Molecule 2 is a protein called human_BID_BH3_SAHB.

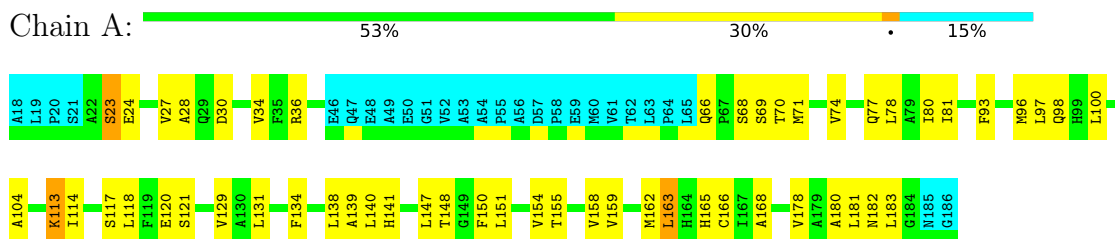
Mol	Chain	Residues	Atoms					Trace
2	B	23	Total	C	H	N	O	1
			343	111	165	35	32	

4 Residue-property plots

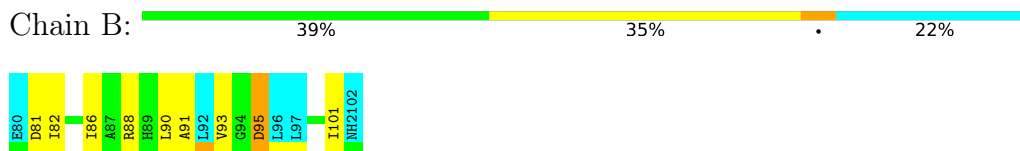
4.1 Average score per residue in the NMR ensemble

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: Bcl-2 homologous antagonist/killer



- Molecule 2: human_BID_BH3_SAHB

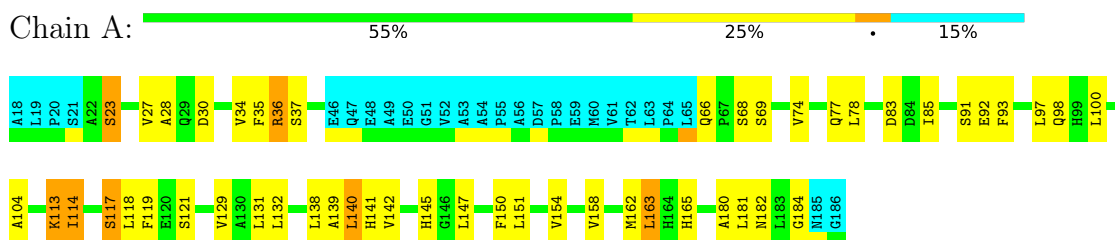


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Bcl-2 homologous antagonist/killer

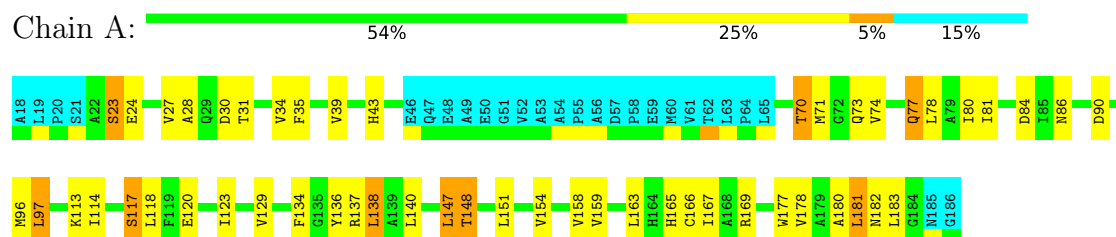


- Molecule 2: human_BID_BH3_SAHB



4.2.2 Score per residue for model 2

- Molecule 1: Bcl-2 homologous antagonist/killer

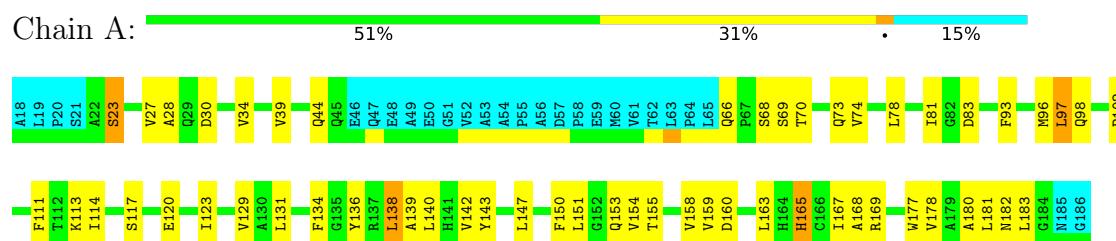


- Molecule 2: human_BID_BH3_SAHB



4.2.3 Score per residue for model 3

- Molecule 1: Bcl-2 homologous antagonist/killer

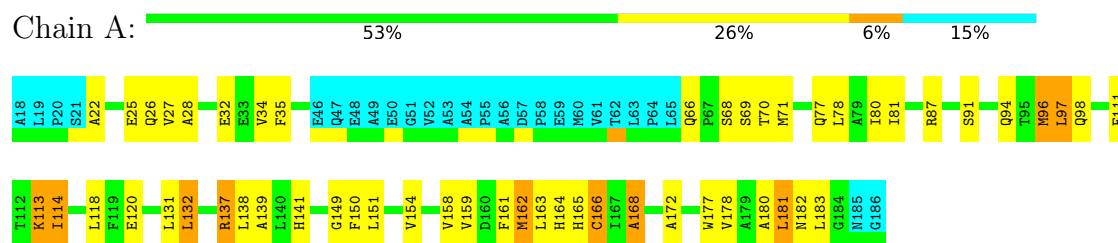


- Molecule 2: human_BID_BH3_SAHB

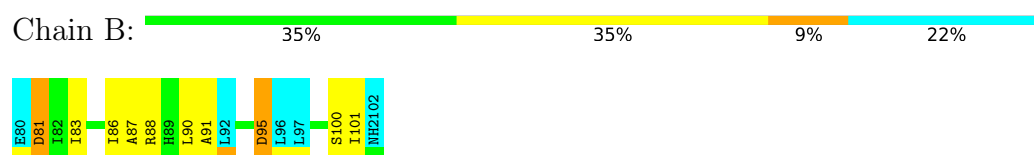


4.2.4 Score per residue for model 4

- Molecule 1: Bcl-2 homologous antagonist/killer

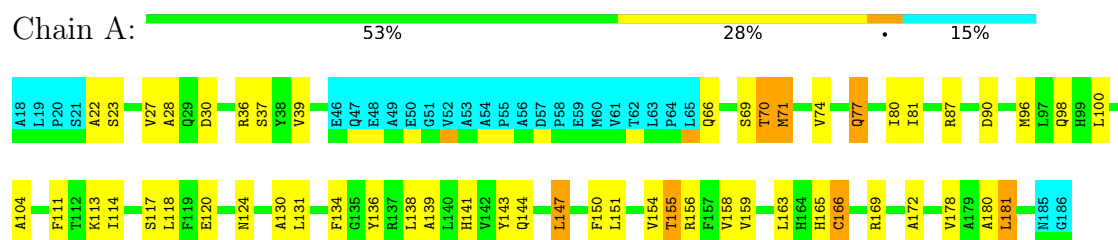


- Molecule 2: human_BID_BH3_SAHB

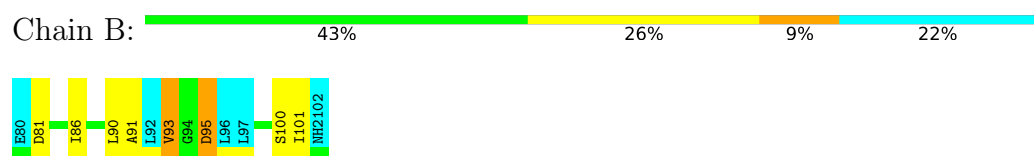


4.2.5 Score per residue for model 5

- Molecule 1: Bcl-2 homologous antagonist/killer

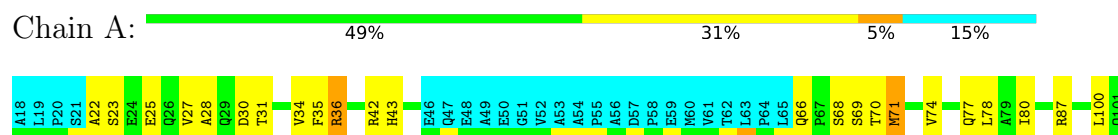


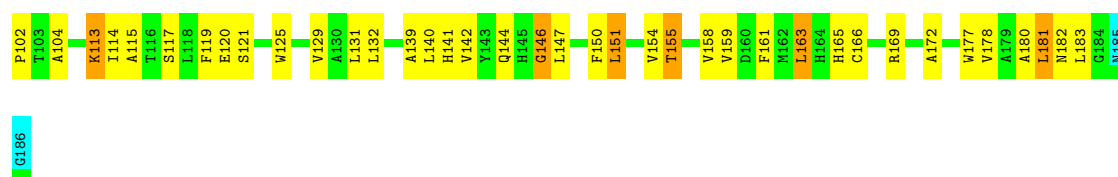
- Molecule 2: human_BID_BH3_SAHB



4.2.6 Score per residue for model 6

- Molecule 1: Bcl-2 homologous antagonist/killer



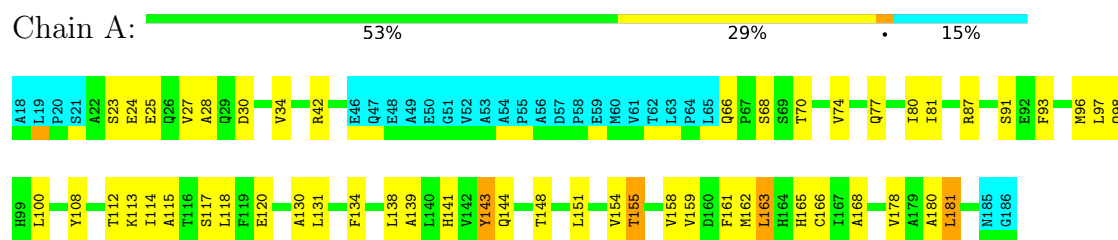


- Molecule 2: human_BID_BH3_SAHB



4.2.7 Score per residue for model 7

- Molecule 1: Bcl-2 homologous antagonist/killer

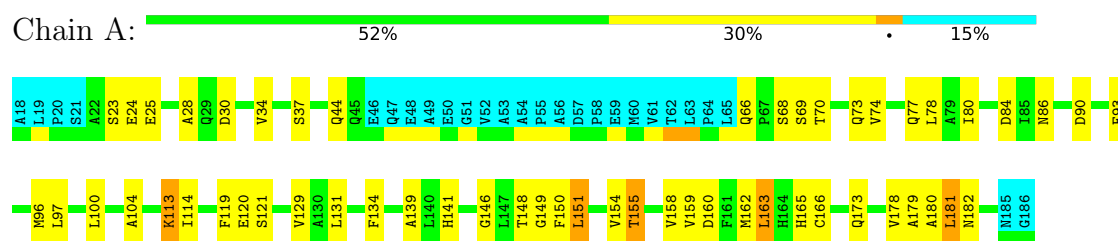


- Molecule 2: human_BID_BH3_SAHB



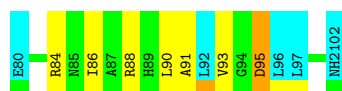
4.2.8 Score per residue for model 8

- Molecule 1: Bcl-2 homologous antagonist/killer



- Molecule 2: human_BID_BH3_SAHB

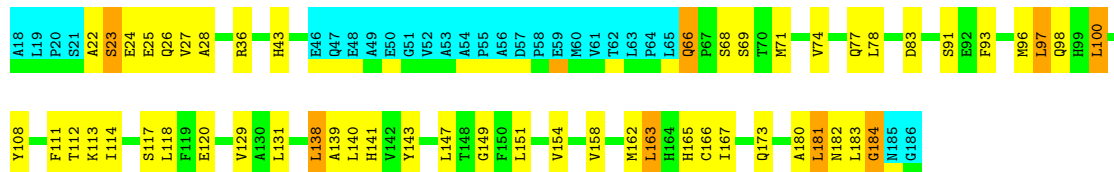




4.2.9 Score per residue for model 9

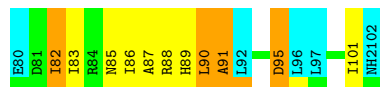
- Molecule 1: Bcl-2 homologous antagonist/killer

Chain A: 53% 27% 5% 15%



- Molecule 2: human_BID_BH3_SAHB

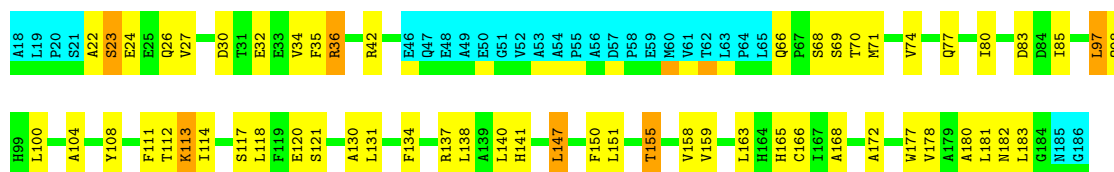
Chain B: 30% 30% 17% 22%



4.2.10 Score per residue for model 10

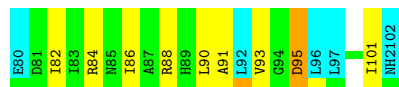
- Molecule 1: Bcl-2 homologous antagonist/killer

Chain A: 50% 31% 15% 4%



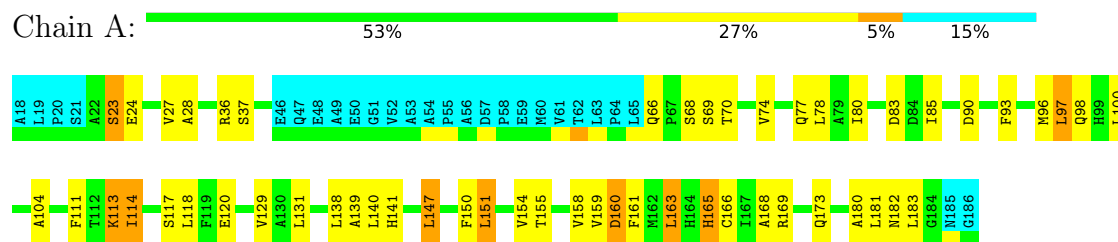
- Molecule 2: human_BID_BH3_SAHB

Chain B: 39% 35% 22% 4%

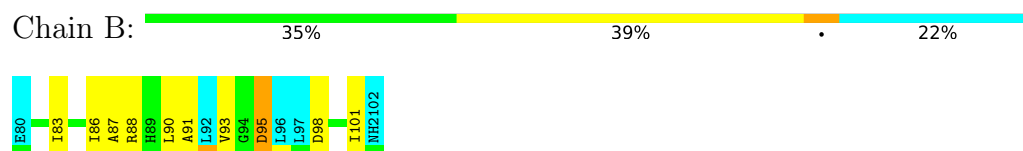


4.2.11 Score per residue for model 11

- Molecule 1: Bcl-2 homologous antagonist/killer

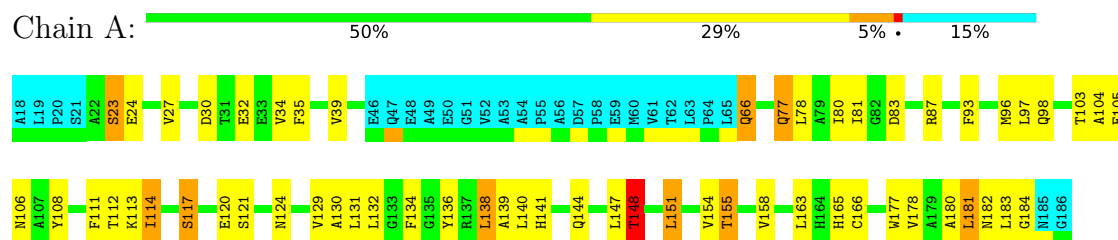


- Molecule 2: human_BID_BH3_SAHB

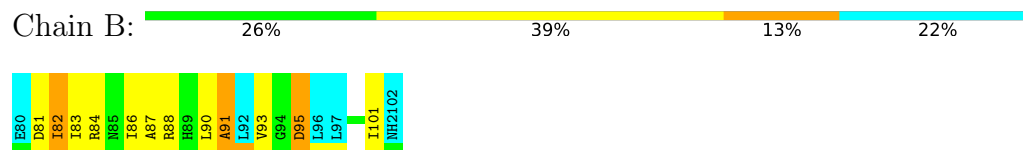


4.2.12 Score per residue for model 12

- Molecule 1: Bcl-2 homologous antagonist/killer

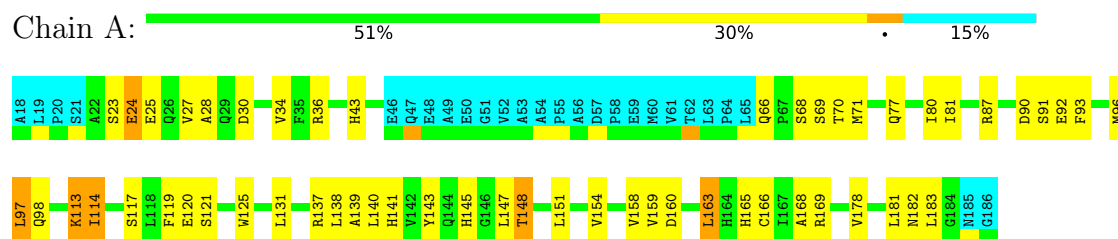


- Molecule 2: human_BID_BH3_SAHB

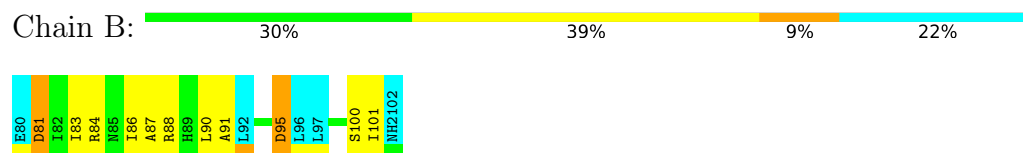


4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Bcl-2 homologous antagonist/killer

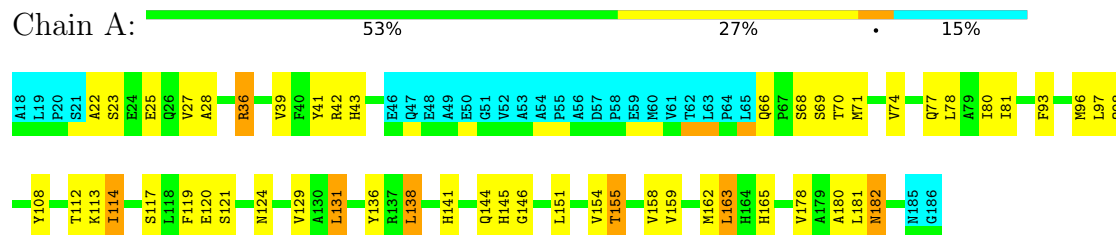


- Molecule 2: human_BID_BH3_SAHB



4.2.14 Score per residue for model 14

- Molecule 1: Bcl-2 homologous antagonist/killer

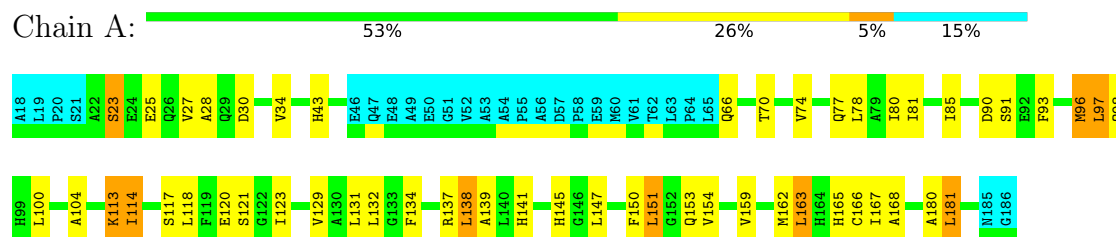


- Molecule 2: human_BID_BH3_SAHB



4.2.15 Score per residue for model 15

- Molecule 1: Bcl-2 homologous antagonist/killer

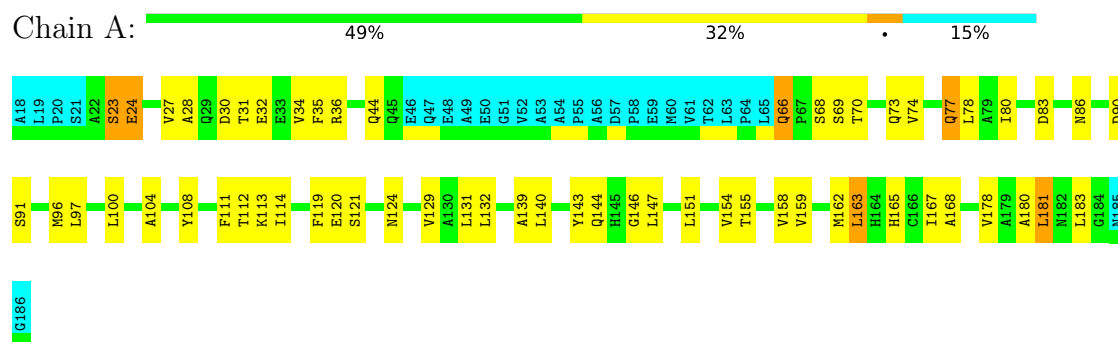


- Molecule 2: human_BID_BH3_SAHB

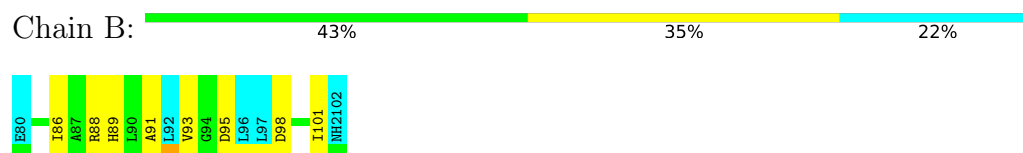


4.2.16 Score per residue for model 16

- Molecule 1: Bcl-2 homologous antagonist/killer

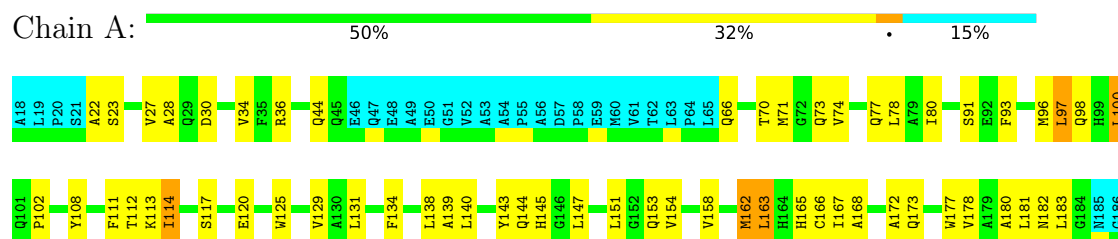


- Molecule 2: human_BID_BH3_SAHB



4.2.17 Score per residue for model 17

- Molecule 1: Bcl-2 homologous antagonist/killer



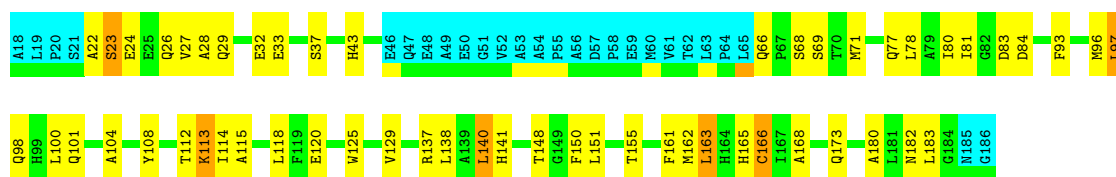
- Molecule 2: human_BID_BH3_SAHB



4.2.18 Score per residue for model 18

- Molecule 1: Bcl-2 homologous antagonist/killer





- Molecule 2: human_BID_BH3_SAHB



4.2.19 Score per residue for model 19

- Molecule 1: Bcl-2 homologous antagonist/killer



- Molecule 2: human_BID_BH3_SAHB



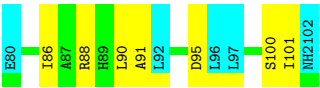
4.2.20 Score per residue for model 20

- Molecule 1: Bcl-2 homologous antagonist/killer



- Molecule 2: human_BID_BH3_SAHB





5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, simulated annealing, molecular dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
TopSpin	structure solution	
TopSpin	structure solution	
TopSpin	structure solution	
CYANA	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	2098
Number of shifts mapped to atoms	1898
Number of unparsed shifts	0
Number of shifts with mapping errors	200
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MK8, NLE, NH2

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
2	B	0.0±0.0	2.0±0.0
All	All	0	40

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
2	B	91	ALA	Peptide	20
2	B	95	ASP	Peptide	20

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	1156	960	1110	34±5
2	B	142	126	146	9±3
All	All	25960	21720	25120	690

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:ILE:HD12	2:B:86:ILE:HG21	0.98	1.33	6	10
1:A:70:THR:HG21	1:A:178:VAL:HG13	0.95	1.35	17	8
1:A:183:LEU:HD22	2:B:101:ILE:HD12	0.94	1.32	2	8
1:A:104:ALA:HB2	1:A:147:LEU:HD13	0.94	1.39	6	1
1:A:97:LEU:HD11	1:A:138:LEU:HD12	0.85	1.44	3	3
1:A:78:LEU:HD21	1:A:180:ALA:HB1	0.83	1.48	14	9
1:A:97:LEU:HD21	1:A:138:LEU:HD12	0.82	1.49	2	2
1:A:100:LEU:HD22	2:B:86:ILE:HD11	0.81	1.51	19	3
1:A:114:ILE:HD12	2:B:86:ILE:HD13	0.80	1.53	18	12
1:A:74:VAL:HG13	1:A:180:ALA:HB3	0.80	1.53	7	12
1:A:28:ALA:HB2	1:A:163:LEU:HD13	0.74	1.60	6	7
1:A:100:LEU:HD12	2:B:86:ILE:HD11	0.73	1.59	7	1
1:A:114:ILE:HD12	2:B:86:ILE:HD12	0.72	1.61	1	1
1:A:74:VAL:HG22	1:A:181:LEU:HD12	0.72	1.61	5	1
1:A:39:VAL:HG21	1:A:136:TYR:CG	0.72	2.20	12	6
2:B:87:ALA:HA	2:B:90:LEU:HD22	0.71	1.63	9	1
1:A:104:ALA:HB2	1:A:147:LEU:HD11	0.71	1.61	1	2
1:A:178:VAL:O	1:A:181:LEU:HD22	0.70	1.85	6	8
1:A:28:ALA:HB2	1:A:163:LEU:HD21	0.69	1.63	3	5
1:A:96:MET:HE3	2:B:86:ILE:HG13	0.69	1.63	17	1
1:A:183:LEU:HD22	2:B:101:ILE:HG22	0.68	1.65	6	2
1:A:96:MET:HE2	1:A:97:LEU:HD22	0.68	1.63	13	1
1:A:35:PHE:CE2	1:A:158:VAL:HG21	0.67	2.24	20	3
1:A:114:ILE:CD1	2:B:86:ILE:HD13	0.67	2.19	14	13
1:A:111:PHE:CZ	1:A:158:VAL:HG22	0.66	2.26	16	8
1:A:28:ALA:CB	1:A:163:LEU:HD21	0.66	2.21	3	1
1:A:96:MET:HE1	2:B:86:ILE:HB	0.65	1.69	13	6
1:A:114:ILE:HD12	2:B:86:ILE:CG2	0.65	2.21	19	7
1:A:39:VAL:HG21	1:A:136:TYR:CD2	0.65	2.26	2	3
1:A:181:LEU:HD23	1:A:182:ASN:N	0.65	2.05	6	7
2:B:82:ILE:HD13	2:B:82:ILE:O	0.65	1.92	9	1
1:A:28:ALA:HB2	1:A:163:LEU:HD11	0.64	1.69	18	4
1:A:154:VAL:O	1:A:158:VAL:HG23	0.64	1.92	13	11
2:B:90:LEU:C	2:B:90:LEU:HD23	0.64	2.17	9	1
1:A:93:PHE:CZ	2:B:90:LEU:HD21	0.64	2.27	17	5
1:A:100:LEU:HA	2:B:82:ILE:HD12	0.64	1.69	17	1
1:A:78:LEU:HD22	1:A:129:VAL:HG22	0.64	1.69	2	5
1:A:111:PHE:CZ	1:A:158:VAL:HG12	0.64	2.26	10	1
1:A:131:LEU:HD21	1:A:158:VAL:HG13	0.64	1.70	12	1
1:A:28:ALA:HB2	1:A:163:LEU:CD2	0.64	2.23	11	3
1:A:23:SER:O	1:A:27:VAL:HG23	0.63	1.93	6	15
2:B:82:ILE:HG23	2:B:83:ILE:HD12	0.63	1.68	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:GLN:OE1	1:A:81:ILE:HG23	0.63	1.94	4	1
1:A:74:VAL:HG13	1:A:180:ALA:CB	0.63	2.24	1	8
1:A:139:ALA:CB	1:A:154:VAL:HG21	0.63	2.22	1	13
1:A:70:THR:O	1:A:74:VAL:HG23	0.63	1.93	11	6
1:A:78:LEU:HD22	1:A:129:VAL:CG2	0.63	2.23	15	3
1:A:147:LEU:HD23	1:A:150:PHE:CD1	0.63	2.29	19	1
1:A:139:ALA:HB1	1:A:154:VAL:HG21	0.62	1.70	13	9
1:A:104:ALA:CB	1:A:147:LEU:HD21	0.62	2.24	11	2
1:A:118:LEU:HD13	2:B:90:LEU:HB3	0.62	1.71	18	9
1:A:34:VAL:HG11	1:A:177:TRP:CE3	0.62	2.29	6	8
1:A:181:LEU:HD13	1:A:181:LEU:H	0.62	1.55	8	5
1:A:181:LEU:HD12	1:A:182:ASN:N	0.61	2.10	11	5
1:A:28:ALA:HB2	1:A:163:LEU:CD1	0.61	2.25	17	9
1:A:183:LEU:CD2	2:B:101:ILE:HD12	0.61	2.24	3	2
1:A:77:GLN:HA	1:A:80:ILE:HD12	0.61	1.73	4	17
1:A:97:LEU:HD12	1:A:138:LEU:HD23	0.61	1.71	15	1
1:A:97:LEU:CD1	1:A:138:LEU:HD13	0.59	2.27	17	2
1:A:113:LYS:HD3	1:A:114:ILE:HD13	0.59	1.72	6	17
1:A:97:LEU:CD1	1:A:138:LEU:HD12	0.59	2.26	12	2
1:A:119:PHE:CE1	1:A:131:LEU:HD12	0.59	2.33	1	5
1:A:93:PHE:CD1	1:A:96:MET:HE2	0.59	2.32	17	1
1:A:30:ASP:OD2	1:A:71:MET:HE2	0.59	1.97	2	3
1:A:97:LEU:HD13	1:A:137:ARG:NH1	0.59	2.13	4	1
2:B:82:ILE:HG22	2:B:83:ILE:HD12	0.59	1.73	9	1
1:A:39:VAL:HG21	1:A:136:TYR:CD1	0.59	2.32	14	2
1:A:78:LEU:CD2	1:A:180:ALA:HB1	0.59	2.27	14	1
1:A:70:THR:HG23	1:A:181:LEU:HD23	0.58	1.75	11	1
1:A:74:VAL:HG13	1:A:180:ALA:HB2	0.58	1.74	9	2
1:A:27:VAL:CG2	1:A:172:ALA:HB2	0.58	2.29	4	2
1:A:104:ALA:HB2	1:A:147:LEU:HD21	0.58	1.75	11	4
1:A:113:LYS:HE2	2:B:87:ALA:HB2	0.58	1.75	12	4
1:A:22:ALA:O	1:A:172:ALA:HB1	0.58	1.98	6	2
1:A:96:MET:HE2	1:A:97:LEU:CD2	0.58	2.28	13	1
1:A:24:GLU:HG3	1:A:163:LEU:HD22	0.58	1.74	10	1
1:A:183:LEU:HB3	2:B:101:ILE:HG23	0.57	1.74	16	2
1:A:28:ALA:CB	1:A:163:LEU:HD11	0.57	2.29	5	2
1:A:27:VAL:HG11	1:A:168:ALA:HA	0.57	1.75	17	11
1:A:96:MET:HE1	2:B:86:ILE:CA	0.57	2.29	20	7
1:A:81:ILE:CG2	2:B:101:ILE:HG22	0.57	2.30	19	11
1:A:93:PHE:CE1	2:B:90:LEU:HD21	0.57	2.34	8	1
1:A:146:GLY:O	1:A:147:LEU:HD23	0.57	2.00	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:LEU:HD22	2:B:101:ILE:CG2	0.57	2.29	16	3
1:A:113:LYS:HD2	1:A:114:ILE:HD13	0.56	1.77	1	1
1:A:78:LEU:HD22	1:A:129:VAL:CG1	0.56	2.29	6	7
1:A:70:THR:HG23	1:A:73:GLN:OE1	0.56	1.99	16	4
2:B:82:ILE:CG2	2:B:83:ILE:HD12	0.56	2.31	2	4
1:A:32:GLU:HA	1:A:155:THR:HG22	0.56	1.78	12	2
1:A:96:MET:HE1	2:B:86:ILE:CB	0.56	2.30	12	5
1:A:150:PHE:O	1:A:154:VAL:HG23	0.56	2.01	4	4
1:A:93:PHE:O	1:A:97:LEU:HD12	0.56	2.01	9	3
1:A:114:ILE:HG21	1:A:134:PHE:CE1	0.56	2.36	7	6
1:A:39:VAL:HG11	1:A:136:TYR:CD2	0.56	2.36	3	2
1:A:74:VAL:HG22	1:A:181:LEU:CD1	0.56	2.29	5	1
1:A:104:ALA:HB1	1:A:150:PHE:CE1	0.55	2.37	18	5
1:A:102:PRO:O	1:A:142:VAL:HG12	0.55	2.01	6	1
1:A:22:ALA:HB1	1:A:26:GLN:CG	0.55	2.31	9	3
1:A:139:ALA:HB2	1:A:154:VAL:HG21	0.55	1.76	1	4
1:A:138:LEU:HD13	1:A:139:ALA:N	0.55	2.17	15	1
1:A:35:PHE:HA	1:A:132:LEU:HD13	0.54	1.79	16	2
1:A:117:SER:OG	2:B:87:ALA:HB1	0.54	2.02	1	3
1:A:93:PHE:CZ	2:B:90:LEU:HD11	0.54	2.37	8	1
1:A:32:GLU:HB3	1:A:159:VAL:HG21	0.54	1.78	4	2
1:A:104:ALA:HB2	1:A:147:LEU:CD1	0.54	2.33	20	2
1:A:155:THR:O	1:A:159:VAL:HG23	0.53	2.03	8	8
1:A:113:LYS:CE	2:B:87:ALA:HB2	0.53	2.34	12	1
1:A:93:PHE:CD1	2:B:90:LEU:HD21	0.53	2.39	8	1
1:A:147:LEU:HD13	1:A:150:PHE:CG	0.53	2.39	11	1
1:A:31:THR:HG21	1:A:159:VAL:HA	0.52	1.80	2	3
1:A:97:LEU:CD1	1:A:138:LEU:HD23	0.52	2.33	15	1
1:A:159:VAL:O	1:A:163:LEU:HD23	0.52	2.03	3	1
2:B:98:ASP:HA	2:B:101:ILE:HD12	0.52	1.81	16	2
1:A:138:LEU:O	1:A:142:VAL:HG23	0.52	2.04	20	1
1:A:34:VAL:HG11	1:A:177:TRP:CZ3	0.52	2.40	20	2
1:A:22:ALA:HB1	1:A:26:GLN:HG2	0.52	1.81	10	3
1:A:147:LEU:O	1:A:148:THR:HG22	0.52	2.04	2	1
1:A:103:THR:HG23	1:A:106:ASN:H	0.52	1.63	12	1
1:A:125:TRP:CD2	1:A:183:LEU:HD11	0.52	2.39	13	2
1:A:93:PHE:O	1:A:97:LEU:HD23	0.52	2.05	7	6
1:A:100:LEU:HG	2:B:82:ILE:HD12	0.52	1.82	9	2
1:A:36:ARG:HG3	1:A:155:THR:HG21	0.51	1.82	6	1
1:A:96:MET:HE1	2:B:86:ILE:HA	0.51	1.81	7	6
1:A:143:TYR:HA	1:A:147:LEU:HD13	0.51	1.83	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ALA:HB1	1:A:159:VAL:CG1	0.51	2.36	14	4
1:A:97:LEU:HD21	1:A:138:LEU:HD13	0.51	1.82	4	1
1:A:114:ILE:CG2	2:B:90:LEU:HD11	0.51	2.35	13	8
1:A:102:PRO:HG3	1:A:138:LEU:HD11	0.51	1.81	17	1
1:A:104:ALA:HB2	1:A:147:LEU:CD2	0.51	2.36	12	1
1:A:114:ILE:CD1	2:B:86:ILE:HG21	0.50	2.28	19	3
1:A:143:TYR:HA	1:A:147:LEU:HD12	0.50	1.83	17	3
2:B:87:ALA:HA	2:B:90:LEU:HD12	0.49	1.85	18	3
1:A:100:LEU:HA	2:B:82:ILE:HD13	0.49	1.82	15	1
1:A:114:ILE:HD13	1:A:114:ILE:N	0.49	2.22	1	17
1:A:123:ILE:HD13	1:A:167:ILE:HD13	0.49	1.83	2	3
1:A:118:LEU:HD13	2:B:90:LEU:CB	0.48	2.38	1	1
1:A:39:VAL:HG23	1:A:43:HIS:CE1	0.48	2.43	2	1
1:A:115:ALA:HB1	1:A:161:PHE:CE1	0.48	2.43	6	2
1:A:74:VAL:CG1	1:A:180:ALA:HB3	0.48	2.37	10	1
1:A:119:PHE:CZ	1:A:131:LEU:HD12	0.48	2.43	1	5
1:A:130:ALA:CB	2:B:93:VAL:HG22	0.48	2.38	19	3
1:A:27:VAL:HG11	1:A:168:ALA:CA	0.48	2.39	10	1
1:A:138:LEU:HD13	1:A:138:LEU:C	0.48	2.33	15	1
1:A:147:LEU:HD13	1:A:150:PHE:CD1	0.48	2.44	11	1
1:A:35:PHE:HD2	1:A:132:LEU:HD22	0.48	1.68	4	3
1:A:130:ALA:CB	2:B:93:VAL:HG12	0.48	2.39	5	1
1:A:102:PRO:HG2	1:A:142:VAL:HG11	0.47	1.86	3	1
1:A:96:MET:HE2	1:A:97:LEU:HG	0.47	1.85	18	1
2:B:87:ALA:CA	2:B:90:LEU:HD22	0.47	2.37	9	1
1:A:24:GLU:CD	1:A:163:LEU:HD13	0.47	2.35	9	1
1:A:97:LEU:CD2	1:A:138:LEU:HD12	0.47	2.40	9	1
1:A:114:ILE:HG23	2:B:90:LEU:HD11	0.47	1.85	19	4
1:A:143:TYR:C	1:A:143:TYR:CD1	0.47	2.92	7	1
1:A:24:GLU:O	1:A:163:LEU:HD11	0.47	2.10	13	1
1:A:143:TYR:CA	1:A:147:LEU:HD22	0.47	2.40	5	1
1:A:97:LEU:HD11	1:A:138:LEU:HD13	0.47	1.85	10	1
1:A:28:ALA:HB2	1:A:163:LEU:HD23	0.47	1.86	11	1
1:A:96:MET:HE3	2:B:86:ILE:CG1	0.47	2.39	17	1
1:A:147:LEU:HD22	1:A:150:PHE:CD1	0.46	2.45	1	1
1:A:125:TRP:CH2	1:A:180:ALA:HB2	0.46	2.45	17	1
1:A:93:PHE:CD2	1:A:96:MET:HE2	0.46	2.45	15	1
1:A:114:ILE:HG23	2:B:86:ILE:CD1	0.46	2.39	1	1
1:A:29:GLN:O	1:A:32:GLU:CG	0.46	2.64	18	1
1:A:160:ASP:CG	1:A:161:PHE:N	0.46	2.73	20	2
1:A:86:ASN:O	1:A:90:ASP:N	0.45	2.50	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:181:LEU:CD2	1:A:181:LEU:C	0.45	2.89	7	5
1:A:114:ILE:HG22	2:B:90:LEU:HD11	0.45	1.88	1	1
1:A:30:ASP:O	1:A:34:VAL:HG23	0.45	2.11	16	11
1:A:93:PHE:CE2	1:A:97:LEU:HD11	0.45	2.47	11	1
1:A:131:LEU:HD12	1:A:134:PHE:HE2	0.45	1.72	3	8
1:A:130:ALA:HB1	2:B:93:VAL:HG12	0.45	1.88	5	1
1:A:140:LEU:HD23	1:A:140:LEU:O	0.45	2.11	16	1
1:A:142:VAL:HG21	1:A:150:PHE:CE2	0.44	2.48	1	1
1:A:156:ARG:HA	1:A:159:VAL:CG2	0.44	2.42	5	1
1:A:78:LEU:HD21	1:A:180:ALA:CB	0.44	2.32	14	2
1:A:162:MET:HE2	1:A:167:ILE:CG2	0.44	2.43	9	1
1:A:125:TRP:O	1:A:129:VAL:HG23	0.44	2.12	18	1
1:A:100:LEU:CD1	2:B:86:ILE:HD11	0.44	2.37	7	1
1:A:162:MET:HE2	1:A:167:ILE:HG21	0.44	1.89	9	2
1:A:130:ALA:HB1	2:B:93:VAL:HB	0.44	1.90	10	1
1:A:70:THR:CG2	1:A:181:LEU:HD23	0.44	2.42	11	1
1:A:140:LEU:C	1:A:140:LEU:HD13	0.44	2.38	3	1
1:A:131:LEU:CD2	1:A:158:VAL:HG13	0.44	2.41	12	1
1:A:130:ALA:HB1	2:B:93:VAL:HG22	0.43	1.90	7	1
1:A:147:LEU:O	1:A:148:THR:HG23	0.43	2.12	12	1
1:A:22:ALA:C	1:A:172:ALA:HB1	0.43	2.39	4	2
1:A:139:ALA:HB1	1:A:154:VAL:CG2	0.43	2.43	20	1
1:A:131:LEU:O	1:A:131:LEU:HD23	0.43	2.12	16	2
1:A:147:LEU:HD22	1:A:150:PHE:HD2	0.43	1.74	10	1
1:A:35:PHE:CD1	1:A:132:LEU:HD22	0.43	2.49	16	2
1:A:138:LEU:HD23	1:A:139:ALA:N	0.43	2.28	3	1
1:A:96:MET:HE3	1:A:97:LEU:CD2	0.43	2.44	15	1
1:A:22:ALA:HB3	1:A:172:ALA:CB	0.43	2.43	17	1
1:A:35:PHE:CD2	1:A:132:LEU:HD22	0.43	2.49	4	1
1:A:74:VAL:HG21	1:A:177:TRP:O	0.43	2.14	10	1
1:A:78:LEU:HB3	1:A:129:VAL:HG13	0.42	1.91	18	1
1:A:115:ALA:HB1	1:A:161:PHE:CE2	0.42	2.49	18	1
1:A:131:LEU:HD12	1:A:134:PHE:CE2	0.42	2.50	3	1
1:A:161:PHE:CG	1:A:162:MET:N	0.42	2.87	4	1
1:A:111:PHE:HZ	1:A:158:VAL:HG22	0.42	1.74	12	1
1:A:138:LEU:C	1:A:138:LEU:HD22	0.42	2.40	15	1
1:A:35:PHE:CD1	1:A:155:THR:HG23	0.42	2.50	10	2
2:B:90:LEU:C	2:B:90:LEU:CD2	0.42	2.85	9	1
1:A:81:ILE:HB	2:B:101:ILE:HG22	0.42	1.91	19	1
1:A:181:LEU:HD22	1:A:181:LEU:N	0.42	2.29	8	1
1:A:36:ARG:HD3	1:A:155:THR:HG21	0.42	1.92	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:LEU:HD22	1:A:150:PHE:CD2	0.42	2.50	10	1
1:A:35:PHE:CD1	1:A:35:PHE:C	0.42	2.97	4	1
1:A:178:VAL:O	1:A:181:LEU:HD21	0.42	2.15	8	3
1:A:108:TYR:O	1:A:112:THR:HG23	0.42	2.15	14	8
1:A:125:TRP:CE2	1:A:183:LEU:HD11	0.41	2.50	6	1
1:A:130:ALA:HB1	2:B:93:VAL:CG1	0.41	2.44	5	1
1:A:31:THR:HG21	1:A:162:MET:SD	0.41	2.56	16	1
1:A:147:LEU:O	1:A:148:THR:CG2	0.41	2.68	2	1
1:A:24:GLU:HA	1:A:168:ALA:HB1	0.41	1.92	19	2
1:A:93:PHE:CE2	2:B:90:LEU:HD21	0.41	2.50	11	1
1:A:94:GLN:N	1:A:137:ARG:HH22	0.41	2.14	4	1
1:A:22:ALA:N	1:A:172:ALA:HB1	0.41	2.31	17	1
1:A:104:ALA:CB	1:A:147:LEU:HD11	0.41	2.39	1	1
1:A:24:GLU:CG	1:A:163:LEU:HD22	0.41	2.44	10	1
1:A:96:MET:HE1	2:B:86:ILE:N	0.41	2.31	2	2
1:A:158:VAL:HG23	1:A:159:VAL:N	0.41	2.31	10	1
1:A:162:MET:HG3	1:A:167:ILE:HG21	0.41	1.92	17	1
1:A:138:LEU:HD12	1:A:138:LEU:O	0.40	2.16	17	1
1:A:147:LEU:HD23	1:A:150:PHE:CB	0.40	2.46	5	1
1:A:183:LEU:O	1:A:184:GLY:C	0.40	2.64	9	1
1:A:132:LEU:N	1:A:132:LEU:HD23	0.40	2.31	4	1
1:A:155:THR:O	1:A:159:VAL:HG22	0.40	2.16	5	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	143/169 (85%)	132±2 (92±1%)	10±2 (7±1%)	1±1 (1±1%)	18	68
2	B	18/23 (78%)	15±1 (84±5%)	3±1 (16±5%)	0±0 (0±0%)	100	100
All	All	3220/3840 (84%)	2933 (91%)	264 (8%)	23 (1%)	20	70

All 9 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	149	GLY	4
1	A	166	CYS	4
1	A	146	GLY	4
1	A	184	GLY	3
1	A	148	THR	3
1	A	165	HIS	2
1	A	168	ALA	1
1	A	147	LEU	1
1	A	22	ALA	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	118/137 (86%)	94±4 (79±3%)	24±4 (21±3%)	3	32
2	B	15/16 (94%)	11±1 (72±8%)	4±1 (28±8%)	1	19
All	All	2660/3060 (87%)	2088 (78%)	572 (22%)	3	30

All 76 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	151	LEU	20
1	A	165	HIS	20
1	A	120	GLU	19
1	A	66	GLN	18
1	A	117	SER	16
2	B	88	ARG	16
1	A	23	SER	15
1	A	98	GLN	15
1	A	141	HIS	15
1	A	166	CYS	15
1	A	68	SER	14
1	A	97	LEU	14
1	A	69	SER	13
1	A	163	LEU	13
1	A	36	ARG	12
1	A	113	LYS	12

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Mol	Chain	Res	Type	Models (Total)
1	A	138	LEU	12
2	B	95	ASP	12
1	A	121	SER	11
1	A	162	MET	10
1	A	181	LEU	10
2	B	100	SER	10
1	A	71	MET	10
1	A	83	ASP	9
1	A	114	ILE	9
2	B	82	ILE	9
1	A	25	GLU	9
1	A	91	SER	8
1	A	140	LEU	8
2	B	93	VAL	8
1	A	24	GLU	8
2	B	84	ARG	8
1	A	155	THR	8
1	A	100	LEU	7
1	A	169	ARG	7
1	A	87	ARG	7
2	B	81	ASP	7
1	A	144	GLN	7
1	A	77	GLN	6
1	A	145	HIS	6
1	A	137	ARG	6
1	A	160	ASP	6
1	A	43	HIS	6
1	A	148	THR	6
1	A	173	GLN	6
1	A	85	ILE	5
1	A	70	THR	5
1	A	147	LEU	5
1	A	44	GLN	5
1	A	96	MET	5
1	A	131	LEU	5
1	A	124	ASN	5
1	A	84	ASP	4
1	A	132	LEU	4
1	A	90	ASP	4
1	A	42	ARG	4
1	A	182	ASN	4
2	B	89	HIS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	153	GLN	3
2	B	83	ILE	3
1	A	37	SER	3
2	B	85	ASN	3
1	A	92	GLU	2
1	A	118	LEU	2
2	B	101	ILE	2
2	B	99	ARG	2
1	A	101	GLN	2
1	A	93	PHE	1
2	B	86	ILE	1
1	A	73	GLN	1
1	A	26	GLN	1
1	A	164	HIS	1
1	A	143	TYR	1
2	B	90	LEU	1
1	A	105	GLU	1
1	A	33	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	MK8	B	92	2	5,8,9	1.12±0.02	0±0 (0±0%)
2	NLE	B	97	2	6,7,8	0.66±0.01	0±0 (0±0%)
2	MK8	B	96	2	5,8,9	1.12±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	MK8	B	92	2	6,10,12	0.95±0.03	1±0 (15±5%)
2	NLE	B	97	2	2,7,9	0.68±0.00	0±0 (0±0%)
2	MK8	B	96	2	6,10,12	0.49±0.03	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MK8	B	92	2	-	0±0,6,8,11	-
2	MK8	B	96	2	-	0±0,6,8,11	-
2	NLE	B	97	2	-	0±0,5,6,8	-

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	92	MK8	CB1-CA-C	2.23	100.82	109.75	10	18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 80% 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	2098
Number of shifts mapped to atoms	1898
Number of unparsed shifts	0
Number of shifts with mapping errors	200
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 200 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	19	LEU	HB2	1.482	0.020	1
1	A	20	PRO	HB2	2.182	0.020	2
1	A	20	PRO	HD2	3.754	0.020	2
1	A	20	PRO	HG2	1.915	0.020	1
1	A	21	SER	HB2	3.801	0.020	1
1	A	23	SER	HB2	4.088	0.020	2
1	A	24	GLU	HB2	1.861	0.020	1
1	A	24	GLU	HG2	1.956	0.020	2
1	A	25	GLU	HB2	1.89	0.020	1
1	A	25	GLU	HG2	2.23	0.020	1
1	A	26	GLN	HB2	2.152	0.020	1
1	A	26	GLN	HG2	2.423	0.020	1
1	A	29	GLN	HB2	2.178	0.020	1
1	A	29	GLN	HG2	2.426	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	ASP	HB2	3.295	0.020	2
1	A	32	GLU	HB2	2.059	0.020	1
1	A	32	GLU	HG2	2.237	0.020	2
1	A	33	GLU	HB2	1.983	0.020	1
1	A	33	GLU	HG2	2.02	0.020	1
1	A	35	PHE	HB2	2.964	0.020	1
1	A	36	ARG	HB2	1.798	0.020	2
1	A	36	ARG	HD2	3.072	0.020	1
1	A	36	ARG	HG2	1.588	0.020	1
1	A	37	SER	HB2	4.032	0.020	1
1	A	38	TYR	HB2	3.233	0.020	2
1	A	40	PHE	HB2	2.903	0.020	1
1	A	41	TYR	HB2	2.881	0.020	2
1	A	42	ARG	HB2	0.675	0.020	1
1	A	42	ARG	HD2	2.643	0.020	1
1	A	42	ARG	HG2	0.794	0.020	1
1	A	43	HIS	HB2	3.415	0.020	2
1	A	44	GLN	HB2	1.85	0.020	2
1	A	44	GLN	HG2	1.938	0.020	2
1	A	45	GLN	HB2	2.064	0.020	1
1	A	45	GLN	HG2	2.35	0.020	1
1	A	46	GLU	HB2	1.924	0.020	1
1	A	46	GLU	HG2	2.45	0.020	2
1	A	47	GLN	HB2	1.882	0.020	1
1	A	47	GLN	HG2	1.919	0.020	1
1	A	48	GLU	HB2	1.966	0.020	1
1	A	48	GLU	HG2	2.286	0.020	2
1	A	50	GLU	HB2	1.89	0.020	1
1	A	50	GLU	HG2	2.233	0.020	1
1	A	55	PRO	HB2	2.177	0.020	2
1	A	55	PRO	HD2	3.705	0.020	2
1	A	55	PRO	HG2	1.941	0.020	1
1	A	57	ASP	HB2	2.881	0.020	2
1	A	58	PRO	HB2	2.255	0.020	1
1	A	58	PRO	HD2	3.643	0.020	2
1	A	58	PRO	HG2	1.925	0.020	1
1	A	60	MET	HB2	1.626	0.020	2
1	A	60	MET	HG2	2.129	0.020	1
1	A	63	LEU	HB2	1.208	0.020	1
1	A	64	PRO	HB2	1.959	0.020	2
1	A	64	PRO	HD2	3.603	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	64	PRO	HG2	1.82	0.020	1
1	A	65	LEU	HB2	1.283	0.020	2
1	A	66	GLN	HB2	1.978	0.020	2
1	A	66	GLN	HG2	2.264	0.020	2
1	A	67	PRO	HB2	2.246	0.020	2
1	A	67	PRO	HD2	3.703	0.020	2
1	A	67	PRO	HG2	1.937	0.020	2
1	A	68	SER	HB2	3.876	0.020	2
1	A	69	SER	HB2	4.174	0.020	2
1	A	71	MET	HB2	1.91	0.020	2
1	A	71	MET	HG2	2.965	0.020	2
1	A	73	GLN	HB2	2.273	0.020	2
1	A	73	GLN	HG2	2.429	0.020	1
1	A	76	ARG	HB2	1.5	0.020	2
1	A	76	ARG	HD2	2.595	0.020	2
1	A	76	ARG	HG2	0.303	0.020	2
1	A	77	GLN	HB2	2.027	0.020	1
1	A	77	GLN	HG2	2.276	0.020	1
1	A	78	LEU	HB2	2.053	0.020	2
1	A	80	ILE	HG12	1.498	0.020	2
1	A	81	ILE	HG12	1.473	0.020	2
1	A	83	ASP	HB2	2.799	0.020	2
1	A	84	ASP	HB2	2.611	0.020	1
1	A	85	ILE	HG12	1.519	0.020	2
1	A	86	ASN	HB2	2.784	0.020	1
1	A	87	ARG	HB2	1.766	0.020	1
1	A	87	ARG	HD2	3.103	0.020	1
1	A	87	ARG	HG2	1.745	0.020	2
1	A	88	ARG	HB2	1.62	0.020	2
1	A	88	ARG	HD2	2.938	0.020	2
1	A	88	ARG	HG2	1.203	0.020	2
1	A	89	TYR	HB2	3.274	0.020	2
1	A	90	ASP	HB2	2.999	0.020	2
1	A	91	SER	HB2	3.883	0.020	1
1	A	92	GLU	HB2	1.835	0.020	1
1	A	92	GLU	HG2	2.183	0.020	1
1	A	93	PHE	HB2	3.226	0.020	2
1	A	94	GLN	HB2	2.188	0.020	1
1	A	94	GLN	HG2	2.463	0.020	2
1	A	96	MET	HB2	1.676	0.020	1
1	A	96	MET	HG2	2.679	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	97	LEU	HB2	1.55	0.020	2
1	A	98	GLN	HB2	2.229	0.020	2
1	A	98	GLN	HG2	2.467	0.020	1
1	A	99	HIS	HB2	3.16	0.020	1
1	A	100	LEU	HB2	1.671	0.020	2
1	A	101	GLN	HB2	2.053	0.020	1
1	A	101	GLN	HG2	2.243	0.020	1
1	A	102	PRO	HB2	1.834	0.020	2
1	A	102	PRO	HD2	3.337	0.020	1
1	A	102	PRO	HG2	1.456	0.020	1
1	A	105	GLU	HB2	1.881	0.020	1
1	A	105	GLU	HG2	2.263	0.020	2
1	A	106	ASN	HB2	2.255	0.020	1
1	A	108	TYR	HB2	2.67	0.020	2
1	A	109	GLU	HB2	1.981	0.020	2
1	A	109	GLU	HG2	2.212	0.020	1
1	A	110	TYR	HB2	3.022	0.020	2
1	A	111	PHE	HB2	2.951	0.020	1
1	A	113	LYS	HB2	1.771	0.020	1
1	A	113	LYS	HD2	1.624	0.020	2
1	A	113	LYS	HE2	2.874	0.020	1
1	A	113	LYS	HG2	1.333	0.020	1
1	A	114	ILE	HG12	1.732	0.020	2
1	A	117	SER	HB2	3.661	0.020	2
1	A	118	LEU	HB2	1.688	0.020	2
1	A	119	PHE	HB2	3.283	0.020	2
1	A	120	GLU	HB2	2.139	0.020	2
1	A	120	GLU	HG2	2.273	0.020	1
1	A	121	SER	HB2	4.097	0.020	2
1	A	123	ILE	HG12	1.303	0.020	2
1	A	124	ASN	HB2	3.318	0.020	2
1	A	125	TRP	HB2	3.404	0.020	2
1	A	127	ARG	HB2	1.326	0.020	1
1	A	127	ARG	HD2	2.66	0.020	2
1	A	127	ARG	HG2	1.013	0.020	1
1	A	131	LEU	HB2	2.589	0.020	2
1	A	132	LEU	HB2	1.495	0.020	2
1	A	134	PHE	HB2	3.372	0.020	1
1	A	136	TYR	HB2	3.654	0.020	2
1	A	137	ARG	HB2	1.959	0.020	2
1	A	137	ARG	HD2	3.159	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	137	ARG	HG2	1.742	0.020	1
1	A	138	LEU	HB2	1.87	0.020	2
1	A	140	LEU	HB2	1.553	0.020	2
1	A	141	HIS	HB2	3.193	0.020	2
1	A	143	TYR	HB2	3.174	0.020	1
1	A	144	GLN	HB2	2.082	0.020	2
1	A	144	GLN	HG2	2.658	0.020	2
1	A	145	HIS	HB2	3.463	0.020	2
1	A	147	LEU	HB2	1.457	0.020	2
1	A	150	PHE	HB2	2.906	0.020	2
1	A	151	LEU	HB2	1.571	0.020	1
1	A	153	GLN	HB2	0.837	0.020	2
1	A	153	GLN	HG2	1.859	0.020	2
1	A	156	ARG	HB2	1.838	0.020	2
1	A	156	ARG	HD2	3.066	0.020	1
1	A	156	ARG	HG2	1.626	0.020	2
1	A	157	PHE	HB2	2.681	0.020	2
1	A	160	ASP	HB2	2.946	0.020	2
1	A	161	PHE	HB2	3.68	0.020	2
1	A	162	MET	HB2	2.455	0.020	2
1	A	162	MET	HG2	3.19	0.020	2
1	A	163	LEU	HB2	1.377	0.020	1
1	A	164	HIS	HB2	3.109	0.020	2
1	A	165	HIS	HB2	2.764	0.020	2
1	A	166	CYS	HB2	3.035	0.020	2
1	A	167	ILE	HG12	0.821	0.020	2
1	A	169	ARG	HB2	1.759	0.020	2
1	A	169	ARG	HD2	3.098	0.020	1
1	A	169	ARG	HG2	1.426	0.020	1
1	A	170	TRP	HB2	3.232	0.020	2
1	A	171	ILE	HG12	1.58	0.020	2
1	A	173	GLN	HB2	1.923	0.020	2
1	A	173	GLN	HG2	2.254	0.020	1
1	A	174	ARG	HB2	1.928	0.020	2
1	A	174	ARG	HD2	2.122	0.020	2
1	A	174	ARG	HG2	0.953	0.020	2
1	A	177	TRP	HB2	3.292	0.020	2
1	A	181	LEU	HB2	1.682	0.020	2
1	A	182	ASN	HB2	2.897	0.020	2
1	A	183	LEU	HB2	1.531	0.020	2
1	A	185	ASN	HB2	2.774	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	80	GLU	HB2	1.928	0.020	2
1	B	80	GLU	HG2	2.204	0.020	1
1	B	81	ASP	HB2	2.629	0.020	2
1	B	82	ILE	HG12	1.355	0.020	2
1	B	83	ILE	HG12	1.417	0.020	2
1	B	84	ARG	HB2	1.781	0.020	1
1	B	84	ARG	HD2	3.112	0.020	1
1	B	84	ARG	HG2	1.693	0.020	2
1	B	85	ASN	HB2	2.859	0.020	2
1	B	86	ILE	HG12	0.819	0.020	2
1	B	88	ARG	HB2	1.855	0.020	2
1	B	88	ARG	HD2	3.122	0.020	1
1	B	88	ARG	HG2	1.575	0.020	1
1	B	89	HIS	HB2	3.136	0.020	2
1	B	90	LEU	HB2	1.511	0.020	2
1	B	95	ASP	HB2	2.754	0.020	2
1	B	98	ASP	HB2	2.97	0.020	2
1	B	99	ARG	HB2	2.01	0.020	2
1	B	99	ARG	HD2	3.209	0.020	1
1	B	99	ARG	HG2	1.831	0.020	2
1	B	100	SER	HB2	4.081	0.020	1
1	B	101	ILE	HG12	1.684	0.020	2

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	168	-0.32 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	154	0.39 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	155	0.76 ± 0.35	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 1797 atoms were assigned a chemical shift out of a possible 2255. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	611/815 (75%)	333/334 (100%)	143/322 (44%)	135/159 (85%)
Sidechain	1012/1202 (84%)	728/783 (93%)	267/361 (74%)	17/58 (29%)
Aromatic	174/238 (73%)	103/119 (87%)	68/109 (62%)	3/10 (30%)
Overall	1797/2255 (80%)	1164/1236 (94%)	478/792 (60%)	155/227 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 2066 atoms were assigned a chemical shift out of a possible 2574. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	705/944 (75%)	382/386 (99%)	168/376 (45%)	155/182 (85%)
Sidechain	1187/1392 (85%)	849/908 (94%)	320/424 (75%)	18/60 (30%)
Aromatic	174/238 (73%)	103/119 (87%)	68/109 (62%)	3/10 (30%)
Overall	2066/2574 (80%)	1334/1413 (94%)	556/909 (61%)	176/252 (70%)

7.1.4 Statistically unusual chemical shifts [i](#)

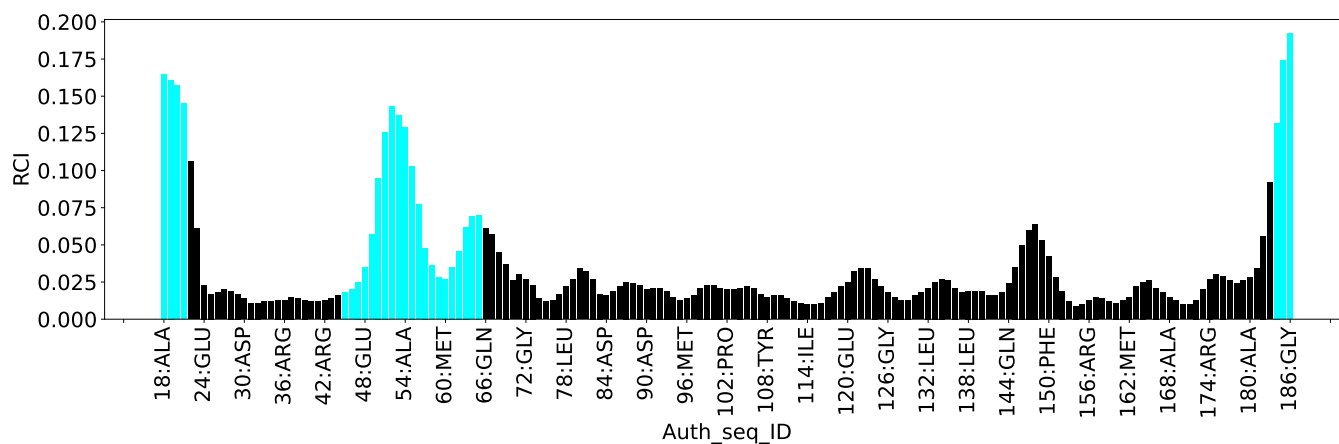
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	127	ARG	NE	117.95	76.53 – 92.65	20.7
1	A	115	ALA	HB1	-0.20	0.14 – 2.58	-6.4
1	A	115	ALA	HB2	-0.20	0.14 – 2.58	-6.4
1	A	115	ALA	HB3	-0.20	0.14 – 2.58	-6.4
1	A	174	ARG	HD3	1.46	1.81 – 4.39	-6.4
1	A	123	ILE	HG21	-0.83	-0.56 – 2.11	-6.0
1	A	123	ILE	HG22	-0.83	-0.56 – 2.11	-6.0
1	A	123	ILE	HG23	-0.83	-0.56 – 2.11	-6.0
1	A	153	GLN	HB3	0.64	0.71 – 3.33	-5.2
1	A	76	ARG	HG3	0.15	0.15 – 2.94	-5.0

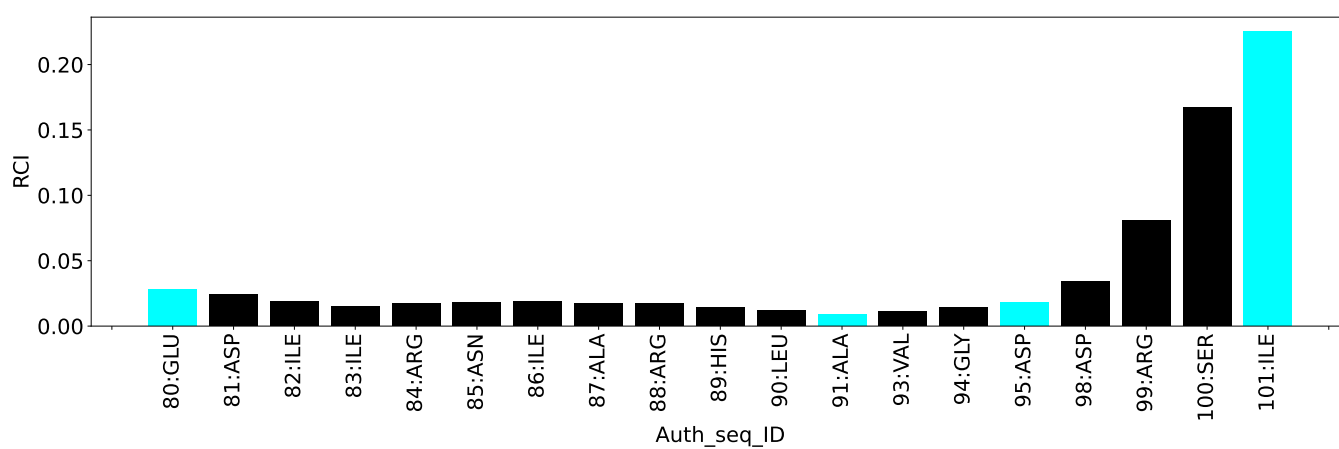
7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	3311
Intra-residue ($ i-j =0$)	1108
Sequential ($ i-j =1$)	695
Medium range ($ i-j >1$ and $ i-j <5$)	622
Long range ($ i-j \geq 5$)	535
Inter-chain	188
Hydrogen bond restraints	163
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	17.2
Number of long range restraints per residue ¹	2.8

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	54.1	0.2
0.2-0.5 (Medium)	78.5	0.5
>0.5 (Large)	119.3	3.11

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

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

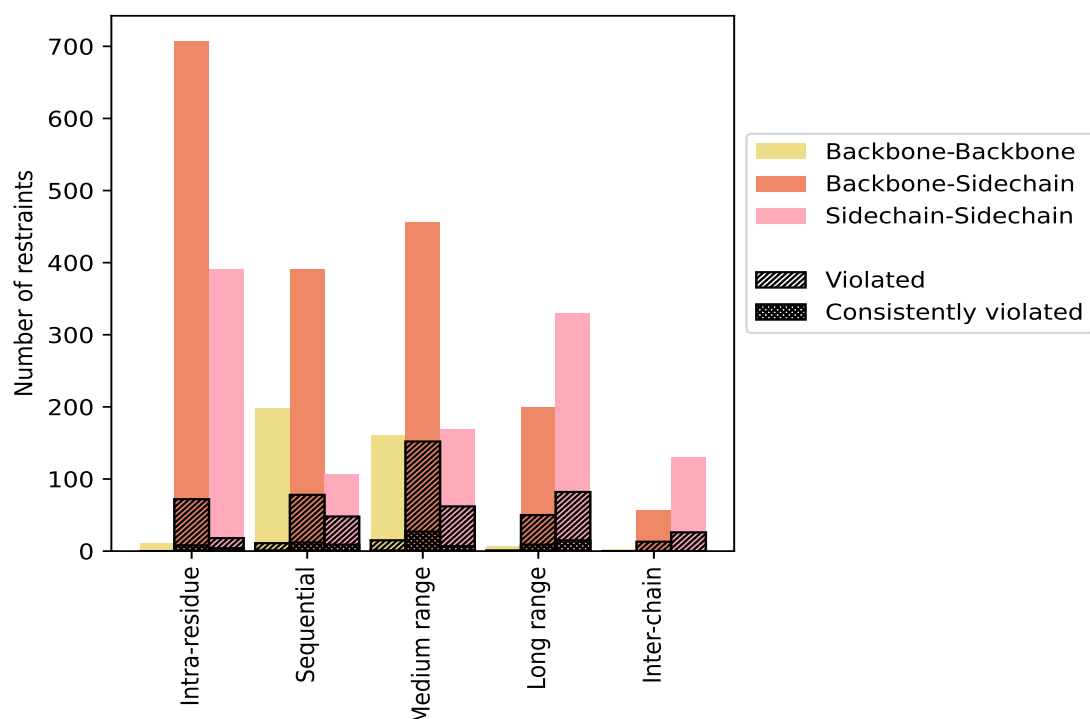
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1108	33.5	90	8.1	2.7	12	1.1	0.4
Backbone-Backbone	11	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	707	21.4	72	10.2	2.2	8	1.1	0.2
Sidechain-Sidechain	390	11.8	18	4.6	0.5	4	1.0	0.1
Sequential ($i-j =1$)	695	21.0	137	19.7	4.1	22	3.2	0.7
Backbone-Backbone	198	6.0	11	5.6	0.3	1	0.5	0.0
Backbone-Sidechain	391	11.8	78	19.9	2.4	12	3.1	0.4
Sidechain-Sidechain	106	3.2	48	45.3	1.4	9	8.5	0.3
Medium range ($i-j >1$ & $i-j <5$)	622	18.8	143	23.0	4.3	18	2.9	0.5
Backbone-Backbone	160	4.8	15	9.4	0.5	1	0.6	0.0
Backbone-Sidechain	293	8.8	66	22.5	2.0	10	3.4	0.3
Sidechain-Sidechain	169	5.1	62	36.7	1.9	7	4.1	0.2
Long range ($i-j \geq 5$)	535	16.2	133	24.9	4.0	24	4.5	0.7
Backbone-Backbone	7	0.2	1	14.3	0.0	0	0.0	0.0
Backbone-Sidechain	199	6.0	50	25.1	1.5	9	4.5	0.3
Sidechain-Sidechain	329	9.9	82	24.9	2.5	15	4.6	0.5
Inter-chain	188	5.7	39	20.7	1.2	0	0.0	0.0
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	56	1.7	13	23.2	0.4	0	0.0	0.0
Sidechain-Sidechain	130	3.9	26	20.0	0.8	0	0.0	0.0
Hydrogen bond	163	4.9	86	52.8	2.6	17	10.4	0.5
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3311	100.0	628	19.0	19.0	93	2.8	2.8
Backbone-Backbone	378	11.4	27	7.1	0.8	2	0.5	0.1
Backbone-Sidechain	1809	54.6	365	20.2	11.0	56	3.1	1.7
Sidechain-Sidechain	1124	33.9	236	21.0	7.1	35	3.1	1.1

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	30	70	101	57	14	272	0.59	2.36	0.52	0.37
2	29	59	92	56	5	241	0.65	2.8	0.56	0.43
3	28	66	98	65	10	267	0.67	2.92	0.57	0.46
4	32	68	104	60	10	274	0.64	2.33	0.54	0.42
5	30	62	91	46	9	238	0.63	3.11	0.55	0.4
6	28	53	87	62	12	242	0.63	2.34	0.53	0.42
7	31	64	92	56	4	247	0.67	2.28	0.53	0.49
8	30	64	87	58	9	248	0.64	2.84	0.55	0.4
9	37	69	94	61	10	271	0.65	2.69	0.55	0.46
10	28	62	107	66	10	273	0.63	2.83	0.55	0.42

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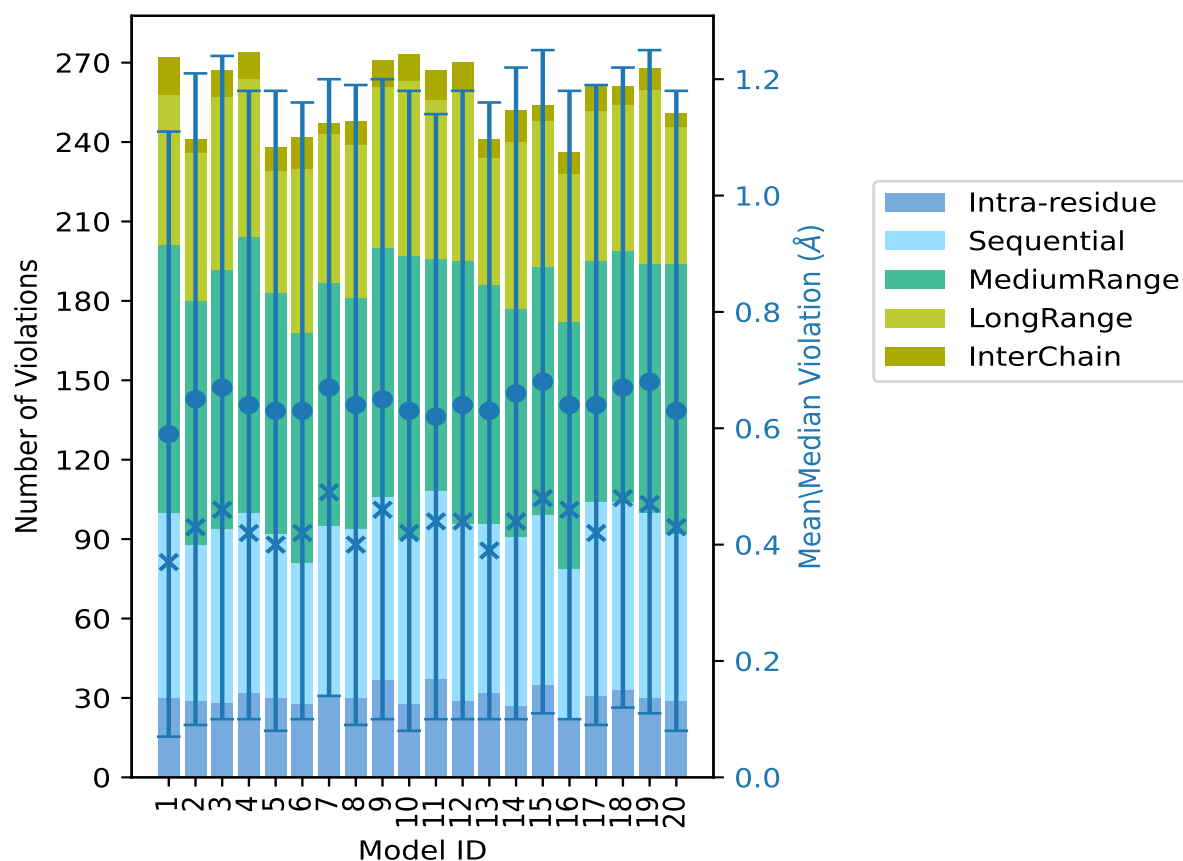
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	37	71	88	60	11	267	0.62	2.85	0.52	0.44
12	29	67	99	64	11	270	0.64	3.11	0.54	0.44
13	32	64	90	48	7	241	0.63	2.36	0.53	0.39
14	27	64	86	63	12	252	0.66	2.66	0.56	0.44
15	35	64	94	55	6	254	0.68	2.67	0.57	0.48
16	22	57	93	56	8	236	0.64	2.61	0.54	0.46
17	31	73	91	57	10	262	0.64	2.78	0.55	0.42
18	33	71	95	55	7	261	0.67	2.54	0.55	0.48
19	30	70	94	66	8	268	0.68	2.84	0.57	0.47
20	29	63	102	52	5	251	0.63	2.84	0.55	0.43

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

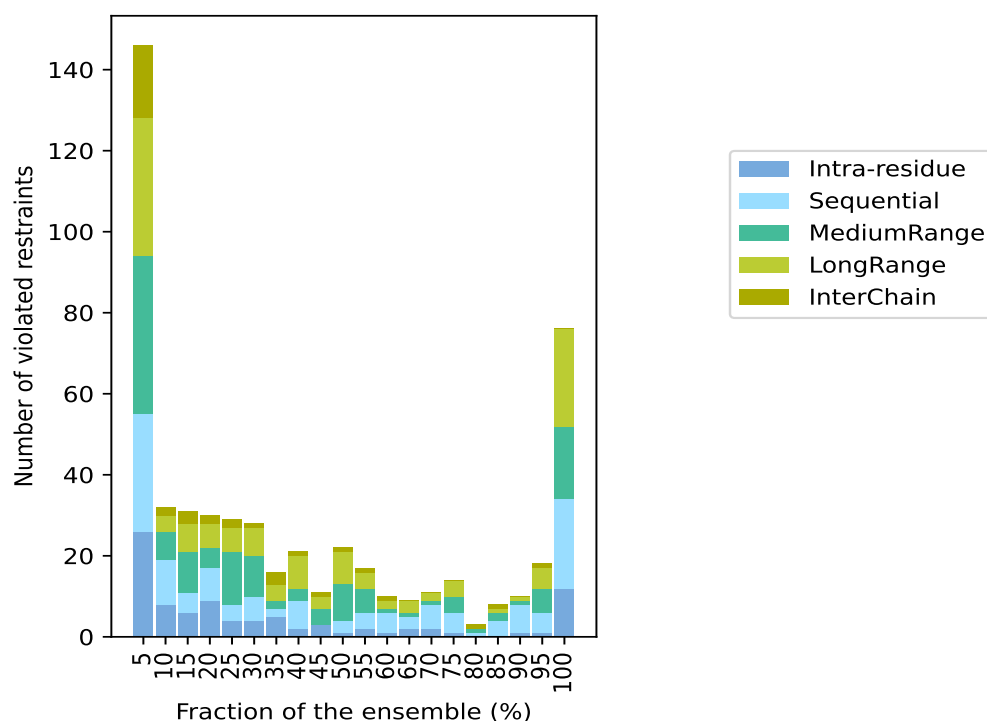
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2606(IR:1018, SQ:558, MR:479, LR:402, IC:149) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
26	29	39	34	18	146	1	5.0
8	11	7	4	2	32	2	10.0
6	5	10	7	3	31	3	15.0
9	8	5	6	2	30	4	20.0
4	4	13	6	2	29	5	25.0
4	6	10	7	1	28	6	30.0
5	2	2	4	3	16	7	35.0
2	7	3	8	1	21	8	40.0
3	0	4	3	1	11	9	45.0
1	3	9	8	1	22	10	50.0
2	4	6	4	1	17	11	55.0
1	5	1	2	1	10	12	60.0
2	3	1	3	0	9	13	65.0
2	6	1	2	0	11	14	70.0
1	5	4	4	0	14	15	75.0
0	1	1	0	1	3	16	80.0
0	4	2	1	1	8	17	85.0
1	7	1	1	0	10	18	90.0
1	5	6	5	1	18	19	95.0
12	22	18	24	0	76	20	100.0

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

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

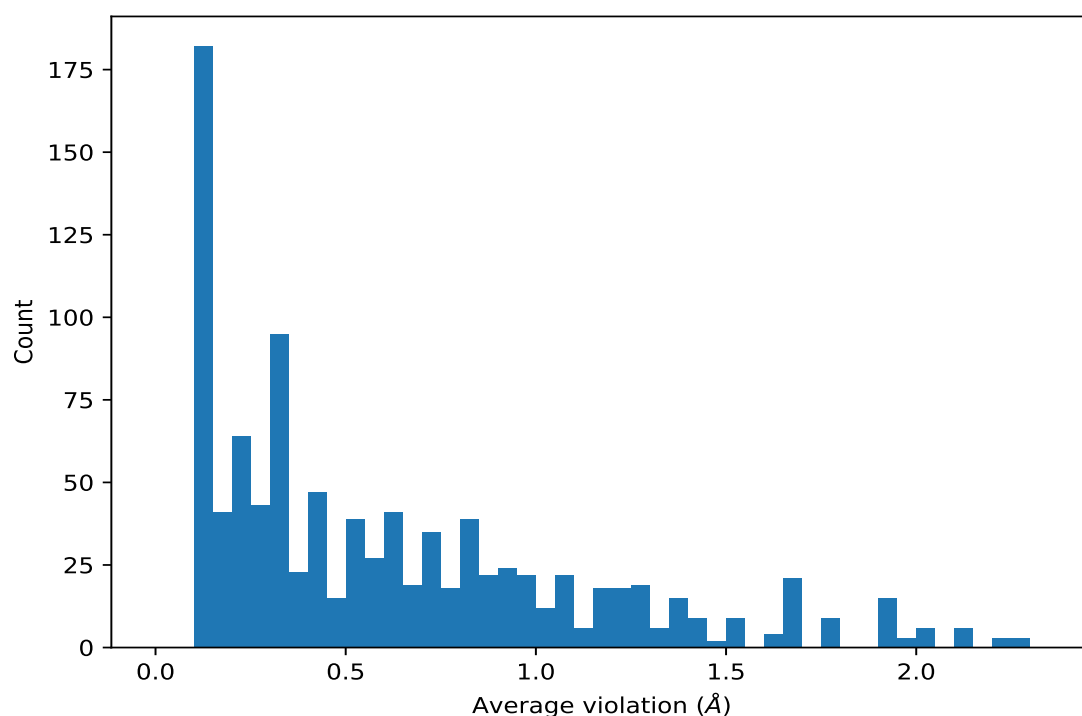
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	20	2.3	0.06	2.32
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	20	2.3	0.06	2.32
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	20	2.3	0.06	2.32
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	20	2.14	0.1	2.16
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	20	2.14	0.1	2.16
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	20	2.14	0.1	2.16
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	20	2.0	0.26	2.09
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	20	2.0	0.26	2.09
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	20	2.0	0.26	2.09
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	20	1.96	0.19	2.01
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	20	1.96	0.19	2.01
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	20	1.96	0.19	2.01
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	20	1.95	0.31	2.06
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	20	1.95	0.31	2.06
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	20	1.95	0.31	2.06
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	20	1.95	0.31	2.06

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	20	1.95	0.31	2.06
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	20	1.95	0.31	2.06
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	20	1.95	0.31	2.06
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	20	1.95	0.31	2.06
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	20	1.95	0.31	2.06
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	20	1.77	0.2	1.82
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	20	1.77	0.2	1.82
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	20	1.77	0.2	1.82
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	20	1.77	0.2	1.82
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	20	1.77	0.2	1.82
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	20	1.77	0.2	1.82
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	20	1.77	0.2	1.82
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	20	1.77	0.2	1.82
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	20	1.77	0.2	1.82
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	20	1.6	0.47	1.88
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	20	1.6	0.09	1.65
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	20	1.6	0.09	1.65
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	20	1.6	0.09	1.65
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	20	1.43	0.07	1.41
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	20	1.43	0.07	1.41
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	20	1.43	0.07	1.41
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	20	1.39	0.26	1.48
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	20	1.39	0.26	1.48
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	20	1.39	0.26	1.48
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	20	1.3	0.41	1.34
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	20	1.3	0.41	1.34
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	20	1.3	0.41	1.34
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	20	1.27	0.01	1.27
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	20	1.25	0.58	0.98
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	20	1.25	0.58	0.98
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	20	1.25	0.58	0.98
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	20	1.25	0.58	0.98
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	20	1.25	0.58	0.98
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	20	1.25	0.58	0.98
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	20	1.25	0.58	0.98
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	20	1.25	0.58	0.98
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	20	1.25	0.58	0.98
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	20	1.24	0.2	1.31
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	20	1.24	0.2	1.31
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	20	1.24	0.2	1.31
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	20	1.19	0.43	1.1
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	20	1.19	0.43	1.1

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	20	1.19	0.43	1.1
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	20	1.18	0.1	1.18
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	20	1.18	0.1	1.18
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	20	1.18	0.1	1.18
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	20	1.18	0.1	1.19
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	20	1.18	0.1	1.19
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	20	1.18	0.1	1.19
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	20	1.14	0.39	1.22
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	20	1.12	0.14	1.11
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	20	1.12	0.14	1.11
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	20	1.12	0.14	1.11
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	20	1.11	0.13	1.13
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	20	1.08	0.59	0.88
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	20	1.08	0.59	0.88
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	20	1.08	0.59	0.88
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	20	1.07	0.34	1.14
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	20	1.07	0.34	1.14
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	20	0.99	0.38	0.92
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	20	0.99	0.38	0.92
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	20	0.99	0.38	0.92
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	20	0.94	0.13	0.94
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	20	0.94	0.13	0.94
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	20	0.94	0.13	0.94
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	20	0.93	0.14	0.95
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	20	0.93	0.14	0.95
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	20	0.93	0.14	0.95
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	20	0.9	0.0	0.9
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	20	0.9	0.0	0.9
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	20	0.9	0.0	0.9
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	20	0.9	0.11	0.89
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	20	0.89	0.09	0.9
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	20	0.89	0.09	0.9
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	20	0.89	0.09	0.9
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	20	0.87	0.12	0.87
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	20	0.87	0.12	0.87
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	20	0.87	0.12	0.87
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	20	0.83	0.18	0.86
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	20	0.83	0.18	0.86
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	20	0.83	0.18	0.86
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	20	0.78	0.4	0.62
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	20	0.76	0.02	0.75
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	20	0.76	0.02	0.75

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	20	0.76	0.02	0.75
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	20	0.74	0.29	0.82
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	20	0.74	0.29	0.82
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	20	0.74	0.29	0.82
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	20	0.73	0.03	0.73
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	20	0.72	0.0	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	20	0.72	0.0	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	20	0.72	0.0	0.72
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	20	0.72	0.07	0.72
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	20	0.72	0.07	0.72
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	20	0.72	0.07	0.72
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	20	0.72	0.07	0.72
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	20	0.72	0.07	0.72
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	20	0.72	0.07	0.72
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	20	0.72	0.07	0.72
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	20	0.72	0.07	0.72
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	20	0.72	0.07	0.72
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	20	0.72	0.07	0.72
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	20	0.72	0.07	0.72
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	20	0.72	0.07	0.72
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	20	0.72	0.07	0.72
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	20	0.72	0.07	0.72
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	20	0.72	0.07	0.72
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	20	0.72	0.07	0.72
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	20	0.72	0.07	0.72
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	20	0.72	0.07	0.72
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	20	0.65	0.29	0.72
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	20	0.65	0.29	0.72
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	20	0.65	0.29	0.72
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	20	0.64	0.01	0.64
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	20	0.62	0.01	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	20	0.62	0.01	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	20	0.62	0.01	0.62
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	20	0.58	0.15	0.57
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	20	0.58	0.15	0.57
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	20	0.58	0.01	0.58
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	20	0.52	0.23	0.52
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	20	0.52	0.23	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	20	0.52	0.01	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	20	0.52	0.01	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	20	0.52	0.01	0.52
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	20	0.44	0.04	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	20	0.44	0.04	0.42
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	20	0.44	0.04	0.42
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	20	0.42	0.11	0.44
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	20	0.42	0.11	0.44
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	20	0.42	0.11	0.44
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	20	0.42	0.11	0.44
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	20	0.42	0.11	0.44
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	20	0.42	0.11	0.44
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	20	0.42	0.11	0.44
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	20	0.42	0.11	0.44
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	20	0.42	0.11	0.44
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	20	0.4	0.06	0.38
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	20	0.38	0.06	0.4
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	20	0.38	0.07	0.36
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	20	0.38	0.07	0.36
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	20	0.38	0.07	0.36
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	20	0.37	0.02	0.37
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	20	0.34	0.02	0.34
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	20	0.33	0.03	0.34
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	20	0.32	0.06	0.32
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	20	0.32	0.06	0.32
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	20	0.32	0.06	0.32
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	20	0.32	0.03	0.31
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	20	0.32	0.03	0.32
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	20	0.32	0.03	0.32
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	20	0.31	0.03	0.32
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	20	0.31	0.04	0.31
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	20	0.31	0.04	0.32
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	20	0.31	0.03	0.32
(2,149)	1:112:A:THR:O	1:116:A:THR:N	20	0.3	0.02	0.3
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	20	0.27	0.07	0.3
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	20	0.25	0.06	0.26
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	20	0.25	0.03	0.26
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	20	0.25	0.05	0.26
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	20	0.25	0.05	0.24
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	20	0.24	0.05	0.24
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	20	0.22	0.05	0.21
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	20	0.19	0.03	0.19
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	20	0.16	0.02	0.16
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	20	0.14	0.01	0.15
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	19	1.21	0.44	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	19	1.21	0.44	1.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	19	1.21	0.44	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	19	1.21	0.44	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	19	1.21	0.44	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	19	1.21	0.44	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	19	1.21	0.44	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	19	1.21	0.44	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	19	1.21	0.44	1.35
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	19	1.09	0.33	1.3
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	19	1.09	0.33	1.3
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	19	1.09	0.33	1.3
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	19	1.06	0.34	1.19
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	19	0.97	0.15	1.01
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	19	0.97	0.15	1.01
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	19	0.97	0.15	1.01
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	19	0.91	0.2	0.93
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	19	0.83	0.19	0.83
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	19	0.83	0.19	0.83
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	19	0.83	0.19	0.83
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	19	0.76	0.32	0.75
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	19	0.58	0.23	0.66
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	19	0.58	0.23	0.66
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	19	0.52	0.07	0.52
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	19	0.52	0.07	0.52
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	19	0.52	0.07	0.52
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	19	0.5	0.01	0.5
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	19	0.49	0.26	0.45
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	19	0.32	0.12	0.35
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	19	0.32	0.12	0.35
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	19	0.32	0.12	0.35
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	19	0.32	0.08	0.31
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	19	0.32	0.08	0.31
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	19	0.32	0.08	0.31
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	19	0.32	0.08	0.32
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	19	0.26	0.06	0.25
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	19	0.26	0.04	0.25
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	19	0.24	0.06	0.23
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	19	0.24	0.06	0.23
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	19	0.24	0.06	0.23
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	19	0.24	0.06	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	19	0.23	0.02	0.23
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	19	0.21	0.04	0.21
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	19	0.19	0.03	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	18	0.73	0.12	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	18	0.73	0.12	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	18	0.73	0.12	0.69
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	18	0.58	0.27	0.55
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	18	0.58	0.27	0.55
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	18	0.58	0.27	0.55
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	18	0.58	0.27	0.55
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	18	0.58	0.27	0.55
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	18	0.58	0.27	0.55
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	18	0.58	0.27	0.55
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	18	0.58	0.27	0.55
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	18	0.58	0.27	0.55
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	18	0.34	0.18	0.3
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	18	0.34	0.18	0.3
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	18	0.24	0.02	0.25
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	18	0.24	0.05	0.26
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	18	0.22	0.05	0.22
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	18	0.22	0.05	0.22
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	18	0.22	0.05	0.22
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	18	0.21	0.05	0.22
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	18	0.2	0.05	0.21
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	18	0.14	0.03	0.13
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	18	0.12	0.01	0.12
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	18	0.11	0.01	0.11
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	17	1.07	0.8	0.65
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	17	1.07	0.8	0.65
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	17	1.07	0.8	0.65
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	17	0.75	0.1	0.74
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	17	0.68	0.48	0.44
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	17	0.68	0.48	0.44
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	17	0.68	0.48	0.44
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	17	0.46	0.17	0.45
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	17	0.32	0.13	0.29
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	17	0.29	0.05	0.29
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	17	0.22	0.05	0.21
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	17	0.22	0.05	0.21
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	17	0.22	0.05	0.21
(1,410)	1:94:A:GLN:HE22	1:95:A:THR:H	16	0.52	0.28	0.55
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB1	16	0.14	0.02	0.14
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB2	16	0.14	0.02	0.14
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB3	16	0.14	0.02	0.14
(2,88)	1:132:A:LEU:O	1:136:A:TYR:N	16	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,256)	1:159:A:VAL:HG11	1:158:A:VAL:H	15	1.68	0.08	1.68
(1,256)	1:159:A:VAL:HG12	1:158:A:VAL:H	15	1.68	0.08	1.68
(1,256)	1:159:A:VAL:HG13	1:158:A:VAL:H	15	1.68	0.08	1.68
(1,963)	1:159:A:VAL:HG21	1:160:A:ASP:HA	15	1.52	0.01	1.52
(1,963)	1:159:A:VAL:HG22	1:160:A:ASP:HA	15	1.52	0.01	1.52
(1,963)	1:159:A:VAL:HG23	1:160:A:ASP:HA	15	1.52	0.01	1.52
(1,854)	1:159:A:VAL:HG11	1:32:A:GLU:HA	15	1.4	0.23	1.43
(1,854)	1:159:A:VAL:HG12	1:32:A:GLU:HA	15	1.4	0.23	1.43
(1,854)	1:159:A:VAL:HG13	1:32:A:GLU:HA	15	1.4	0.23	1.43
(1,1570)	1:159:A:VAL:HG11	1:158:A:VAL:HB	15	1.24	0.18	1.21
(1,1570)	1:159:A:VAL:HG12	1:158:A:VAL:HB	15	1.24	0.18	1.21
(1,1570)	1:159:A:VAL:HG13	1:158:A:VAL:HB	15	1.24	0.18	1.21
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG21	15	0.8	0.28	0.81
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG22	15	0.8	0.28	0.81
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG23	15	0.8	0.28	0.81
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG21	15	0.8	0.28	0.81
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG22	15	0.8	0.28	0.81
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG23	15	0.8	0.28	0.81
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG21	15	0.8	0.28	0.81
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG22	15	0.8	0.28	0.81
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG23	15	0.8	0.28	0.81
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG21	15	0.8	0.28	0.81
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG22	15	0.8	0.28	0.81
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG23	15	0.8	0.28	0.81
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG21	15	0.8	0.28	0.81
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG22	15	0.8	0.28	0.81
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG23	15	0.8	0.28	0.81
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG21	15	0.8	0.28	0.81
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG22	15	0.8	0.28	0.81
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG23	15	0.8	0.28	0.81
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG11	15	0.79	0.0	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG12	15	0.79	0.0	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG13	15	0.79	0.0	0.79
(1,2556)	1:183:A:LEU:HD21	1:125:A:TRP:HE3	15	0.61	0.29	0.57
(1,2556)	1:183:A:LEU:HD22	1:125:A:TRP:HE3	15	0.61	0.29	0.57
(1,2556)	1:183:A:LEU:HD23	1:125:A:TRP:HE3	15	0.61	0.29	0.57
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB1	15	0.53	0.26	0.44
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB2	15	0.53	0.26	0.44
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB3	15	0.53	0.26	0.44
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB1	15	0.53	0.26	0.44
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB2	15	0.53	0.26	0.44
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB3	15	0.53	0.26	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB1	15	0.53	0.26	0.44
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB2	15	0.53	0.26	0.44
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB3	15	0.53	0.26	0.44
(1,934)	1:159:A:VAL:HG11	1:156:A:ARG:HA	15	0.49	0.18	0.48
(1,934)	1:159:A:VAL:HG12	1:156:A:ARG:HA	15	0.49	0.18	0.48
(1,934)	1:159:A:VAL:HG13	1:156:A:ARG:HA	15	0.49	0.18	0.48
(2,140)	1:78:A:LEU:O	1:82:A:GLY:N	15	0.18	0.04	0.2
(2,11)	1:29:A:GLN:O	1:33:A:GLU:H	15	0.14	0.03	0.13
(1,1483)	1:143:A:TYR:HE1	1:144:A:GLN:HG3	14	1.49	0.38	1.58
(1,1483)	1:143:A:TYR:HE2	1:144:A:GLN:HG3	14	1.49	0.38	1.58
(1,921)	1:98:A:GLN:HE22	1:98:A:GLN:HA	14	0.96	0.3	1.09
(1,1746)	1:86:A:ASN:HB3	1:87:A:ARG:HG3	14	0.86	0.11	0.85
(1,190)	1:183:A:LEU:HD21	1:125:A:TRP:H	14	0.57	0.27	0.6
(1,190)	1:183:A:LEU:HD22	1:125:A:TRP:H	14	0.57	0.27	0.6
(1,190)	1:183:A:LEU:HD23	1:125:A:TRP:H	14	0.57	0.27	0.6
(1,1495)	1:153:A:GLN:H	1:153:A:GLN:HG3	14	0.41	0.06	0.4
(2,146)	1:107:A:ALA:O	1:111:A:PHE:N	14	0.21	0.06	0.22
(2,153)	1:134:A:PHE:O	1:138:A:LEU:N	14	0.21	0.08	0.2
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG11	13	2.14	0.89	2.54
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG12	13	2.14	0.89	2.54
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG13	13	2.14	0.89	2.54
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG21	13	0.45	0.27	0.37
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG22	13	0.45	0.27	0.37
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG23	13	0.45	0.27	0.37
(1,1842)	1:165:A:HIS:HA	1:166:A:CYS:HB3	13	0.45	0.21	0.49
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	13	0.44	0.13	0.49
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	13	0.44	0.13	0.49
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	13	0.44	0.13	0.49
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG11	13	0.4	0.16	0.41
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG12	13	0.4	0.16	0.41
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG13	13	0.4	0.16	0.41
(2,157)	1:153:A:GLN:O	1:157:A:PHE:N	13	0.23	0.07	0.25
(1,1428)	1:31:A:THR:HB	1:32:A:GLU:HG3	13	0.15	0.03	0.16
(1,154)	1:32:A:GLU:HG3	1:32:A:GLU:H	13	0.14	0.02	0.14
(2,63)	1:110:A:TYR:O	1:114:A:ILE:H	13	0.12	0.01	0.12
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD21	12	1.93	0.39	2.05
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD22	12	1.93	0.39	2.05
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD23	12	1.93	0.39	2.05
(1,542)	1:172:A:ALA:HB1	1:173:A:GLN:HE22	12	0.49	0.16	0.5
(1,542)	1:172:A:ALA:HB2	1:173:A:GLN:HE22	12	0.49	0.16	0.5
(1,542)	1:172:A:ALA:HB3	1:173:A:GLN:HE22	12	0.49	0.16	0.5
(1,171)	1:162:A:MET:HB3	1:161:A:PHE:H	12	0.44	0.14	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1730)	1:144:A:GLN:H	1:145:A:HIS:HB3	12	0.35	0.12	0.34
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG11	12	0.35	0.14	0.31
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG12	12	0.35	0.14	0.31
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG13	12	0.35	0.14	0.31
(2,159)	1:158:A:VAL:O	1:162:A:MET:N	12	0.21	0.06	0.2
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD11	12	0.18	0.0	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD12	12	0.18	0.0	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD13	12	0.18	0.0	0.18
(2,9)	1:28:A:ALA:O	1:32:A:GLU:H	12	0.16	0.07	0.12
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD11	12	0.13	0.04	0.12
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD12	12	0.13	0.04	0.12
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD13	12	0.13	0.04	0.12
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD11	12	0.13	0.04	0.12
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD12	12	0.13	0.04	0.12
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD13	12	0.13	0.04	0.12
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD11	12	0.13	0.04	0.12
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD12	12	0.13	0.04	0.12
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD13	12	0.13	0.04	0.12
(2,17)	1:32:A:GLU:O	1:36:A:ARG:H	12	0.11	0.01	0.11
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG11	11	2.22	0.19	2.31
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG12	11	2.22	0.19	2.31
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG13	11	2.22	0.19	2.31
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD1	11	1.69	0.22	1.76
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD2	11	1.69	0.22	1.76
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD1	11	1.69	0.22	1.76
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD2	11	1.69	0.22	1.76
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD1	11	1.69	0.22	1.76
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD2	11	1.69	0.22	1.76
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD21	11	1.45	0.71	1.98
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD22	11	1.45	0.71	1.98
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD23	11	1.45	0.71	1.98
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG11	11	1.34	0.02	1.34
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG12	11	1.34	0.02	1.34
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG13	11	1.34	0.02	1.34
(1,1627)	1:129:A:VAL:HG11	1:125:A:TRP:HB3	11	1.26	0.1	1.27
(1,1627)	1:129:A:VAL:HG12	1:125:A:TRP:HB3	11	1.26	0.1	1.27
(1,1627)	1:129:A:VAL:HG13	1:125:A:TRP:HB3	11	1.26	0.1	1.27
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD11	11	1.26	0.19	1.31
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD12	11	1.26	0.19	1.31
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD13	11	1.26	0.19	1.31
(1,90)	1:97:A:LEU:HD21	1:138:A:LEU:H	11	1.02	0.28	1.1
(1,90)	1:97:A:LEU:HD22	1:138:A:LEU:H	11	1.02	0.28	1.1

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,90)	1:97:A:LEU:HD23	1:138:A:LEU:H	11	1.02	0.28	1.1
(1,841)	1:97:A:LEU:HD11	1:93:A:PHE:HA	11	0.99	0.1	0.97
(1,841)	1:97:A:LEU:HD12	1:93:A:PHE:HA	11	0.99	0.1	0.97
(1,841)	1:97:A:LEU:HD13	1:93:A:PHE:HA	11	0.99	0.1	0.97
(1,1043)	1:182:A:ASN:HB3	1:179:A:ALA:HA	11	0.92	0.57	0.81
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD21	11	0.89	0.3	0.86
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD22	11	0.89	0.3	0.86
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD23	11	0.89	0.3	0.86
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD21	11	0.89	0.3	0.86
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD22	11	0.89	0.3	0.86
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD23	11	0.89	0.3	0.86
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD21	11	0.89	0.3	0.86
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD22	11	0.89	0.3	0.86
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD23	11	0.89	0.3	0.86
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG11	11	0.88	0.15	0.93
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG12	11	0.88	0.15	0.93
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG13	11	0.88	0.15	0.93
(1,1588)	1:129:A:VAL:HG11	1:128:A:VAL:HB	11	0.82	0.08	0.86
(1,1588)	1:129:A:VAL:HG12	1:128:A:VAL:HB	11	0.82	0.08	0.86
(1,1588)	1:129:A:VAL:HG13	1:128:A:VAL:HB	11	0.82	0.08	0.86
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG11	11	0.64	0.0	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG12	11	0.64	0.0	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG13	11	0.64	0.0	0.64
(2,139)	1:40:A:PHE:O	1:44:A:GLN:N	11	0.2	0.07	0.19
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD11	11	0.13	0.02	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD12	11	0.13	0.02	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD13	11	0.13	0.02	0.13
(2,75)	1:124:A:ASN:O	1:128:A:VAL:H	11	0.12	0.01	0.12
(1,757)	1:41:A:TYR:HE1	1:41:A:TYR:HA	11	0.12	0.01	0.11
(1,757)	1:41:A:TYR:HE2	1:41:A:TYR:HA	11	0.12	0.01	0.11
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD1	10	1.35	0.03	1.36
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD2	10	1.35	0.03	1.36
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD1	10	1.35	0.03	1.36
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD2	10	1.35	0.03	1.36
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD1	10	1.35	0.03	1.36
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD2	10	1.35	0.03	1.36
(1,593)	1:131:A:LEU:HD21	1:135:A:GLY:H	10	1.23	0.06	1.22
(1,593)	1:131:A:LEU:HD22	1:135:A:GLY:H	10	1.23	0.06	1.22
(1,593)	1:131:A:LEU:HD23	1:135:A:GLY:H	10	1.23	0.06	1.22
(1,139)	1:131:A:LEU:HD21	1:115:A:ALA:H	10	0.91	0.18	0.9
(1,139)	1:131:A:LEU:HD22	1:115:A:ALA:H	10	0.91	0.18	0.9
(1,139)	1:131:A:LEU:HD23	1:115:A:ALA:H	10	0.91	0.18	0.9

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2483)	1:147:A:LEU:HD21	1:150:A:PHE:HZ	10	0.84	0.55	0.78
(1,2483)	1:147:A:LEU:HD22	1:150:A:PHE:HZ	10	0.84	0.55	0.78
(1,2483)	1:147:A:LEU:HD23	1:150:A:PHE:HZ	10	0.84	0.55	0.78
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG11	10	0.79	0.36	0.66
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG12	10	0.79	0.36	0.66
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG13	10	0.79	0.36	0.66
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG11	10	0.79	0.36	0.66
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG12	10	0.79	0.36	0.66
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG13	10	0.79	0.36	0.66
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG11	10	0.79	0.36	0.66
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG12	10	0.79	0.36	0.66
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG13	10	0.79	0.36	0.66
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD11	10	0.69	0.06	0.66
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD12	10	0.69	0.06	0.66
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD13	10	0.69	0.06	0.66
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG11	10	0.58	0.36	0.52
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG12	10	0.58	0.36	0.52
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG13	10	0.58	0.36	0.52
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD11	10	0.41	0.23	0.36
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD12	10	0.41	0.23	0.36
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD13	10	0.41	0.23	0.36
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD11	10	0.41	0.23	0.36
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD12	10	0.41	0.23	0.36
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD13	10	0.41	0.23	0.36
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD11	10	0.41	0.23	0.36
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD12	10	0.41	0.23	0.36
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD13	10	0.41	0.23	0.36
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG11	10	0.41	0.21	0.36
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG12	10	0.41	0.21	0.36
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG13	10	0.41	0.21	0.36
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG11	10	0.41	0.21	0.36
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG12	10	0.41	0.21	0.36
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG13	10	0.41	0.21	0.36
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD11	10	0.36	0.03	0.36
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD12	10	0.36	0.03	0.36
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD13	10	0.36	0.03	0.36
(1,123)	1:34:A:VAL:HG11	1:74:A:VAL:H	10	0.35	0.23	0.25
(1,123)	1:34:A:VAL:HG12	1:74:A:VAL:H	10	0.35	0.23	0.25
(1,123)	1:34:A:VAL:HG13	1:74:A:VAL:H	10	0.35	0.23	0.25
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG21	10	0.33	0.12	0.31
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG22	10	0.33	0.12	0.31
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG23	10	0.33	0.12	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG21	10	0.33	0.12	0.31
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG22	10	0.33	0.12	0.31
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG23	10	0.33	0.12	0.31
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG21	10	0.33	0.12	0.31
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG22	10	0.33	0.12	0.31
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG23	10	0.33	0.12	0.31
(1,733)	1:26:A:GLN:HG3	1:23:A:SER:HB3	10	0.31	0.33	0.21
(1,1032)	1:131:A:LEU:HD21	1:115:A:ALA:HA	10	0.3	0.13	0.34
(1,1032)	1:131:A:LEU:HD22	1:115:A:ALA:HA	10	0.3	0.13	0.34
(1,1032)	1:131:A:LEU:HD23	1:115:A:ALA:HA	10	0.3	0.13	0.34
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG21	10	0.23	0.09	0.2
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG22	10	0.23	0.09	0.2
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG23	10	0.23	0.09	0.2
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE1	10	0.22	0.03	0.22
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE2	10	0.22	0.03	0.22
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE1	10	0.22	0.03	0.22
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE2	10	0.22	0.03	0.22
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE1	10	0.22	0.03	0.22
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE2	10	0.22	0.03	0.22
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD11	10	0.14	0.03	0.12
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD12	10	0.14	0.03	0.12
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD13	10	0.14	0.03	0.12
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB1	9	1.69	0.57	1.89
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB2	9	1.69	0.57	1.89
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB3	9	1.69	0.57	1.89
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB1	9	1.69	0.57	1.89
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB2	9	1.69	0.57	1.89
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB3	9	1.69	0.57	1.89
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB1	9	1.69	0.57	1.89
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB2	9	1.69	0.57	1.89
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB3	9	1.69	0.57	1.89
(1,1350)	1:179:A:ALA:HB1	1:182:A:ASN:HB3	9	0.86	0.41	0.74
(1,1350)	1:179:A:ALA:HB2	1:182:A:ASN:HB3	9	0.86	0.41	0.74
(1,1350)	1:179:A:ALA:HB3	1:182:A:ASN:HB3	9	0.86	0.41	0.74
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE1	9	0.5	0.17	0.63
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE2	9	0.5	0.17	0.63
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE1	9	0.5	0.17	0.63
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE2	9	0.5	0.17	0.63
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE1	9	0.5	0.17	0.63
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE2	9	0.5	0.17	0.63
(1,1326)	1:182:A:ASN:H	1:182:A:ASN:HB3	9	0.32	0.01	0.32
(1,1027)	1:27:A:VAL:HG21	1:168:A:ALA:HA	9	0.31	0.13	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1027)	1:27:A:VAL:HG22	1:168:A:ALA:HA	9	0.31	0.13	0.29
(1,1027)	1:27:A:VAL:HG23	1:168:A:ALA:HA	9	0.31	0.13	0.29
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB1	9	0.26	0.16	0.19
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB2	9	0.26	0.16	0.19
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB3	9	0.26	0.16	0.19
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB1	9	0.26	0.16	0.19
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB2	9	0.26	0.16	0.19
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB3	9	0.26	0.16	0.19
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB1	9	0.26	0.16	0.19
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB2	9	0.26	0.16	0.19
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB3	9	0.26	0.16	0.19
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD11	9	0.2	0.05	0.24
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD12	9	0.2	0.05	0.24
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD13	9	0.2	0.05	0.24
(1,1494)	1:44:A:GLN:HB3	1:44:A:GLN:HG3	9	0.14	0.01	0.15
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HD	9	0.13	0.02	0.13
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HDA	9	0.13	0.02	0.13
(1,34)	1:118:A:LEU:HD21	1:134:A:PHE:H	8	2.03	0.08	2.04
(1,34)	1:118:A:LEU:HD22	1:134:A:PHE:H	8	2.03	0.08	2.04
(1,34)	1:118:A:LEU:HD23	1:134:A:PHE:H	8	2.03	0.08	2.04
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE1	8	1.5	0.2	1.48
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE2	8	1.5	0.2	1.48
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE1	8	1.5	0.2	1.48
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE2	8	1.5	0.2	1.48
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE1	8	1.5	0.2	1.48
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE2	8	1.5	0.2	1.48
(1,3031)	1:118:A:LEU:HD11	2:91:B:ALA:HA	8	1.37	0.09	1.38
(1,3031)	1:118:A:LEU:HD12	2:91:B:ALA:HA	8	1.37	0.09	1.38
(1,3031)	1:118:A:LEU:HD13	2:91:B:ALA:HA	8	1.37	0.09	1.38
(1,1020)	1:118:A:LEU:HD21	1:130:A:ALA:HA	8	1.25	0.15	1.3
(1,1020)	1:118:A:LEU:HD22	1:130:A:ALA:HA	8	1.25	0.15	1.3
(1,1020)	1:118:A:LEU:HD23	1:130:A:ALA:HA	8	1.25	0.15	1.3
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD1	8	1.2	0.1	1.23
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD2	8	1.2	0.1	1.23
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD1	8	1.2	0.1	1.23
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD2	8	1.2	0.1	1.23
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD1	8	1.2	0.1	1.23
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD2	8	1.2	0.1	1.23
(1,625)	1:118:A:LEU:HD21	1:128:A:VAL:HA	8	1.18	0.26	1.22
(1,625)	1:118:A:LEU:HD22	1:128:A:VAL:HA	8	1.18	0.26	1.22
(1,625)	1:118:A:LEU:HD23	1:128:A:VAL:HA	8	1.18	0.26	1.22
(1,1329)	1:118:A:LEU:HD21	1:134:A:PHE:HB3	8	1.09	0.08	1.09

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1329)	1:118:A:LEU:HD22	1:134:A:PHE:HB3	8	1.09	0.08	1.09
(1,1329)	1:118:A:LEU:HD23	1:134:A:PHE:HB3	8	1.09	0.08	1.09
(1,178)	1:118:A:LEU:HD21	1:131:A:LEU:H	8	1.04	0.17	1.08
(1,178)	1:118:A:LEU:HD22	1:131:A:LEU:H	8	1.04	0.17	1.08
(1,178)	1:118:A:LEU:HD23	1:131:A:LEU:H	8	1.04	0.17	1.08
(1,1033)	1:118:A:LEU:HD21	1:115:A:ALA:HA	8	0.97	0.15	1.0
(1,1033)	1:118:A:LEU:HD22	1:115:A:ALA:HA	8	0.97	0.15	1.0
(1,1033)	1:118:A:LEU:HD23	1:115:A:ALA:HA	8	0.97	0.15	1.0
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG21	8	0.93	0.05	0.94
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG22	8	0.93	0.05	0.94
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG23	8	0.93	0.05	0.94
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG21	8	0.93	0.05	0.94
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG22	8	0.93	0.05	0.94
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG23	8	0.93	0.05	0.94
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG21	8	0.93	0.05	0.94
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG22	8	0.93	0.05	0.94
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG23	8	0.93	0.05	0.94
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE1	8	0.82	0.2	0.84
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE2	8	0.82	0.2	0.84
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE1	8	0.82	0.2	0.84
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE2	8	0.82	0.2	0.84
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE1	8	0.82	0.2	0.84
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE2	8	0.82	0.2	0.84
(1,298)	1:88:A:ARG:HD3	1:88:A:ARG:H	8	0.71	0.12	0.7
(1,2493)	1:118:A:LEU:HD21	1:119:A:PHE:HZ	8	0.61	0.23	0.62
(1,2493)	1:118:A:LEU:HD22	1:119:A:PHE:HZ	8	0.61	0.23	0.62
(1,2493)	1:118:A:LEU:HD23	1:119:A:PHE:HZ	8	0.61	0.23	0.62
(1,1349)	1:181:A:LEU:HD11	1:182:A:ASN:HB3	8	0.52	0.05	0.52
(1,1349)	1:181:A:LEU:HD12	1:182:A:ASN:HB3	8	0.52	0.05	0.52
(1,1349)	1:181:A:LEU:HD13	1:182:A:ASN:HB3	8	0.52	0.05	0.52
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD11	8	0.36	0.01	0.36
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD12	8	0.36	0.01	0.36
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD13	8	0.36	0.01	0.36
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE1	8	0.3	0.16	0.3
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE2	8	0.3	0.16	0.3
(2,130)	1:30:A:ASP:O	1:34:A:VAL:N	8	0.22	0.07	0.25
(1,96)	1:29:A:GLN:HB3	1:30:A:ASP:H	8	0.18	0.02	0.18
(1,531)	1:23:A:SER:H	1:26:A:GLN:HE22	8	0.16	0.04	0.16
(1,1740)	1:63:A:LEU:HD11	1:64:A:PRO:HG3	7	1.41	0.63	1.78
(1,1740)	1:63:A:LEU:HD12	1:64:A:PRO:HG3	7	1.41	0.63	1.78
(1,1740)	1:63:A:LEU:HD13	1:64:A:PRO:HG3	7	1.41	0.63	1.78
(1,2365)	2:93:B:VAL:HG21	1:89:A:TYR:HD1	7	1.04	0.47	1.03

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2365)	2:93:B:VAL:HG21	1:89:A:TYR:HD2	7	1.04	0.47	1.03
(1,2365)	2:93:B:VAL:HG22	1:89:A:TYR:HD1	7	1.04	0.47	1.03
(1,2365)	2:93:B:VAL:HG22	1:89:A:TYR:HD2	7	1.04	0.47	1.03
(1,2365)	2:93:B:VAL:HG23	1:89:A:TYR:HD1	7	1.04	0.47	1.03
(1,2365)	2:93:B:VAL:HG23	1:89:A:TYR:HD2	7	1.04	0.47	1.03
(1,74)	1:63:A:LEU:HD11	1:65:A:LEU:H	7	0.55	0.37	0.41
(1,74)	1:63:A:LEU:HD12	1:65:A:LEU:H	7	0.55	0.37	0.41
(1,74)	1:63:A:LEU:HD13	1:65:A:LEU:H	7	0.55	0.37	0.41
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD11	7	0.49	0.38	0.29
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD12	7	0.49	0.38	0.29
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD13	7	0.49	0.38	0.29
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD11	7	0.37	0.12	0.38
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD12	7	0.37	0.12	0.38
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD13	7	0.37	0.12	0.38
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD21	7	0.33	0.13	0.33
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD22	7	0.33	0.13	0.33
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD23	7	0.33	0.13	0.33
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD21	7	0.32	0.12	0.34
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD22	7	0.32	0.12	0.34
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD23	7	0.32	0.12	0.34
(1,994)	1:50:A:GLU:HG3	1:50:A:GLU:HA	7	0.26	0.03	0.25
(2,158)	1:156:A:ARG:O	1:160:A:ASP:N	7	0.19	0.04	0.19
(2,136)	1:37:A:SER:O	1:41:A:TYR:N	7	0.17	0.05	0.16
(1,3097)	1:126:A:GLY:H	2:101:B:ILE:HG13	7	0.16	0.05	0.14
(2,53)	1:93:A:PHE:O	1:97:A:LEU:H	7	0.15	0.04	0.16
(1,3086)	1:129:A:VAL:H	2:97:B:NLE:HD2	7	0.15	0.02	0.14
(1,3086)	1:129:A:VAL:H	2:97:B:NLE:HD3	7	0.15	0.02	0.14
(1,941)	1:68:A:SER:HB3	1:68:A:SER:HA	7	0.13	0.01	0.13
(2,91)	1:135:A:GLY:O	1:139:A:ALA:H	7	0.13	0.03	0.13
(1,868)	1:25:A:GLU:HG3	1:25:A:GLU:HA	7	0.11	0.01	0.11
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG21	6	1.92	0.02	1.92
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG22	6	1.92	0.02	1.92
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG23	6	1.92	0.02	1.92
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG21	6	1.66	0.51	1.78
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG22	6	1.66	0.51	1.78
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG23	6	1.66	0.51	1.78
(1,528)	1:55:A:PRO:HD3	1:47:A:GLN:HE21	6	1.08	0.36	1.14
(1,1103)	1:39:A:VAL:HG11	1:133:A:GLY:HA2	6	1.06	0.11	1.05
(1,1103)	1:39:A:VAL:HG11	1:133:A:GLY:HA3	6	1.06	0.11	1.05
(1,1103)	1:39:A:VAL:HG12	1:133:A:GLY:HA2	6	1.06	0.11	1.05
(1,1103)	1:39:A:VAL:HG12	1:133:A:GLY:HA3	6	1.06	0.11	1.05
(1,1103)	1:39:A:VAL:HG13	1:133:A:GLY:HA2	6	1.06	0.11	1.05

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1103)	1:39:A:VAL:HG13	1:133:A:GLY:HA3	6	1.06	0.11	1.05
(1,883)	1:39:A:VAL:HG21	1:36:A:ARG:HA	6	0.8	0.07	0.8
(1,883)	1:39:A:VAL:HG22	1:36:A:ARG:HA	6	0.8	0.07	0.8
(1,883)	1:39:A:VAL:HG23	1:36:A:ARG:HA	6	0.8	0.07	0.8
(1,2497)	1:39:A:VAL:HG21	1:35:A:PHE:HZ	6	0.64	0.09	0.61
(1,2497)	1:39:A:VAL:HG22	1:35:A:PHE:HZ	6	0.64	0.09	0.61
(1,2497)	1:39:A:VAL:HG23	1:35:A:PHE:HZ	6	0.64	0.09	0.61
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD11	6	0.63	0.42	0.49
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD12	6	0.63	0.42	0.49
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD13	6	0.63	0.42	0.49
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD11	6	0.63	0.42	0.49
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD12	6	0.63	0.42	0.49
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD13	6	0.63	0.42	0.49
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD11	6	0.63	0.42	0.49
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD12	6	0.63	0.42	0.49
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD13	6	0.63	0.42	0.49
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD11	6	0.63	0.42	0.49
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD12	6	0.63	0.42	0.49
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD13	6	0.63	0.42	0.49
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD11	6	0.63	0.42	0.49
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD12	6	0.63	0.42	0.49
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD13	6	0.63	0.42	0.49
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD11	6	0.63	0.42	0.49
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD12	6	0.63	0.42	0.49
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD13	6	0.63	0.42	0.49
(1,2433)	1:97:A:LEU:HD11	1:93:A:PHE:HE1	6	0.54	0.27	0.44
(1,2433)	1:97:A:LEU:HD11	1:93:A:PHE:HE2	6	0.54	0.27	0.44
(1,2433)	1:97:A:LEU:HD12	1:93:A:PHE:HE1	6	0.54	0.27	0.44
(1,2433)	1:97:A:LEU:HD12	1:93:A:PHE:HE2	6	0.54	0.27	0.44
(1,2433)	1:97:A:LEU:HD13	1:93:A:PHE:HE1	6	0.54	0.27	0.44
(1,2433)	1:97:A:LEU:HD13	1:93:A:PHE:HE2	6	0.54	0.27	0.44
(1,2354)	1:76:A:ARG:HB3	1:41:A:TYR:HD1	6	0.52	0.14	0.5
(1,2354)	1:76:A:ARG:HB3	1:41:A:TYR:HD2	6	0.52	0.14	0.5
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG21	6	0.5	0.27	0.54
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG22	6	0.5	0.27	0.54
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG23	6	0.5	0.27	0.54
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG21	6	0.38	0.0	0.38
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG22	6	0.38	0.0	0.38
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG23	6	0.38	0.0	0.38
(1,896)	1:142:A:VAL:HG21	1:103:A:THR:HA	6	0.3	0.17	0.24
(1,896)	1:142:A:VAL:HG22	1:103:A:THR:HA	6	0.3	0.17	0.24
(1,896)	1:142:A:VAL:HG23	1:103:A:THR:HA	6	0.3	0.17	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD11	6	0.27	0.05	0.26
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD12	6	0.27	0.05	0.26
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD13	6	0.27	0.05	0.26
(1,1663)	1:27:A:VAL:HG11	1:24:A:GLU:HB3	6	0.26	0.16	0.21
(1,1663)	1:27:A:VAL:HG12	1:24:A:GLU:HB3	6	0.26	0.16	0.21
(1,1663)	1:27:A:VAL:HG13	1:24:A:GLU:HB3	6	0.26	0.16	0.21
(1,839)	1:63:A:LEU:HB3	1:62:A:THR:HA	6	0.24	0.09	0.2
(1,1138)	1:52:A:VAL:HG11	1:51:A:GLY:HA3	6	0.23	0.06	0.24
(1,1138)	1:52:A:VAL:HG12	1:51:A:GLY:HA3	6	0.23	0.06	0.24
(1,1138)	1:52:A:VAL:HG13	1:51:A:GLY:HA3	6	0.23	0.06	0.24
(1,1138)	1:52:A:VAL:HG21	1:51:A:GLY:HA3	6	0.23	0.06	0.24
(1,1138)	1:52:A:VAL:HG22	1:51:A:GLY:HA3	6	0.23	0.06	0.24
(1,1138)	1:52:A:VAL:HG23	1:51:A:GLY:HA3	6	0.23	0.06	0.24
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD21	6	0.22	0.07	0.26
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD22	6	0.22	0.07	0.26
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD23	6	0.22	0.07	0.26
(1,1189)	1:159:A:VAL:HG11	1:156:A:ARG:HD3	6	0.2	0.1	0.19
(1,1189)	1:159:A:VAL:HG12	1:156:A:ARG:HD3	6	0.2	0.1	0.19
(1,1189)	1:159:A:VAL:HG13	1:156:A:ARG:HD3	6	0.2	0.1	0.19
(2,10)	1:28:A:ALA:O	1:32:A:GLU:N	6	0.18	0.05	0.18
(1,2779)	2:88:B:ARG:HB3	2:88:B:ARG:HD3	6	0.15	0.01	0.15
(1,2758)	2:82:B:ILE:HB	2:83:B:ILE:H	6	0.15	0.02	0.15
(1,2636)	2:90:B:LEU:HA	2:93:B:VAL:HB	6	0.15	0.02	0.16
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD21	6	0.13	0.01	0.12
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD22	6	0.13	0.01	0.12
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD23	6	0.13	0.01	0.12
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD21	6	0.13	0.01	0.12
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD22	6	0.13	0.01	0.12
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD23	6	0.13	0.01	0.12
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD21	6	0.13	0.01	0.12
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD22	6	0.13	0.01	0.12
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD23	6	0.13	0.01	0.12
(2,47)	1:83:A:ASP:O	1:87:A:ARG:N	6	0.13	0.02	0.12
(1,2454)	1:147:A:LEU:HD21	1:150:A:PHE:HE1	5	0.73	0.3	0.85
(1,2454)	1:147:A:LEU:HD21	1:150:A:PHE:HE2	5	0.73	0.3	0.85
(1,2454)	1:147:A:LEU:HD22	1:150:A:PHE:HE1	5	0.73	0.3	0.85
(1,2454)	1:147:A:LEU:HD22	1:150:A:PHE:HE2	5	0.73	0.3	0.85
(1,2454)	1:147:A:LEU:HD23	1:150:A:PHE:HE1	5	0.73	0.3	0.85
(1,2454)	1:147:A:LEU:HD23	1:150:A:PHE:HE2	5	0.73	0.3	0.85
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD21	5	0.7	0.29	0.7
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD22	5	0.7	0.29	0.7
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD23	5	0.7	0.29	0.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,543)	1:181:A:LEU:HD11	1:73:A:GLN:HE21	5	0.66	0.46	0.39
(1,543)	1:181:A:LEU:HD12	1:73:A:GLN:HE21	5	0.66	0.46	0.39
(1,543)	1:181:A:LEU:HD13	1:73:A:GLN:HE21	5	0.66	0.46	0.39
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD21	5	0.65	0.25	0.48
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD22	5	0.65	0.25	0.48
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD23	5	0.65	0.25	0.48
(1,2382)	1:147:A:LEU:HD21	1:150:A:PHE:HD1	5	0.62	0.3	0.61
(1,2382)	1:147:A:LEU:HD21	1:150:A:PHE:HD2	5	0.62	0.3	0.61
(1,2382)	1:147:A:LEU:HD22	1:150:A:PHE:HD1	5	0.62	0.3	0.61
(1,2382)	1:147:A:LEU:HD22	1:150:A:PHE:HD2	5	0.62	0.3	0.61
(1,2382)	1:147:A:LEU:HD23	1:150:A:PHE:HD1	5	0.62	0.3	0.61
(1,2382)	1:147:A:LEU:HD23	1:150:A:PHE:HD2	5	0.62	0.3	0.61
(1,1535)	1:156:A:ARG:HA	1:159:A:VAL:HB	5	0.58	0.14	0.52
(1,1029)	1:147:A:LEU:HD21	1:104:A:ALA:HA	5	0.44	0.22	0.37
(1,1029)	1:147:A:LEU:HD22	1:104:A:ALA:HA	5	0.44	0.22	0.37
(1,1029)	1:147:A:LEU:HD23	1:104:A:ALA:HA	5	0.44	0.22	0.37
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD11	5	0.42	0.17	0.51
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD12	5	0.42	0.17	0.51
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD13	5	0.42	0.17	0.51
(1,1002)	1:181:A:LEU:HD21	1:181:A:LEU:HA	5	0.4	0.01	0.4
(1,1002)	1:181:A:LEU:HD22	1:181:A:LEU:HA	5	0.4	0.01	0.4
(1,1002)	1:181:A:LEU:HD23	1:181:A:LEU:HA	5	0.4	0.01	0.4
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD21	5	0.35	0.2	0.43
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD22	5	0.35	0.2	0.43
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD23	5	0.35	0.2	0.43
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD21	5	0.35	0.2	0.43
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD22	5	0.35	0.2	0.43
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD23	5	0.35	0.2	0.43
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD21	5	0.35	0.2	0.43
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD22	5	0.35	0.2	0.43
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD23	5	0.35	0.2	0.43
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD21	5	0.35	0.2	0.43
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD22	5	0.35	0.2	0.43
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD23	5	0.35	0.2	0.43
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD21	5	0.35	0.2	0.43
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD22	5	0.35	0.2	0.43
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD23	5	0.35	0.2	0.43
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD21	5	0.35	0.2	0.43
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD22	5	0.35	0.2	0.43
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD23	5	0.35	0.2	0.43
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG21	5	0.35	0.07	0.33
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG22	5	0.35	0.07	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG23	5	0.35	0.07	0.33
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG21	5	0.35	0.07	0.33
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG22	5	0.35	0.07	0.33
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG23	5	0.35	0.07	0.33
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG21	5	0.34	0.05	0.32
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG22	5	0.34	0.05	0.32
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG23	5	0.34	0.05	0.32
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG21	5	0.34	0.05	0.32
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG22	5	0.34	0.05	0.32
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG23	5	0.34	0.05	0.32
(1,1709)	1:98:A:GLN:HE22	1:98:A:GLN:HB3	5	0.27	0.1	0.27
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG21	5	0.22	0.03	0.21
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG22	5	0.22	0.03	0.21
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG23	5	0.22	0.03	0.21
(2,109)	1:155:A:THR:O	1:159:A:VAL:H	5	0.19	0.04	0.19
(1,2494)	1:131:A:LEU:HD21	1:119:A:PHE:HZ	5	0.18	0.03	0.17
(1,2494)	1:131:A:LEU:HD22	1:119:A:PHE:HZ	5	0.18	0.03	0.17
(1,2494)	1:131:A:LEU:HD23	1:119:A:PHE:HZ	5	0.18	0.03	0.17
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG21	5	0.14	0.04	0.13
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG22	5	0.14	0.04	0.13
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG23	5	0.14	0.04	0.13
(2,95)	1:137:A:ARG:O	1:141:A:HIS:H	5	0.14	0.03	0.12
(2,77)	1:126:A:GLY:O	1:130:A:ALA:H	5	0.13	0.03	0.11
(1,1111)	2:97:B:NLE:HB2	1:126:A:GLY:HA3	5	0.13	0.02	0.14
(1,1111)	2:97:B:NLE:HB3	1:126:A:GLY:HA3	5	0.13	0.02	0.14
(1,2795)	2:88:B:ARG:HA	2:91:B:ALA:H	5	0.13	0.02	0.13
(2,50)	1:85:A:ILE:O	1:89:A:TYR:H	5	0.12	0.01	0.12
(1,901)	1:94:A:GLN:H	1:92:A:GLU:HA	5	0.12	0.01	0.11
(2,71)	1:114:A:ILE:O	1:118:A:LEU:H	5	0.11	0.01	0.1
(1,1867)	1:73:A:GLN:HG3	1:181:A:LEU:HD11	4	0.97	0.38	1.0
(1,1867)	1:73:A:GLN:HG3	1:181:A:LEU:HD12	4	0.97	0.38	1.0
(1,1867)	1:73:A:GLN:HG3	1:181:A:LEU:HD13	4	0.97	0.38	1.0
(1,1087)	1:47:A:GLN:HE22	1:55:A:PRO:HD3	4	0.65	0.51	0.61
(1,390)	1:63:A:LEU:HD11	1:36:A:ARG:H	4	0.55	0.2	0.52
(1,390)	1:63:A:LEU:HD12	1:36:A:ARG:H	4	0.55	0.2	0.52
(1,390)	1:63:A:LEU:HD13	1:36:A:ARG:H	4	0.55	0.2	0.52
(1,2443)	1:153:A:GLN:HB3	1:150:A:PHE:HE1	4	0.43	0.18	0.38
(1,2443)	1:153:A:GLN:HB3	1:150:A:PHE:HE2	4	0.43	0.18	0.38
(1,874)	1:63:A:LEU:HD21	1:36:A:ARG:HA	4	0.38	0.06	0.38
(1,874)	1:63:A:LEU:HD22	1:36:A:ARG:HA	4	0.38	0.06	0.38
(1,874)	1:63:A:LEU:HD23	1:36:A:ARG:HA	4	0.38	0.06	0.38
(1,1050)	1:19:A:LEU:HD21	1:19:A:LEU:HA	4	0.34	0.05	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1050)	1:19:A:LEU:HD22	1:19:A:LEU:HA	4	0.34	0.05	0.32
(1,1050)	1:19:A:LEU:HD23	1:19:A:LEU:HA	4	0.34	0.05	0.32
(1,3011)	1:100:A:LEU:HD21	2:82:B:ILE:HD11	4	0.33	0.01	0.33
(1,3011)	1:100:A:LEU:HD21	2:82:B:ILE:HD12	4	0.33	0.01	0.33
(1,3011)	1:100:A:LEU:HD21	2:82:B:ILE:HD13	4	0.33	0.01	0.33
(1,3011)	1:100:A:LEU:HD22	2:82:B:ILE:HD11	4	0.33	0.01	0.33
(1,3011)	1:100:A:LEU:HD22	2:82:B:ILE:HD12	4	0.33	0.01	0.33
(1,3011)	1:100:A:LEU:HD22	2:82:B:ILE:HD13	4	0.33	0.01	0.33
(1,3011)	1:100:A:LEU:HD23	2:82:B:ILE:HD11	4	0.33	0.01	0.33
(1,3011)	1:100:A:LEU:HD23	2:82:B:ILE:HD12	4	0.33	0.01	0.33
(1,3011)	1:100:A:LEU:HD23	2:82:B:ILE:HD13	4	0.33	0.01	0.33
(1,1877)	1:101:A:GLN:H	1:100:A:LEU:HD11	4	0.32	0.1	0.38
(1,1877)	1:101:A:GLN:H	1:100:A:LEU:HD12	4	0.32	0.1	0.38
(1,1877)	1:101:A:GLN:H	1:100:A:LEU:HD13	4	0.32	0.1	0.38
(1,2559)	1:145:A:HIS:H	1:145:A:HIS:HD2	4	0.21	0.02	0.22
(1,2336)	1:145:A:HIS:HA	1:145:A:HIS:HE1	4	0.2	0.01	0.2
(1,1427)	1:92:A:GLU:HA	1:92:A:GLU:HG3	4	0.18	0.01	0.18
(2,110)	1:155:A:THR:O	1:159:A:VAL:N	4	0.17	0.03	0.18
(1,2201)	1:97:A:LEU:HA	1:96:A:MET:HE1	4	0.17	0.05	0.15
(1,2201)	1:97:A:LEU:HA	1:96:A:MET:HE2	4	0.17	0.05	0.15
(1,2201)	1:97:A:LEU:HA	1:96:A:MET:HE3	4	0.17	0.05	0.15
(1,1660)	1:47:A:GLN:HE21	1:46:A:GLU:HB3	4	0.16	0.04	0.15
(1,442)	1:181:A:LEU:HD11	1:182:A:ASN:H	4	0.15	0.01	0.15
(1,442)	1:181:A:LEU:HD12	1:182:A:ASN:H	4	0.15	0.01	0.15
(1,442)	1:181:A:LEU:HD13	1:182:A:ASN:H	4	0.15	0.01	0.15
(1,1534)	1:160:A:ASP:H	1:159:A:VAL:HB	4	0.15	0.02	0.15
(1,490)	1:164:A:HIS:HB3	1:164:A:HIS:H	4	0.14	0.01	0.14
(2,12)	1:29:A:GLN:O	1:33:A:GLU:N	4	0.14	0.06	0.11
(1,2014)	1:159:A:VAL:HA	1:159:A:VAL:HG11	4	0.13	0.0	0.13
(1,2014)	1:159:A:VAL:HA	1:159:A:VAL:HG12	4	0.13	0.0	0.13
(1,2014)	1:159:A:VAL:HA	1:159:A:VAL:HG13	4	0.13	0.0	0.13
(1,2206)	1:129:A:VAL:HB	1:130:A:ALA:HB1	4	0.12	0.0	0.12
(1,2206)	1:129:A:VAL:HB	1:130:A:ALA:HB2	4	0.12	0.0	0.12
(1,2206)	1:129:A:VAL:HB	1:130:A:ALA:HB3	4	0.12	0.0	0.12
(2,5)	1:26:A:GLN:O	1:30:A:ASP:H	4	0.12	0.02	0.12
(1,2983)	1:85:A:ILE:HG21	2:93:B:VAL:HB	4	0.12	0.01	0.12
(1,2983)	1:85:A:ILE:HG22	2:93:B:VAL:HB	4	0.12	0.01	0.12
(1,2983)	1:85:A:ILE:HG23	2:93:B:VAL:HB	4	0.12	0.01	0.12
(2,57)	1:106:A:ASN:O	1:110:A:TYR:H	4	0.12	0.0	0.12
(2,31)	1:39:A:VAL:O	1:43:A:HIS:H	4	0.11	0.01	0.12
(2,81)	1:129:A:VAL:O	1:133:A:GLY:H	4	0.11	0.0	0.11
(1,2344)	1:160:A:ASP:HB3	1:164:A:HIS:HE1	3	1.14	0.25	1.01

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1898)	1:143:A:TYR:HD1	1:147:A:LEU:HD21	3	0.96	0.3	0.89
(1,1898)	1:143:A:TYR:HD1	1:147:A:LEU:HD22	3	0.96	0.3	0.89
(1,1898)	1:143:A:TYR:HD1	1:147:A:LEU:HD23	3	0.96	0.3	0.89
(1,1898)	1:143:A:TYR:HD2	1:147:A:LEU:HD21	3	0.96	0.3	0.89
(1,1898)	1:143:A:TYR:HD2	1:147:A:LEU:HD22	3	0.96	0.3	0.89
(1,1898)	1:143:A:TYR:HD2	1:147:A:LEU:HD23	3	0.96	0.3	0.89
(1,1750)	1:142:A:VAL:HG21	1:102:A:PRO:HG3	3	0.36	0.06	0.34
(1,1750)	1:142:A:VAL:HG22	1:102:A:PRO:HG3	3	0.36	0.06	0.34
(1,1750)	1:142:A:VAL:HG23	1:102:A:PRO:HG3	3	0.36	0.06	0.34
(1,106)	1:162:A:MET:HG3	1:168:A:ALA:H	3	0.3	0.24	0.15
(1,268)	1:50:A:GLU:HB3	1:52:A:VAL:H	3	0.28	0.15	0.25
(1,2658)	2:89:B:HIS:HA	2:92:B:MK8:HB	3	0.21	0.06	0.22
(1,2759)	2:82:B:ILE:H	2:82:B:ILE:HB	3	0.2	0.04	0.18
(1,320)	1:163:A:LEU:HD11	1:29:A:GLN:H	3	0.18	0.04	0.19
(1,320)	1:163:A:LEU:HD12	1:29:A:GLN:H	3	0.18	0.04	0.19
(1,320)	1:163:A:LEU:HD13	1:29:A:GLN:H	3	0.18	0.04	0.19
(1,320)	1:163:A:LEU:HD21	1:29:A:GLN:H	3	0.18	0.04	0.19
(1,320)	1:163:A:LEU:HD22	1:29:A:GLN:H	3	0.18	0.04	0.19
(1,320)	1:163:A:LEU:HD23	1:29:A:GLN:H	3	0.18	0.04	0.19
(1,1424)	1:163:A:LEU:HD11	1:25:A:GLU:HG3	3	0.18	0.05	0.16
(1,1424)	1:163:A:LEU:HD12	1:25:A:GLU:HG3	3	0.18	0.05	0.16
(1,1424)	1:163:A:LEU:HD13	1:25:A:GLU:HG3	3	0.18	0.05	0.16
(1,1424)	1:163:A:LEU:HD21	1:25:A:GLU:HG3	3	0.18	0.05	0.16
(1,1424)	1:163:A:LEU:HD22	1:25:A:GLU:HG3	3	0.18	0.05	0.16
(1,1424)	1:163:A:LEU:HD23	1:25:A:GLU:HG3	3	0.18	0.05	0.16
(1,1923)	1:147:A:LEU:HA	1:147:A:LEU:HD11	3	0.16	0.05	0.15
(1,1923)	1:147:A:LEU:HA	1:147:A:LEU:HD12	3	0.16	0.05	0.15
(1,1923)	1:147:A:LEU:HA	1:147:A:LEU:HD13	3	0.16	0.05	0.15
(1,735)	1:26:A:GLN:H	1:23:A:SER:HB3	3	0.16	0.01	0.15
(1,1893)	1:147:A:LEU:H	1:147:A:LEU:HD21	3	0.15	0.04	0.13
(1,1893)	1:147:A:LEU:H	1:147:A:LEU:HD22	3	0.15	0.04	0.13
(1,1893)	1:147:A:LEU:H	1:147:A:LEU:HD23	3	0.15	0.04	0.13
(1,2394)	1:107:A:ALA:HB1	1:150:A:PHE:HD1	3	0.14	0.01	0.13
(1,2394)	1:107:A:ALA:HB1	1:150:A:PHE:HD2	3	0.14	0.01	0.13
(1,2394)	1:107:A:ALA:HB2	1:150:A:PHE:HD1	3	0.14	0.01	0.13
(1,2394)	1:107:A:ALA:HB2	1:150:A:PHE:HD2	3	0.14	0.01	0.13
(1,2394)	1:107:A:ALA:HB3	1:150:A:PHE:HD1	3	0.14	0.01	0.13
(1,2394)	1:107:A:ALA:HB3	1:150:A:PHE:HD2	3	0.14	0.01	0.13
(1,2772)	2:83:B:ILE:HB	2:84:B:ARG:H	3	0.14	0.01	0.14
(1,3069)	1:118:A:LEU:HD11	2:91:B:ALA:HA	3	0.13	0.0	0.13
(1,3069)	1:118:A:LEU:HD12	2:91:B:ALA:HA	3	0.13	0.0	0.13
(1,3069)	1:118:A:LEU:HD13	2:91:B:ALA:HA	3	0.13	0.0	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3069)	1:118:A:LEU:HD21	2:91:B:ALA:HA	3	0.13	0.0	0.13
(1,3069)	1:118:A:LEU:HD22	2:91:B:ALA:HA	3	0.13	0.0	0.13
(1,3069)	1:118:A:LEU:HD23	2:91:B:ALA:HA	3	0.13	0.0	0.13
(2,97)	1:139:A:ALA:O	1:143:A:TYR:H	3	0.12	0.02	0.11
(1,2812)	2:97:B:NLE:HB2	2:101:B:ILE:HG21	3	0.12	0.02	0.11
(1,2812)	2:97:B:NLE:HB2	2:101:B:ILE:HG22	3	0.12	0.02	0.11
(1,2812)	2:97:B:NLE:HB2	2:101:B:ILE:HG23	3	0.12	0.02	0.11
(1,2812)	2:97:B:NLE:HB3	2:101:B:ILE:HG21	3	0.12	0.02	0.11
(1,2812)	2:97:B:NLE:HB3	2:101:B:ILE:HG22	3	0.12	0.02	0.11
(1,2812)	2:97:B:NLE:HB3	2:101:B:ILE:HG23	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD11	2:86:B:ILE:HG21	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD11	2:86:B:ILE:HG22	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD11	2:86:B:ILE:HG23	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD12	2:86:B:ILE:HG21	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD12	2:86:B:ILE:HG22	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD12	2:86:B:ILE:HG23	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD13	2:86:B:ILE:HG21	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD13	2:86:B:ILE:HG22	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD13	2:86:B:ILE:HG23	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD21	2:86:B:ILE:HG21	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD21	2:86:B:ILE:HG22	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD21	2:86:B:ILE:HG23	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD22	2:86:B:ILE:HG21	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD22	2:86:B:ILE:HG22	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD22	2:86:B:ILE:HG23	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD23	2:86:B:ILE:HG21	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD23	2:86:B:ILE:HG22	3	0.12	0.02	0.11
(1,3049)	1:97:A:LEU:HD23	2:86:B:ILE:HG23	3	0.12	0.02	0.11
(1,2241)	1:28:A:ALA:H	1:168:A:ALA:HB1	3	0.12	0.01	0.12
(1,2241)	1:28:A:ALA:H	1:168:A:ALA:HB2	3	0.12	0.01	0.12
(1,2241)	1:28:A:ALA:H	1:168:A:ALA:HB3	3	0.12	0.01	0.12
(2,125)	1:170:A:TRP:O	1:174:A:ARG:H	3	0.12	0.01	0.11
(1,3044)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	3	0.11	0.0	0.11
(1,3044)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	3	0.11	0.0	0.11
(1,3044)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	3	0.11	0.0	0.11
(1,499)	1:119:A:PHE:HD1	1:116:A:THR:H	3	0.11	0.01	0.11
(1,499)	1:119:A:PHE:HD2	1:116:A:THR:H	3	0.11	0.01	0.11
(2,79)	1:127:A:ARG:O	1:131:A:LEU:H	3	0.11	0.0	0.11
(1,1003)	1:182:A:ASN:HA	1:181:A:LEU:HA	3	0.11	0.01	0.1
(1,2495)	1:128:A:VAL:HG21	1:119:A:PHE:HZ	3	0.11	0.0	0.11
(1,2495)	1:128:A:VAL:HG22	1:119:A:PHE:HZ	3	0.11	0.0	0.11
(1,2495)	1:128:A:VAL:HG23	1:119:A:PHE:HZ	3	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,85)	1:131:A:LEU:O	1:135:A:GLY:H	3	0.11	0.0	0.11
(1,732)	1:66:A:GLN:HG3	1:69:A:SER:HB3	2	0.63	0.32	0.63
(1,1395)	1:46:A:GLU:H	1:46:A:GLU:HG3	2	0.34	0.01	0.34
(1,2683)	2:84:B:ARG:HA	2:84:B:ARG:HD3	2	0.28	0.13	0.28
(1,1467)	1:61:A:VAL:HA	1:60:A:MET:HG3	2	0.26	0.01	0.26
(1,611)	1:63:A:LEU:H	1:62:A:THR:HB	2	0.26	0.0	0.26
(1,65)	1:18:A:ALA:HA	1:19:A:LEU:H	2	0.25	0.0	0.25
(1,1995)	1:97:A:LEU:HA	1:100:A:LEU:HD21	2	0.25	0.08	0.25
(1,1995)	1:97:A:LEU:HA	1:100:A:LEU:HD22	2	0.25	0.08	0.25
(1,1995)	1:97:A:LEU:HA	1:100:A:LEU:HD23	2	0.25	0.08	0.25
(1,1307)	2:93:B:VAL:HG21	1:89:A:TYR:HB3	2	0.23	0.0	0.23
(1,1307)	2:93:B:VAL:HG22	1:89:A:TYR:HB3	2	0.23	0.0	0.23
(1,1307)	2:93:B:VAL:HG23	1:89:A:TYR:HB3	2	0.23	0.0	0.23
(1,2675)	2:82:B:ILE:HG21	2:83:B:ILE:H	2	0.2	0.03	0.2
(1,2675)	2:82:B:ILE:HG22	2:83:B:ILE:H	2	0.2	0.03	0.2
(1,2675)	2:82:B:ILE:HG23	2:83:B:ILE:H	2	0.2	0.03	0.2
(1,1115)	1:35:A:PHE:HE1	1:135:A:GLY:HA2	2	0.2	0.01	0.2
(1,1115)	1:35:A:PHE:HE2	1:135:A:GLY:HA2	2	0.2	0.01	0.2
(1,2939)	2:99:B:ARG:HG3	2:100:B:SER:H	2	0.18	0.04	0.18
(1,1117)	1:139:A:ALA:H	1:135:A:GLY:HA3	2	0.15	0.0	0.15
(1,674)	1:74:A:VAL:HG21	1:34:A:VAL:HA	2	0.14	0.02	0.14
(1,674)	1:74:A:VAL:HG22	1:34:A:VAL:HA	2	0.14	0.02	0.14
(1,674)	1:74:A:VAL:HG23	1:34:A:VAL:HA	2	0.14	0.02	0.14
(1,960)	1:163:A:LEU:HD11	1:164:A:HIS:HA	2	0.14	0.0	0.14
(1,960)	1:163:A:LEU:HD12	1:164:A:HIS:HA	2	0.14	0.0	0.14
(1,960)	1:163:A:LEU:HD13	1:164:A:HIS:HA	2	0.14	0.0	0.14
(1,960)	1:163:A:LEU:HD21	1:164:A:HIS:HA	2	0.14	0.0	0.14
(1,960)	1:163:A:LEU:HD22	1:164:A:HIS:HA	2	0.14	0.0	0.14
(1,960)	1:163:A:LEU:HD23	1:164:A:HIS:HA	2	0.14	0.0	0.14
(1,1037)	1:65:A:LEU:HD11	1:65:A:LEU:HA	2	0.14	0.01	0.14
(1,1037)	1:65:A:LEU:HD12	1:65:A:LEU:HA	2	0.14	0.01	0.14
(1,1037)	1:65:A:LEU:HD13	1:65:A:LEU:HA	2	0.14	0.01	0.14
(1,1037)	1:65:A:LEU:HD21	1:65:A:LEU:HA	2	0.14	0.01	0.14
(1,1037)	1:65:A:LEU:HD22	1:65:A:LEU:HA	2	0.14	0.01	0.14
(1,1037)	1:65:A:LEU:HD23	1:65:A:LEU:HA	2	0.14	0.01	0.14
(1,1320)	1:85:A:ILE:HG21	1:89:A:TYR:HB3	2	0.13	0.02	0.13
(1,1320)	1:85:A:ILE:HG22	1:89:A:TYR:HB3	2	0.13	0.02	0.13
(1,1320)	1:85:A:ILE:HG23	1:89:A:TYR:HB3	2	0.13	0.02	0.13
(1,2858)	2:80:B:GLU:HA	2:83:B:ILE:HB	2	0.13	0.02	0.13
(2,113)	1:157:A:PHE:O	1:161:A:PHE:H	2	0.12	0.01	0.12
(1,175)	1:118:A:LEU:HD11	1:131:A:LEU:H	2	0.12	0.02	0.12
(1,175)	1:118:A:LEU:HD12	1:131:A:LEU:H	2	0.12	0.02	0.12

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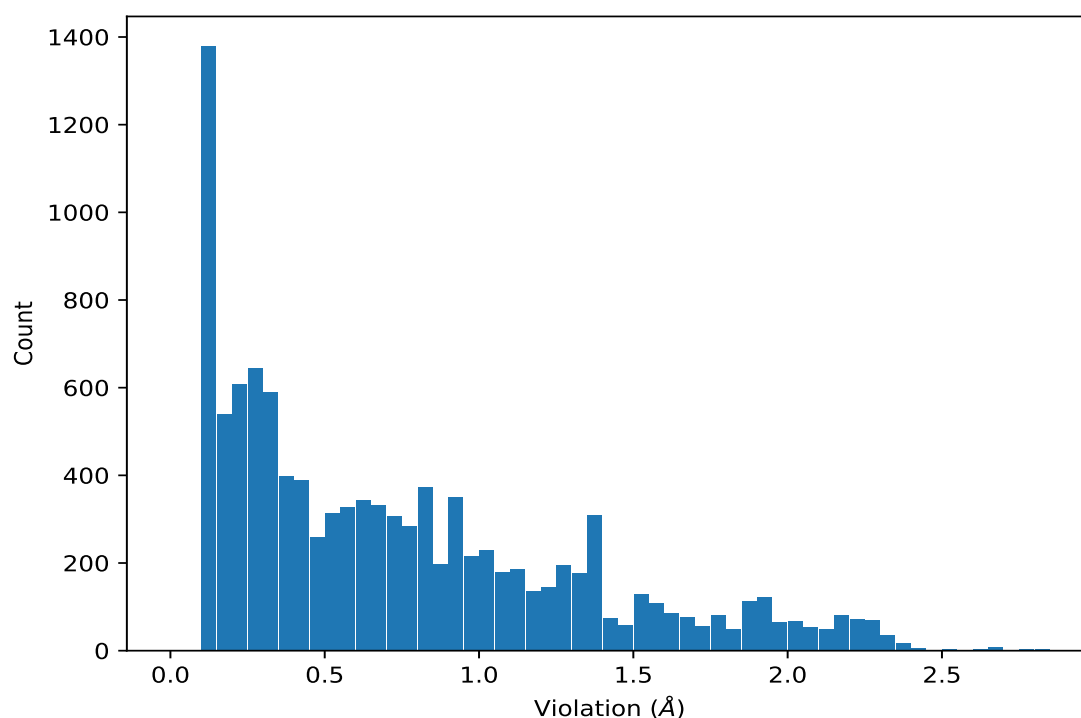
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,175)	1:118:A:LEU:HD13	1:131:A:LEU:H	2	0.12	0.02	0.12
(1,368)	1:119:A:PHE:HA	1:123:A:ILE:H	2	0.12	0.02	0.12
(1,1707)	1:94:A:GLN:HE22	1:94:A:GLN:HB3	2	0.12	0.02	0.12
(1,1315)	1:39:A:VAL:HG11	1:40:A:PHE:HB3	2	0.12	0.0	0.12
(1,1315)	1:39:A:VAL:HG12	1:40:A:PHE:HB3	2	0.12	0.0	0.12
(1,1315)	1:39:A:VAL:HG13	1:40:A:PHE:HB3	2	0.12	0.0	0.12
(2,19)	1:33:A:GLU:O	1:37:A:SER:H	2	0.12	0.0	0.12
(2,142)	1:84:A:ASP:O	1:88:A:ARG:N	2	0.12	0.0	0.12
(1,1098)	2:97:B:NLE:HB2	1:126:A:GLY:HA2	2	0.11	0.0	0.11
(1,1098)	2:97:B:NLE:HB3	1:126:A:GLY:HA2	2	0.11	0.0	0.11
(1,2318)	1:84:A:ASP:HB3	1:85:A:ILE:HD11	2	0.11	0.0	0.11
(1,2318)	1:84:A:ASP:HB3	1:85:A:ILE:HD12	2	0.11	0.0	0.11
(1,2318)	1:84:A:ASP:HB3	1:85:A:ILE:HD13	2	0.11	0.0	0.11
(1,2847)	2:95:B:ASP:HA	2:99:B:ARG:H	2	0.11	0.0	0.11
(2,92)	1:135:A:GLY:O	1:139:A:ALA:N	2	0.11	0.0	0.11
(2,25)	1:36:A:ARG:O	1:40:A:PHE:H	2	0.11	0.0	0.11
(2,117)	1:159:A:VAL:O	1:163:A:LEU:H	2	0.11	0.0	0.11
(1,1063)	1:19:A:LEU:HB3	1:18:A:ALA:HA	2	0.1	0.0	0.1
(1,2599)	1:108:A:TYR:HB3	1:108:A:TYR:HE1	2	0.1	0.0	0.1
(1,2599)	1:108:A:TYR:HB3	1:108:A:TYR:HE2	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG11	10	2.83
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG12	10	2.83
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG13	10	2.83
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG11	2	2.8
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG12	2	2.8
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG13	2	2.8
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG11	9	2.69
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG12	9	2.69
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG13	9	2.69
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG11	3	2.66
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG12	3	2.66
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG13	3	2.66
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG11	14	2.66
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG12	14	2.66
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG13	14	2.66
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG11	11	2.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG12	11	2.6
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG13	11	2.6
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG11	18	2.54
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG12	18	2.54
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG13	18	2.54
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	18	2.44
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	18	2.44
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	18	2.44
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG11	8	2.42
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG12	8	2.42
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG13	8	2.42
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG11	11	2.4
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG12	11	2.4
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG13	11	2.4
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG11	15	2.4
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG12	15	2.4
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG13	15	2.4
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG11	9	2.36
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG12	9	2.36
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG13	9	2.36
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG11	13	2.36
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG12	13	2.36
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG13	13	2.36
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	1	2.36
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	1	2.36
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	1	2.36
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	19	2.36
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	19	2.36
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	19	2.36
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	6	2.34
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	6	2.34
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	6	2.34
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	9	2.33
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	9	2.33
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	9	2.33
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	4	2.33
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	4	2.33
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	4	2.33
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	16	2.33
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	16	2.33
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	16	2.33
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG11	19	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG12	19	2.32
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG13	19	2.32
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	5	2.32
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	5	2.32
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	5	2.32
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	9	2.32
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	9	2.32
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	9	2.32
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	12	2.32
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	12	2.32
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	12	2.32
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	15	2.32
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	15	2.32
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	15	2.32
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	12	2.31
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	12	2.31
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	12	2.31
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG11	2	2.31
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG12	2	2.31
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG13	2	2.31
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	14	2.31
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	14	2.31
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	14	2.31
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	15	2.3
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	15	2.3
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	15	2.3
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	18	2.3
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	18	2.3
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	18	2.3
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	13	2.29
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	13	2.29
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	13	2.29
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	13	2.29
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	13	2.29
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	13	2.29
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	12	2.28
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	12	2.28
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	12	2.28
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	12	2.28
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	12	2.28
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	12	2.28
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	12	2.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	12	2.28
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	12	2.28
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	2	2.28
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	2	2.28
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	2	2.28
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	1	2.27
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	1	2.27
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	1	2.27
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG11	12	2.27
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG12	12	2.27
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG13	12	2.27
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	8	2.27
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	8	2.27
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	8	2.27
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD21	7	2.26
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD22	7	2.26
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD23	7	2.26
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG11	7	2.26
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG12	7	2.26
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG13	7	2.26
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	3	2.26
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	3	2.26
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	3	2.26
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	7	2.26
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	7	2.26
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	7	2.26
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	10	2.26
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	10	2.26
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	10	2.26
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	8	2.25
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	8	2.25
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	8	2.25
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	8	2.25
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	8	2.25
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	8	2.25
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	8	2.25
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	8	2.25
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	8	2.25
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	16	2.25
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	16	2.25
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	16	2.25
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	16	2.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	16	2.25
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	16	2.25
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	16	2.25
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	16	2.25
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	16	2.25
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	17	2.25
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	17	2.25
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	17	2.25
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	15	2.24
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	15	2.24
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	15	2.24
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	1	2.24
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	1	2.24
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	1	2.24
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	1	2.24
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	1	2.24
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	1	2.24
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	1	2.24
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	1	2.24
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	1	2.24
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	15	2.24
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	15	2.24
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	15	2.24
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	15	2.24
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	15	2.24
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	15	2.24
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	15	2.24
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	15	2.24
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	15	2.24
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	6	2.24
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	6	2.24
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	6	2.24
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	13	2.24
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	13	2.24
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	13	2.24
(1,1116)	1:158:A:VAL:HG21	1:135:A:GLY:HA2	10	2.24
(1,1116)	1:158:A:VAL:HG22	1:135:A:GLY:HA2	10	2.24
(1,1116)	1:158:A:VAL:HG23	1:135:A:GLY:HA2	10	2.24
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	6	2.23
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	6	2.23
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	6	2.23
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	9	2.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	9	2.23
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	9	2.23
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	4	2.23
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	4	2.23
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	4	2.23
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD21	20	2.23
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD22	20	2.23
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD23	20	2.23
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	9	2.22
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	9	2.22
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	9	2.22
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	2	2.22
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	2	2.22
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	2	2.22
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	1	2.21
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	1	2.21
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	1	2.21
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG11	20	2.21
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG12	20	2.21
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG13	20	2.21
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD21	16	2.21
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD22	16	2.21
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD23	16	2.21
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	16	2.2
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	16	2.2
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	16	2.2
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	16	2.2
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	16	2.2
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	16	2.2
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	16	2.2
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	16	2.2
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	16	2.2
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	16	2.2
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	16	2.2
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	16	2.2
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG21	2	2.2
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG22	2	2.2
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG23	2	2.2
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	11	2.19
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	11	2.19
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	11	2.19
(1,1364)	1:34:A:VAL:HG21	1:132:A:LEU:HB3	20	2.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1364)	1:34:A:VAL:HG22	1:132:A:LEU:HB3	20	2.19
(1,1364)	1:34:A:VAL:HG23	1:132:A:LEU:HB3	20	2.19
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	20	2.19
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	20	2.19
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	20	2.19
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	5	2.18
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	5	2.18
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	5	2.18
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	2	2.17
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	2	2.17
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	2	2.17
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	7	2.17
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	7	2.17
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	7	2.17
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	17	2.17
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	17	2.17
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	17	2.17
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	17	2.17
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	17	2.17
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	17	2.17
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	17	2.17
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	17	2.17
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	17	2.17
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	14	2.17
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	14	2.17
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	14	2.17
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	14	2.17
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	14	2.17
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	14	2.17
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	14	2.17
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	14	2.17
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	14	2.17
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	20	2.17
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	20	2.17
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	20	2.17
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	20	2.17
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	20	2.17
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	20	2.17
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	20	2.17
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	20	2.17
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	20	2.17
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	2	2.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	2	2.17
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	2	2.17
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	14	2.17
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	14	2.17
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	14	2.17
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	18	2.17
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	18	2.17
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	18	2.17
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	5	2.16
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	5	2.16
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	5	2.16
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	8	2.16
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	8	2.16
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	8	2.16
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	10	2.16
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	10	2.16
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	10	2.16
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	11	2.16
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	11	2.16
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	11	2.16
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	18	2.15
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	18	2.15
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	18	2.15
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	18	2.15
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	18	2.15
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	18	2.15
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	18	2.15
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	18	2.15
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	18	2.15
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	19	2.15
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	19	2.15
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	19	2.15
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD21	1	2.15
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD22	1	2.15
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD23	1	2.15
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	17	2.14
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	17	2.14
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	17	2.14
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	20	2.14
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	20	2.14
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	20	2.14
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	3	2.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	3	2.14
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	3	2.14
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	14	2.13
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	14	2.13
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	14	2.13
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG21	3	2.13
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG22	3	2.13
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG23	3	2.13
(1,34)	1:118:A:LEU:HD21	1:134:A:PHE:H	17	2.13
(1,34)	1:118:A:LEU:HD22	1:134:A:PHE:H	17	2.13
(1,34)	1:118:A:LEU:HD23	1:134:A:PHE:H	17	2.13
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG21	14	2.12
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG22	14	2.12
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG23	14	2.12
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG11	6	2.11
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG12	6	2.11
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG13	6	2.11
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	6	2.11
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	6	2.11
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	6	2.11
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	6	2.11
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	6	2.11
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	6	2.11
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	6	2.11
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	6	2.11
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	6	2.11
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	8	2.11
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	8	2.11
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	8	2.11
(1,34)	1:118:A:LEU:HD21	1:134:A:PHE:H	3	2.11
(1,34)	1:118:A:LEU:HD22	1:134:A:PHE:H	3	2.11
(1,34)	1:118:A:LEU:HD23	1:134:A:PHE:H	3	2.11
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	3	2.1
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	3	2.1
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	3	2.1
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD21	13	2.1
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD22	13	2.1
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD23	13	2.1
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD21	14	2.1
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD22	14	2.1
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD23	14	2.1
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	13	2.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	13	2.09
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	13	2.09
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	5	2.09
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	5	2.09
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	5	2.09
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	5	2.09
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	5	2.09
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	5	2.09
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	5	2.09
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	5	2.09
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	5	2.09
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	19	2.09
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	19	2.09
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	19	2.09
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	19	2.09
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	19	2.09
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	19	2.09
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	19	2.09
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	19	2.09
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	19	2.09
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	14	2.09
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	14	2.09
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	14	2.09
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	15	2.09
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	15	2.09
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	15	2.09
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG11	4	2.09
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG12	4	2.09
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG13	4	2.09
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	7	2.09
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	7	2.09
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	7	2.09
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	10	2.08
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	10	2.08
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	10	2.08
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD21	7	2.08
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD22	7	2.08
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD23	7	2.08
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	19	2.07
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	19	2.07
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	19	2.07
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	5	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	5	2.07
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	5	2.07
(1,34)	1:118:A:LEU:HD21	1:134:A:PHE:H	4	2.07
(1,34)	1:118:A:LEU:HD22	1:134:A:PHE:H	4	2.07
(1,34)	1:118:A:LEU:HD23	1:134:A:PHE:H	4	2.07
(1,34)	1:118:A:LEU:HD21	1:134:A:PHE:H	12	2.07
(1,34)	1:118:A:LEU:HD22	1:134:A:PHE:H	12	2.07
(1,34)	1:118:A:LEU:HD23	1:134:A:PHE:H	12	2.07
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	4	2.06
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	4	2.06
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	4	2.06
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	16	2.05
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	16	2.05
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	16	2.05
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD21	20	2.05
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD22	20	2.05
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD23	20	2.05
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	9	2.04
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	9	2.04
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	9	2.04
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	9	2.04
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	9	2.04
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	9	2.04
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	9	2.04
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	9	2.04
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	9	2.04
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD21	15	2.04
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD22	15	2.04
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD23	15	2.04
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD21	15	2.03
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD22	15	2.03
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD23	15	2.03
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD21	3	2.02
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD22	3	2.02
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD23	3	2.02
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	6	2.02
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	6	2.02
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	6	2.02
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	10	2.02
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	10	2.02
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	10	2.02
(1,34)	1:118:A:LEU:HD21	1:134:A:PHE:H	14	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:118:A:LEU:HD22	1:134:A:PHE:H	14	2.02
(1,34)	1:118:A:LEU:HD23	1:134:A:PHE:H	14	2.02
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	7	2.01
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	7	2.01
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	7	2.01
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	7	2.01
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	7	2.01
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	7	2.01
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	7	2.01
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	7	2.01
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	7	2.01
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	1	2.01
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	1	2.01
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	1	2.01
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	1	2.01
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	1	2.01
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	1	2.01
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB1	4	2.0
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB2	4	2.0
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB3	4	2.0
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB1	4	2.0
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB2	4	2.0
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB3	4	2.0
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB1	4	2.0
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB2	4	2.0
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB3	4	2.0
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	5	2.0
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	5	2.0
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	5	2.0
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	5	2.0
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	5	2.0
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	5	2.0
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	5	2.0
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	5	2.0
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	5	2.0
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	16	2.0
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD21	13	1.99
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD22	13	1.99
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD23	13	1.99
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD21	12	1.99
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD22	12	1.99
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD23	12	1.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:118:A:LEU:HD21	1:134:A:PHE:H	6	1.99
(1,34)	1:118:A:LEU:HD22	1:134:A:PHE:H	6	1.99
(1,34)	1:118:A:LEU:HD23	1:134:A:PHE:H	6	1.99
(1,34)	1:118:A:LEU:HD21	1:134:A:PHE:H	19	1.99
(1,34)	1:118:A:LEU:HD22	1:134:A:PHE:H	19	1.99
(1,34)	1:118:A:LEU:HD23	1:134:A:PHE:H	19	1.99
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	18	1.98
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	18	1.98
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	18	1.98
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	15	1.98
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	15	1.98
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	15	1.98
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	15	1.98
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	15	1.98
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	15	1.98
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	15	1.98
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	15	1.98
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	15	1.98
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD21	4	1.98
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD22	4	1.98
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD23	4	1.98
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD21	17	1.98
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD22	17	1.98
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD23	17	1.98
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	8	1.97
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	4	1.96
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	4	1.96
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	4	1.96
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	4	1.96
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	4	1.96
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	4	1.96
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	4	1.96
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	4	1.96
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	4	1.96
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	6	1.96
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	6	1.96
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	6	1.96
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	6	1.96
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	6	1.96
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	6	1.96
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	6	1.96
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	6	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	6	1.96
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	10	1.96
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	10	1.96
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	10	1.96
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	10	1.96
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	10	1.96
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	10	1.96
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	10	1.96
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	10	1.96
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	10	1.96
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG21	2	1.96
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG22	2	1.96
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG23	2	1.96
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	18	1.96
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	18	1.96
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	18	1.96
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	20	1.95
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	20	1.95
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	20	1.95
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	3	1.95
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	3	1.95
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	3	1.95
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	3	1.95
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	3	1.95
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	3	1.95
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	3	1.95
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	3	1.95
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	3	1.95
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	18	1.95
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE1	19	1.94
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE2	19	1.94
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE1	19	1.94
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE2	19	1.94
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE1	19	1.94
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE2	19	1.94
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	2	1.94
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	2	1.94
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	2	1.94
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	2	1.94
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	2	1.94
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	2	1.94
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	2	1.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	2	1.94
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	2	1.94
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	8	1.94
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	8	1.94
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	8	1.94
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD21	17	1.94
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD22	17	1.94
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD23	17	1.94
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	13	1.94
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	13	1.94
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	13	1.94
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB1	6	1.93
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB2	6	1.93
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB3	6	1.93
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB1	6	1.93
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB2	6	1.93
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB3	6	1.93
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB1	6	1.93
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB2	6	1.93
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB3	6	1.93
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD1	2	1.93
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD2	2	1.93
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD1	2	1.93
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD2	2	1.93
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD1	2	1.93
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD2	2	1.93
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG11	16	1.93
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG12	16	1.93
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG13	16	1.93
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	2	1.93
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	2	1.93
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	2	1.93
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	2	1.93
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	2	1.93
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	2	1.93
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	2	1.93
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	2	1.93
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	2	1.93
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	13	1.93
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	13	1.93
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	13	1.93
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	13	1.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	13	1.93
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	13	1.93
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	13	1.93
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	13	1.93
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	13	1.93
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG21	12	1.93
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG22	12	1.93
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG23	12	1.93
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG21	14	1.93
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG22	14	1.93
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG23	14	1.93
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	13	1.93
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	13	1.93
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	13	1.93
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	13	1.93
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	13	1.93
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	13	1.93
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	13	1.93
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	13	1.93
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	13	1.93
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG21	20	1.92
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG22	20	1.92
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG23	20	1.92
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	10	1.92
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	8	1.92
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	8	1.92
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	8	1.92
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB1	14	1.91
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB2	14	1.91
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB3	14	1.91
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB1	14	1.91
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB2	14	1.91
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB3	14	1.91
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB1	14	1.91
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB2	14	1.91
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB3	14	1.91
(1,2616)	1:27:A:VAL:HG21	1:177:A:TRP:HZ2	4	1.91
(1,2616)	1:27:A:VAL:HG22	1:177:A:TRP:HZ2	4	1.91
(1,2616)	1:27:A:VAL:HG23	1:177:A:TRP:HZ2	4	1.91
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG21	3	1.91
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG22	3	1.91
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG23	3	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	4	1.91
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	4	1.91
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	4	1.91
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	4	1.91
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	4	1.91
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	4	1.91
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	4	1.91
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	4	1.91
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	4	1.91
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	5	1.91
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	20	1.91
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB1	19	1.9
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB2	19	1.9
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB3	19	1.9
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB1	19	1.9
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB2	19	1.9
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB3	19	1.9
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB1	19	1.9
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB2	19	1.9
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB3	19	1.9
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	9	1.9
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	9	1.9
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	9	1.9
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	9	1.9
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	9	1.9
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	9	1.9
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	9	1.9
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	9	1.9
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	9	1.9
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG11	5	1.9
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG12	5	1.9
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG13	5	1.9
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	19	1.9
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB1	17	1.89
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB2	17	1.89
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB3	17	1.89
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB1	17	1.89
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB2	17	1.89
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB3	17	1.89
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB1	17	1.89
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB2	17	1.89
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB3	17	1.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD1	18	1.89
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD2	18	1.89
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD1	18	1.89
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD2	18	1.89
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD1	18	1.89
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD2	18	1.89
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	1	1.89
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	2	1.89
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	4	1.89
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG21	5	1.88
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG22	5	1.88
(1,1980)	1:38:A:TYR:H	1:39:A:VAL:HG23	5	1.88
(1,1570)	1:159:A:VAL:HG11	1:158:A:VAL:HB	10	1.88
(1,1570)	1:159:A:VAL:HG12	1:158:A:VAL:HB	10	1.88
(1,1570)	1:159:A:VAL:HG13	1:158:A:VAL:HB	10	1.88
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	9	1.88
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	12	1.88
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	12	1.88
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	12	1.88
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	20	1.87
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	20	1.87
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	20	1.87
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	20	1.87
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	20	1.87
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	20	1.87
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	20	1.87
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	20	1.87
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	20	1.87
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	19	1.87
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	19	1.87
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	19	1.87
(1,34)	1:118:A:LEU:HD21	1:134:A:PHE:H	9	1.87
(1,34)	1:118:A:LEU:HD22	1:134:A:PHE:H	9	1.87
(1,34)	1:118:A:LEU:HD23	1:134:A:PHE:H	9	1.87
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD1	10	1.86
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD2	10	1.86
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD1	10	1.86
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD2	10	1.86
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD1	10	1.86
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD2	10	1.86
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	14	1.86
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	14	1.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	14	1.86
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	14	1.86
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	14	1.86
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	14	1.86
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	14	1.86
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	14	1.86
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	14	1.86
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	17	1.86
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	17	1.86
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	17	1.86
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	17	1.86
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	17	1.86
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	17	1.86
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	17	1.86
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	17	1.86
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	17	1.86
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	2	1.86
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	2	1.86
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	2	1.86
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	2	1.86
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	2	1.86
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	2	1.86
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	2	1.86
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	2	1.86
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	2	1.86
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	7	1.86
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB1	12	1.85
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB2	12	1.85
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB3	12	1.85
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB1	12	1.85
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB2	12	1.85
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB3	12	1.85
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB1	12	1.85
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB2	12	1.85
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB3	12	1.85
(1,1740)	1:63:A:LEU:HD11	1:64:A:PRO:HG3	15	1.85
(1,1740)	1:63:A:LEU:HD12	1:64:A:PRO:HG3	15	1.85
(1,1740)	1:63:A:LEU:HD13	1:64:A:PRO:HG3	15	1.85
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	6	1.85
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	6	1.85
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	6	1.85
(1,2483)	1:147:A:LEU:HD21	1:150:A:PHE:HZ	7	1.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2483)	1:147:A:LEU:HD22	1:150:A:PHE:HZ	7	1.84
(1,2483)	1:147:A:LEU:HD23	1:150:A:PHE:HZ	7	1.84
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG11	18	1.84
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG12	18	1.84
(1,1864)	1:125:A:TRP:HZ3	1:129:A:VAL:HG13	18	1.84
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB1	3	1.83
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB2	3	1.83
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB3	3	1.83
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB1	3	1.83
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB2	3	1.83
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB3	3	1.83
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB1	3	1.83
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB2	3	1.83
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB3	3	1.83
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	3	1.83
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	3	1.83
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	3	1.83
(1,1740)	1:63:A:LEU:HD11	1:64:A:PRO:HG3	18	1.83
(1,1740)	1:63:A:LEU:HD12	1:64:A:PRO:HG3	18	1.83
(1,1740)	1:63:A:LEU:HD13	1:64:A:PRO:HG3	18	1.83
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	11	1.83
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB1	9	1.82
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB2	9	1.82
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB3	9	1.82
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB1	9	1.82
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB2	9	1.82
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB3	9	1.82
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB1	9	1.82
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB2	9	1.82
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB3	9	1.82
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	16	1.82
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	16	1.82
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	16	1.82
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	16	1.81
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	16	1.81
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	16	1.81
(1,1740)	1:63:A:LEU:HD11	1:64:A:PRO:HG3	13	1.81
(1,1740)	1:63:A:LEU:HD12	1:64:A:PRO:HG3	13	1.81
(1,1740)	1:63:A:LEU:HD13	1:64:A:PRO:HG3	13	1.81
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	13	1.81
(1,256)	1:159:A:VAL:HG11	1:158:A:VAL:H	4	1.81
(1,256)	1:159:A:VAL:HG12	1:158:A:VAL:H	4	1.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:159:A:VAL:HG13	1:158:A:VAL:H	4	1.81
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	4	1.8
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	4	1.8
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	4	1.8
(1,256)	1:159:A:VAL:HG11	1:158:A:VAL:H	15	1.8
(1,256)	1:159:A:VAL:HG12	1:158:A:VAL:H	15	1.8
(1,256)	1:159:A:VAL:HG13	1:158:A:VAL:H	15	1.8
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD1	9	1.78
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD2	9	1.78
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD1	9	1.78
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD2	9	1.78
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD1	9	1.78
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD2	9	1.78
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	12	1.78
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	12	1.78
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	12	1.78
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	12	1.78
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	12	1.78
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	12	1.78
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	12	1.78
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	12	1.78
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	12	1.78
(1,1740)	1:63:A:LEU:HD11	1:64:A:PRO:HG3	9	1.78
(1,1740)	1:63:A:LEU:HD12	1:64:A:PRO:HG3	9	1.78
(1,1740)	1:63:A:LEU:HD13	1:64:A:PRO:HG3	9	1.78
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	2	1.78
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	2	1.78
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	2	1.78
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	17	1.78
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	17	1.78
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	17	1.78
(1,256)	1:159:A:VAL:HG11	1:158:A:VAL:H	16	1.78
(1,256)	1:159:A:VAL:HG12	1:158:A:VAL:H	16	1.78
(1,256)	1:159:A:VAL:HG13	1:158:A:VAL:H	16	1.78
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	8	1.77
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	8	1.77
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	8	1.77
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	14	1.77
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	14	1.77
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	14	1.77
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	15	1.77
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	15	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	15	1.77
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	15	1.77
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	15	1.77
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	15	1.77
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD1	8	1.76
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD2	8	1.76
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD1	8	1.76
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD2	8	1.76
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD1	8	1.76
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD2	8	1.76
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD1	14	1.76
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD2	14	1.76
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD1	14	1.76
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD2	14	1.76
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD1	14	1.76
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD2	14	1.76
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	6	1.76
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	6	1.76
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	6	1.76
(1,256)	1:159:A:VAL:HG11	1:158:A:VAL:H	9	1.76
(1,256)	1:159:A:VAL:HG12	1:158:A:VAL:H	9	1.76
(1,256)	1:159:A:VAL:HG13	1:158:A:VAL:H	9	1.76
(1,256)	1:159:A:VAL:HG11	1:158:A:VAL:H	18	1.76
(1,256)	1:159:A:VAL:HG12	1:158:A:VAL:H	18	1.76
(1,256)	1:159:A:VAL:HG13	1:158:A:VAL:H	18	1.76
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD1	11	1.75
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD2	11	1.75
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD1	11	1.75
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD2	11	1.75
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD1	11	1.75
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD2	11	1.75
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	8	1.75
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	8	1.75
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	8	1.75
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	8	1.75
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	8	1.75
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	8	1.75
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	8	1.75
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	8	1.75
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	8	1.75
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	18	1.75
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	18	1.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	18	1.75
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	16	1.75
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	16	1.75
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	16	1.75
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	18	1.74
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	18	1.74
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	18	1.74
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	18	1.74
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	18	1.74
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	18	1.74
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	18	1.74
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	18	1.74
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	18	1.74
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	16	1.74
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	16	1.74
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	16	1.74
(1,1740)	1:63:A:LEU:HD11	1:64:A:PRO:HG3	1	1.74
(1,1740)	1:63:A:LEU:HD12	1:64:A:PRO:HG3	1	1.74
(1,1740)	1:63:A:LEU:HD13	1:64:A:PRO:HG3	1	1.74
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	7	1.74
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	7	1.74
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	7	1.74
(1,2365)	2:93:B:VAL:HG21	1:89:A:TYR:HD1	6	1.73
(1,2365)	2:93:B:VAL:HG21	1:89:A:TYR:HD2	6	1.73
(1,2365)	2:93:B:VAL:HG22	1:89:A:TYR:HD1	6	1.73
(1,2365)	2:93:B:VAL:HG22	1:89:A:TYR:HD2	6	1.73
(1,2365)	2:93:B:VAL:HG23	1:89:A:TYR:HD1	6	1.73
(1,2365)	2:93:B:VAL:HG23	1:89:A:TYR:HD2	6	1.73
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	19	1.73
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	19	1.73
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	19	1.73
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	19	1.73
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	19	1.73
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	19	1.73
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	19	1.73
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	19	1.73
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	19	1.73
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	1	1.72
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD1	3	1.71
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD2	3	1.71
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD1	3	1.71
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD2	3	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD1	3	1.71
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD2	3	1.71
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	15	1.71
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	15	1.71
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	15	1.71
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	10	1.71
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	10	1.71
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	10	1.71
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	10	1.71
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	10	1.71
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	10	1.71
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	10	1.71
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	10	1.71
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	10	1.71
(1,256)	1:159:A:VAL:HG11	1:158:A:VAL:H	3	1.71
(1,256)	1:159:A:VAL:HG12	1:158:A:VAL:H	3	1.71
(1,256)	1:159:A:VAL:HG13	1:158:A:VAL:H	3	1.71
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	9	1.7
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	9	1.7
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	9	1.7
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	9	1.7
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	9	1.7
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	9	1.7
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD11	13	1.7
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD12	13	1.7
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD13	13	1.7
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	3	1.7
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	3	1.7
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	3	1.7
(1,1483)	1:143:A:TYR:HE1	1:144:A:GLN:HG3	10	1.7
(1,1483)	1:143:A:TYR:HE2	1:144:A:GLN:HG3	10	1.7
(1,854)	1:159:A:VAL:HG11	1:32:A:GLU:HA	10	1.7
(1,854)	1:159:A:VAL:HG12	1:32:A:GLU:HA	10	1.7
(1,854)	1:159:A:VAL:HG13	1:32:A:GLU:HA	10	1.7
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	8	1.69
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	8	1.69
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	8	1.69
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	1	1.68
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	1	1.68
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	1	1.68
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	11	1.68
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	11	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	11	1.68
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	10	1.68
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	10	1.68
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	10	1.68
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	4	1.68
(1,1043)	1:182:A:ASN:HB3	1:179:A:ALA:HA	3	1.68
(1,256)	1:159:A:VAL:HG11	1:158:A:VAL:H	7	1.68
(1,256)	1:159:A:VAL:HG12	1:158:A:VAL:H	7	1.68
(1,256)	1:159:A:VAL:HG13	1:158:A:VAL:H	7	1.68
(1,256)	1:159:A:VAL:HG11	1:158:A:VAL:H	13	1.68
(1,256)	1:159:A:VAL:HG12	1:158:A:VAL:H	13	1.68
(1,256)	1:159:A:VAL:HG13	1:158:A:VAL:H	13	1.68
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	6	1.67
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	6	1.67
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	6	1.67
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	16	1.67
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	16	1.67
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	16	1.67
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	17	1.67
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	17	1.67
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	17	1.67
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	15	1.67
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	15	1.67
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	15	1.67
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	18	1.67
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	18	1.67
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	18	1.67
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	7	1.67
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	7	1.67
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	7	1.67
(1,1483)	1:143:A:TYR:HE1	1:144:A:GLN:HG3	19	1.67
(1,1483)	1:143:A:TYR:HE2	1:144:A:GLN:HG3	19	1.67
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	20	1.66
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	20	1.66
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	20	1.66
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	9	1.66
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	9	1.66
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	9	1.66
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	13	1.66
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	13	1.66
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	13	1.66
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	20	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	20	1.66
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	20	1.66
(1,1483)	1:143:A:TYR:HE1	1:144:A:GLN:HG3	2	1.66
(1,1483)	1:143:A:TYR:HE2	1:144:A:GLN:HG3	2	1.66
(1,854)	1:159:A:VAL:HG11	1:32:A:GLU:HA	11	1.66
(1,854)	1:159:A:VAL:HG12	1:32:A:GLU:HA	11	1.66
(1,854)	1:159:A:VAL:HG13	1:32:A:GLU:HA	11	1.66
(1,256)	1:159:A:VAL:HG11	1:158:A:VAL:H	14	1.66
(1,256)	1:159:A:VAL:HG12	1:158:A:VAL:H	14	1.66
(1,256)	1:159:A:VAL:HG13	1:158:A:VAL:H	14	1.66
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	7	1.65
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	7	1.65
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	7	1.65
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	7	1.65
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	7	1.65
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	7	1.65
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	7	1.65
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	7	1.65
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	7	1.65
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	11	1.65
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	11	1.65
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	11	1.65
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	2	1.65
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	2	1.65
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	2	1.65
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	7	1.65
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	7	1.65
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	7	1.65
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	11	1.65
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	11	1.65
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	11	1.65
(1,256)	1:159:A:VAL:HG11	1:158:A:VAL:H	1	1.65
(1,256)	1:159:A:VAL:HG12	1:158:A:VAL:H	1	1.65
(1,256)	1:159:A:VAL:HG13	1:158:A:VAL:H	1	1.65
(1,256)	1:159:A:VAL:HG11	1:158:A:VAL:H	10	1.65
(1,256)	1:159:A:VAL:HG12	1:158:A:VAL:H	10	1.65
(1,256)	1:159:A:VAL:HG13	1:158:A:VAL:H	10	1.65
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	1	1.64
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	1	1.64
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	1	1.64
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	1	1.64
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	1	1.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	1	1.64
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	1	1.64
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	1	1.64
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	1	1.64
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	5	1.64
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	5	1.64
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	5	1.64
(1,1483)	1:143:A:TYR:HE1	1:144:A:GLN:HG3	15	1.64
(1,1483)	1:143:A:TYR:HE2	1:144:A:GLN:HG3	15	1.64
(1,256)	1:159:A:VAL:HG11	1:158:A:VAL:H	17	1.63
(1,256)	1:159:A:VAL:HG12	1:158:A:VAL:H	17	1.63
(1,256)	1:159:A:VAL:HG13	1:158:A:VAL:H	17	1.63
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	5	1.62
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	5	1.62
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	5	1.62
(1,1483)	1:143:A:TYR:HE1	1:144:A:GLN:HG3	8	1.62
(1,1483)	1:143:A:TYR:HE2	1:144:A:GLN:HG3	8	1.62
(1,854)	1:159:A:VAL:HG11	1:32:A:GLU:HA	19	1.62
(1,854)	1:159:A:VAL:HG12	1:32:A:GLU:HA	19	1.62
(1,854)	1:159:A:VAL:HG13	1:32:A:GLU:HA	19	1.62
(1,256)	1:159:A:VAL:HG11	1:158:A:VAL:H	19	1.62
(1,256)	1:159:A:VAL:HG12	1:158:A:VAL:H	19	1.62
(1,256)	1:159:A:VAL:HG13	1:158:A:VAL:H	19	1.62
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE1	6	1.61
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE2	6	1.61
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE1	6	1.61
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE2	6	1.61
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE1	6	1.61
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE2	6	1.61
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	15	1.61
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	15	1.61
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	15	1.61
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	3	1.61
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	3	1.61
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	3	1.61
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	3	1.61
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	3	1.61
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	3	1.61
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	3	1.61
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	3	1.61
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	3	1.61
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	12	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	12	1.61
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	12	1.61
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	9	1.61
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	9	1.61
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	9	1.61
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	10	1.6
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	14	1.6
(1,1043)	1:182:A:ASN:HB3	1:179:A:ALA:HA	6	1.6
(1,854)	1:159:A:VAL:HG11	1:32:A:GLU:HA	14	1.6
(1,854)	1:159:A:VAL:HG12	1:32:A:GLU:HA	14	1.6
(1,854)	1:159:A:VAL:HG13	1:32:A:GLU:HA	14	1.6
(1,2483)	1:147:A:LEU:HD21	1:150:A:PHE:HZ	8	1.59
(1,2483)	1:147:A:LEU:HD22	1:150:A:PHE:HZ	8	1.59
(1,2483)	1:147:A:LEU:HD23	1:150:A:PHE:HZ	8	1.59
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	1	1.59
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	1	1.59
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	1	1.59
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	1	1.59
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	1	1.59
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	1	1.59
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	1	1.59
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	1	1.59
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	1	1.59
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	18	1.59
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	18	1.59
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	18	1.59
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	18	1.59
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	18	1.59
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	18	1.59
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	18	1.59
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	18	1.59
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	18	1.59
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	10	1.59
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	10	1.59
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	10	1.59
(1,1483)	1:143:A:TYR:HE1	1:144:A:GLN:HG3	17	1.59
(1,1483)	1:143:A:TYR:HE2	1:144:A:GLN:HG3	17	1.59
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	16	1.58
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	16	1.58
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	16	1.58
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	16	1.58
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	16	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	16	1.58
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	16	1.58
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	16	1.58
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	16	1.58
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	3	1.58
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	3	1.58
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	3	1.58
(1,1483)	1:143:A:TYR:HE1	1:144:A:GLN:HG3	11	1.58
(1,1483)	1:143:A:TYR:HE2	1:144:A:GLN:HG3	11	1.58
(1,1043)	1:182:A:ASN:HB3	1:179:A:ALA:HA	12	1.58
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD1	12	1.57
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD2	12	1.57
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD1	12	1.57
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD2	12	1.57
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD1	12	1.57
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD2	12	1.57
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	11	1.57
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	11	1.57
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	11	1.57
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	11	1.57
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	11	1.57
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	11	1.57
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	11	1.57
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	11	1.57
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	11	1.57
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	18	1.57
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	18	1.57
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	18	1.57
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	18	1.57
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	18	1.57
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	18	1.57
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	18	1.57
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	18	1.57
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	18	1.57
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	20	1.57
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	20	1.57
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	20	1.57
(1,1483)	1:143:A:TYR:HE1	1:144:A:GLN:HG3	4	1.57
(1,1483)	1:143:A:TYR:HE2	1:144:A:GLN:HG3	4	1.57
(1,1483)	1:143:A:TYR:HE1	1:144:A:GLN:HG3	5	1.57
(1,1483)	1:143:A:TYR:HE2	1:144:A:GLN:HG3	5	1.57
(1,1483)	1:143:A:TYR:HE1	1:144:A:GLN:HG3	9	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1483)	1:143:A:TYR:HE2	1:144:A:GLN:HG3	9	1.57
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	5	1.56
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	5	1.56
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	5	1.56
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	5	1.56
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	5	1.56
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	5	1.56
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	3	1.56
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	3	1.56
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	3	1.56
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD21	5	1.56
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD22	5	1.56
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD23	5	1.56
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD21	5	1.56
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD22	5	1.56
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD23	5	1.56
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD21	5	1.56
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD22	5	1.56
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD23	5	1.56
(1,854)	1:159:A:VAL:HG11	1:32:A:GLU:HA	17	1.56
(1,854)	1:159:A:VAL:HG12	1:32:A:GLU:HA	17	1.56
(1,854)	1:159:A:VAL:HG13	1:32:A:GLU:HA	17	1.56
(1,347)	1:34:A:VAL:HG11	1:71:A:MET:H	11	1.56
(1,347)	1:34:A:VAL:HG12	1:71:A:MET:H	11	1.56
(1,347)	1:34:A:VAL:HG13	1:71:A:MET:H	11	1.56
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	13	1.55
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	13	1.55
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	13	1.55
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	6	1.55
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	6	1.55
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	6	1.55
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	5	1.55
(1,256)	1:159:A:VAL:HG11	1:158:A:VAL:H	11	1.55
(1,256)	1:159:A:VAL:HG12	1:158:A:VAL:H	11	1.55
(1,256)	1:159:A:VAL:HG13	1:158:A:VAL:H	11	1.55
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	9	1.54
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	9	1.54
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	9	1.54
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	17	1.54
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	17	1.54
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	17	1.54
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	6	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	6	1.54
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	6	1.54
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	18	1.54
(1,625)	1:118:A:LEU:HD21	1:128:A:VAL:HA	19	1.54
(1,625)	1:118:A:LEU:HD22	1:128:A:VAL:HA	19	1.54
(1,625)	1:118:A:LEU:HD23	1:128:A:VAL:HA	19	1.54
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	9	1.54
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	9	1.54
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	9	1.54
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE1	12	1.53
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE2	12	1.53
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE1	12	1.53
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE2	12	1.53
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE1	12	1.53
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE2	12	1.53
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	14	1.53
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	14	1.53
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	14	1.53
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	17	1.53
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	17	1.53
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	17	1.53
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	17	1.53
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	17	1.53
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	17	1.53
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	17	1.53
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	17	1.53
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	17	1.53
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	10	1.53
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	10	1.53
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	10	1.53
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	14	1.53
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	14	1.53
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	14	1.53
(1,1043)	1:182:A:ASN:HB3	1:179:A:ALA:HA	4	1.53
(1,963)	1:159:A:VAL:HG21	1:160:A:ASP:HA	1	1.53
(1,963)	1:159:A:VAL:HG22	1:160:A:ASP:HA	1	1.53
(1,963)	1:159:A:VAL:HG23	1:160:A:ASP:HA	1	1.53
(1,963)	1:159:A:VAL:HG21	1:160:A:ASP:HA	3	1.53
(1,963)	1:159:A:VAL:HG22	1:160:A:ASP:HA	3	1.53
(1,963)	1:159:A:VAL:HG23	1:160:A:ASP:HA	3	1.53
(1,963)	1:159:A:VAL:HG21	1:160:A:ASP:HA	7	1.53
(1,963)	1:159:A:VAL:HG22	1:160:A:ASP:HA	7	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:159:A:VAL:HG23	1:160:A:ASP:HA	7	1.53
(1,963)	1:159:A:VAL:HG21	1:160:A:ASP:HA	9	1.53
(1,963)	1:159:A:VAL:HG22	1:160:A:ASP:HA	9	1.53
(1,963)	1:159:A:VAL:HG23	1:160:A:ASP:HA	9	1.53
(1,963)	1:159:A:VAL:HG21	1:160:A:ASP:HA	11	1.53
(1,963)	1:159:A:VAL:HG22	1:160:A:ASP:HA	11	1.53
(1,963)	1:159:A:VAL:HG23	1:160:A:ASP:HA	11	1.53
(1,963)	1:159:A:VAL:HG21	1:160:A:ASP:HA	18	1.53
(1,963)	1:159:A:VAL:HG22	1:160:A:ASP:HA	18	1.53
(1,963)	1:159:A:VAL:HG23	1:160:A:ASP:HA	18	1.53
(1,963)	1:159:A:VAL:HG21	1:160:A:ASP:HA	19	1.53
(1,963)	1:159:A:VAL:HG22	1:160:A:ASP:HA	19	1.53
(1,963)	1:159:A:VAL:HG23	1:160:A:ASP:HA	19	1.53
(1,256)	1:159:A:VAL:HG11	1:158:A:VAL:H	8	1.53
(1,256)	1:159:A:VAL:HG12	1:158:A:VAL:H	8	1.53
(1,256)	1:159:A:VAL:HG13	1:158:A:VAL:H	8	1.53
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	4	1.52
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	4	1.52
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	4	1.52
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	19	1.52
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	19	1.52
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	19	1.52
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	20	1.52
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	20	1.52
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	20	1.52
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	14	1.52
(1,963)	1:159:A:VAL:HG21	1:160:A:ASP:HA	10	1.52
(1,963)	1:159:A:VAL:HG22	1:160:A:ASP:HA	10	1.52
(1,963)	1:159:A:VAL:HG23	1:160:A:ASP:HA	10	1.52
(1,963)	1:159:A:VAL:HG21	1:160:A:ASP:HA	14	1.52
(1,963)	1:159:A:VAL:HG22	1:160:A:ASP:HA	14	1.52
(1,963)	1:159:A:VAL:HG23	1:160:A:ASP:HA	14	1.52
(1,963)	1:159:A:VAL:HG21	1:160:A:ASP:HA	15	1.52
(1,963)	1:159:A:VAL:HG22	1:160:A:ASP:HA	15	1.52
(1,963)	1:159:A:VAL:HG23	1:160:A:ASP:HA	15	1.52
(1,963)	1:159:A:VAL:HG21	1:160:A:ASP:HA	16	1.52
(1,963)	1:159:A:VAL:HG22	1:160:A:ASP:HA	16	1.52
(1,963)	1:159:A:VAL:HG23	1:160:A:ASP:HA	16	1.52
(1,963)	1:159:A:VAL:HG21	1:160:A:ASP:HA	17	1.52
(1,963)	1:159:A:VAL:HG22	1:160:A:ASP:HA	17	1.52
(1,963)	1:159:A:VAL:HG23	1:160:A:ASP:HA	17	1.52
(1,1483)	1:143:A:TYR:HE1	1:144:A:GLN:HG3	3	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1483)	1:143:A:TYR:HE2	1:144:A:GLN:HG3	3	1.51
(1,1483)	1:143:A:TYR:HE1	1:144:A:GLN:HG3	12	1.51
(1,1483)	1:143:A:TYR:HE2	1:144:A:GLN:HG3	12	1.51
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	2	1.51
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	2	1.51
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	2	1.51
(1,963)	1:159:A:VAL:HG21	1:160:A:ASP:HA	8	1.51
(1,963)	1:159:A:VAL:HG22	1:160:A:ASP:HA	8	1.51
(1,963)	1:159:A:VAL:HG23	1:160:A:ASP:HA	8	1.51
(1,963)	1:159:A:VAL:HG21	1:160:A:ASP:HA	13	1.51
(1,963)	1:159:A:VAL:HG22	1:160:A:ASP:HA	13	1.51
(1,963)	1:159:A:VAL:HG23	1:160:A:ASP:HA	13	1.51
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	6	1.51
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	6	1.51
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	6	1.51
(1,3031)	1:118:A:LEU:HD11	2:91:B:ALA:HA	4	1.5
(1,3031)	1:118:A:LEU:HD12	2:91:B:ALA:HA	4	1.5
(1,3031)	1:118:A:LEU:HD13	2:91:B:ALA:HA	4	1.5
(1,2344)	1:160:A:ASP:HB3	1:164:A:HIS:HE1	20	1.5
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG11	3	1.5
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG12	3	1.5
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG13	3	1.5
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG11	3	1.5
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG12	3	1.5
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG13	3	1.5
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG11	3	1.5
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG12	3	1.5
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG13	3	1.5
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	4	1.5
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	4	1.5
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	4	1.5
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	19	1.5
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	19	1.5
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	19	1.5
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	12	1.5
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	12	1.5
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	12	1.5
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	3	1.49
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	3	1.49
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE1	3	1.49
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE2	3	1.49
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE1	3	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE2	3	1.49
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE1	3	1.49
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE2	3	1.49
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	8	1.49
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	8	1.49
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	8	1.49
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG11	12	1.49
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG12	12	1.49
(1,1932)	1:71:A:MET:H	1:74:A:VAL:HG13	12	1.49
(1,1483)	1:143:A:TYR:HE1	1:144:A:GLN:HG3	13	1.49
(1,1483)	1:143:A:TYR:HE2	1:144:A:GLN:HG3	13	1.49
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	19	1.49
(1,963)	1:159:A:VAL:HG21	1:160:A:ASP:HA	4	1.49
(1,963)	1:159:A:VAL:HG22	1:160:A:ASP:HA	4	1.49
(1,963)	1:159:A:VAL:HG23	1:160:A:ASP:HA	4	1.49
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	15	1.49
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	15	1.49
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	15	1.49
(1,90)	1:97:A:LEU:HD21	1:138:A:LEU:H	3	1.49
(1,90)	1:97:A:LEU:HD22	1:138:A:LEU:H	3	1.49
(1,90)	1:97:A:LEU:HD23	1:138:A:LEU:H	3	1.49
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	1	1.48
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	1	1.48
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE1	17	1.48
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE2	17	1.48
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE1	17	1.48
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE2	17	1.48
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE1	17	1.48
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE2	17	1.48
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	19	1.48
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	19	1.48
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	19	1.48
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	16	1.48
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	16	1.48
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	16	1.48
(1,854)	1:159:A:VAL:HG11	1:32:A:GLU:HA	8	1.48
(1,854)	1:159:A:VAL:HG12	1:32:A:GLU:HA	8	1.48
(1,854)	1:159:A:VAL:HG13	1:32:A:GLU:HA	8	1.48
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	17	1.47
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	17	1.47
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	17	1.47
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	9	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	9	1.47
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	9	1.47
(1,528)	1:55:A:PRO:HD3	1:47:A:GLN:HE21	12	1.47
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	16	1.47
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	16	1.47
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	16	1.47
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	4	1.46
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	4	1.46
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	4	1.46
(1,854)	1:159:A:VAL:HG11	1:32:A:GLU:HA	13	1.46
(1,854)	1:159:A:VAL:HG12	1:32:A:GLU:HA	13	1.46
(1,854)	1:159:A:VAL:HG13	1:32:A:GLU:HA	13	1.46
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	10	1.45
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	10	1.45
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	10	1.45
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	20	1.45
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	20	1.45
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	20	1.45
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD21	10	1.45
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD22	10	1.45
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD23	10	1.45
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	18	1.44
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	18	1.44
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG11	1	1.44
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG12	1	1.44
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG13	1	1.44
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	3	1.44
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	3	1.44
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	3	1.44
(1,1020)	1:118:A:LEU:HD21	1:130:A:ALA:HA	4	1.44
(1,1020)	1:118:A:LEU:HD22	1:130:A:ALA:HA	4	1.44
(1,1020)	1:118:A:LEU:HD23	1:130:A:ALA:HA	4	1.44
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD1	6	1.43
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD2	6	1.43
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD1	6	1.43
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD2	6	1.43
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD1	6	1.43
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD2	6	1.43
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	12	1.43
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	12	1.43
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	12	1.43
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG21	20	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG22	20	1.43
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG23	20	1.43
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	13	1.43
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	13	1.43
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	13	1.43
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	6	1.43
(1,854)	1:159:A:VAL:HG11	1:32:A:GLU:HA	1	1.43
(1,854)	1:159:A:VAL:HG12	1:32:A:GLU:HA	1	1.43
(1,854)	1:159:A:VAL:HG13	1:32:A:GLU:HA	1	1.43
(1,3031)	1:118:A:LEU:HD11	2:91:B:ALA:HA	6	1.42
(1,3031)	1:118:A:LEU:HD12	2:91:B:ALA:HA	6	1.42
(1,3031)	1:118:A:LEU:HD13	2:91:B:ALA:HA	6	1.42
(1,3031)	1:118:A:LEU:HD11	2:91:B:ALA:HA	14	1.42
(1,3031)	1:118:A:LEU:HD12	2:91:B:ALA:HA	14	1.42
(1,3031)	1:118:A:LEU:HD13	2:91:B:ALA:HA	14	1.42
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	2	1.42
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	2	1.42
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	2	1.42
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	15	1.42
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	15	1.42
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	15	1.42
(1,854)	1:159:A:VAL:HG11	1:32:A:GLU:HA	7	1.42
(1,854)	1:159:A:VAL:HG12	1:32:A:GLU:HA	7	1.42
(1,854)	1:159:A:VAL:HG13	1:32:A:GLU:HA	7	1.42
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	16	1.41
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	16	1.41
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG11	18	1.41
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG12	18	1.41
(1,1999)	1:177:A:TRP:HD1	1:34:A:VAL:HG13	18	1.41
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD11	11	1.41
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD12	11	1.41
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD13	11	1.41
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	17	1.41
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	17	1.41
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	17	1.41
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	18	1.41
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	18	1.41
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	18	1.41
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	8	1.41
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	8	1.41
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	8	1.41
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	18	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	18	1.41
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	18	1.41
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD1	2	1.4
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD2	2	1.4
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD1	2	1.4
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD2	2	1.4
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD1	2	1.4
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD2	2	1.4
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD1	18	1.4
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD2	18	1.4
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD1	18	1.4
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD2	18	1.4
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD1	18	1.4
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD2	18	1.4
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	18	1.4
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	18	1.4
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	18	1.4
(1,1867)	1:73:A:GLN:HG3	1:181:A:LEU:HD11	9	1.4
(1,1867)	1:73:A:GLN:HG3	1:181:A:LEU:HD12	9	1.4
(1,1867)	1:73:A:GLN:HG3	1:181:A:LEU:HD13	9	1.4
(1,1627)	1:129:A:VAL:HG11	1:125:A:TRP:HB3	15	1.4
(1,1627)	1:129:A:VAL:HG12	1:125:A:TRP:HB3	15	1.4
(1,1627)	1:129:A:VAL:HG13	1:125:A:TRP:HB3	15	1.4
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	19	1.4
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	19	1.4
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	19	1.4
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	11	1.4
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	11	1.4
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	11	1.4
(1,854)	1:159:A:VAL:HG11	1:32:A:GLU:HA	18	1.4
(1,854)	1:159:A:VAL:HG12	1:32:A:GLU:HA	18	1.4
(1,854)	1:159:A:VAL:HG13	1:32:A:GLU:HA	18	1.4
(1,3031)	1:118:A:LEU:HD11	2:91:B:ALA:HA	17	1.39
(1,3031)	1:118:A:LEU:HD12	2:91:B:ALA:HA	17	1.39
(1,3031)	1:118:A:LEU:HD13	2:91:B:ALA:HA	17	1.39
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	15	1.39
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	15	1.39
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	15	1.39
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	15	1.39
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	15	1.39
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	15	1.39
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	15	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	15	1.39
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	15	1.39
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG21	4	1.39
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG22	4	1.39
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG23	4	1.39
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG21	4	1.39
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG22	4	1.39
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG23	4	1.39
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG21	4	1.39
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG22	4	1.39
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG23	4	1.39
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG21	4	1.39
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG22	4	1.39
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG23	4	1.39
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG21	4	1.39
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG22	4	1.39
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG23	4	1.39
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG21	4	1.39
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG22	4	1.39
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG23	4	1.39
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG11	5	1.39
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG12	5	1.39
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG13	5	1.39
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	18	1.39
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	18	1.39
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	18	1.39
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	7	1.39
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	7	1.39
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	7	1.39
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	8	1.39
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	8	1.39
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	8	1.39
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	10	1.39
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	10	1.39
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	10	1.39
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	11	1.39
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	11	1.39
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	11	1.39
(1,854)	1:159:A:VAL:HG11	1:32:A:GLU:HA	15	1.39
(1,854)	1:159:A:VAL:HG12	1:32:A:GLU:HA	15	1.39
(1,854)	1:159:A:VAL:HG13	1:32:A:GLU:HA	15	1.39
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	12	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	12	1.38
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE1	4	1.38
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE2	4	1.38
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE1	4	1.38
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE2	4	1.38
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE1	4	1.38
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE2	4	1.38
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD1	19	1.38
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD2	19	1.38
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD1	19	1.38
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD2	19	1.38
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD1	19	1.38
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD2	19	1.38
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD11	20	1.38
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD12	20	1.38
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD13	20	1.38
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	17	1.38
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	17	1.38
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	17	1.38
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	10	1.38
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	10	1.38
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	10	1.38
(1,3031)	1:118:A:LEU:HD11	2:91:B:ALA:HA	12	1.37
(1,3031)	1:118:A:LEU:HD12	2:91:B:ALA:HA	12	1.37
(1,3031)	1:118:A:LEU:HD13	2:91:B:ALA:HA	12	1.37
(1,3031)	1:118:A:LEU:HD11	2:91:B:ALA:HA	19	1.37
(1,3031)	1:118:A:LEU:HD12	2:91:B:ALA:HA	19	1.37
(1,3031)	1:118:A:LEU:HD13	2:91:B:ALA:HA	19	1.37
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	20	1.37
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	20	1.37
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD1	7	1.37
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD2	7	1.37
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD1	7	1.37
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD2	7	1.37
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD1	7	1.37
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD2	7	1.37
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD1	19	1.37
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD2	19	1.37
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD1	19	1.37
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD2	19	1.37
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD1	19	1.37
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD2	19	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1627)	1:129:A:VAL:HG11	1:125:A:TRP:HB3	2	1.37
(1,1627)	1:129:A:VAL:HG12	1:125:A:TRP:HB3	2	1.37
(1,1627)	1:129:A:VAL:HG13	1:125:A:TRP:HB3	2	1.37
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	19	1.37
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	19	1.37
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	19	1.37
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	4	1.37
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	4	1.37
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	4	1.37
(1,528)	1:55:A:PRO:HD3	1:47:A:GLN:HE21	5	1.37
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	11	1.37
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	11	1.37
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	11	1.37
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD1	15	1.36
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD2	15	1.36
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD1	15	1.36
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD2	15	1.36
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD1	15	1.36
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD2	15	1.36
(1,2365)	2:93:B:VAL:HG21	1:89:A:TYR:HD1	20	1.36
(1,2365)	2:93:B:VAL:HG21	1:89:A:TYR:HD2	20	1.36
(1,2365)	2:93:B:VAL:HG22	1:89:A:TYR:HD1	20	1.36
(1,2365)	2:93:B:VAL:HG22	1:89:A:TYR:HD2	20	1.36
(1,2365)	2:93:B:VAL:HG23	1:89:A:TYR:HD1	20	1.36
(1,2365)	2:93:B:VAL:HG23	1:89:A:TYR:HD2	20	1.36
(1,1627)	1:129:A:VAL:HG11	1:125:A:TRP:HB3	7	1.36
(1,1627)	1:129:A:VAL:HG12	1:125:A:TRP:HB3	7	1.36
(1,1627)	1:129:A:VAL:HG13	1:125:A:TRP:HB3	7	1.36
(1,1627)	1:129:A:VAL:HG11	1:125:A:TRP:HB3	11	1.36
(1,1627)	1:129:A:VAL:HG12	1:125:A:TRP:HB3	11	1.36
(1,1627)	1:129:A:VAL:HG13	1:125:A:TRP:HB3	11	1.36
(1,1350)	1:179:A:ALA:HB1	1:182:A:ASN:HB3	3	1.36
(1,1350)	1:179:A:ALA:HB2	1:182:A:ASN:HB3	3	1.36
(1,1350)	1:179:A:ALA:HB3	1:182:A:ASN:HB3	3	1.36
(1,1020)	1:118:A:LEU:HD21	1:130:A:ALA:HA	12	1.36
(1,1020)	1:118:A:LEU:HD22	1:130:A:ALA:HA	12	1.36
(1,1020)	1:118:A:LEU:HD23	1:130:A:ALA:HA	12	1.36
(1,3031)	1:118:A:LEU:HD11	2:91:B:ALA:HA	3	1.35
(1,3031)	1:118:A:LEU:HD12	2:91:B:ALA:HA	3	1.35
(1,3031)	1:118:A:LEU:HD13	2:91:B:ALA:HA	3	1.35
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD1	5	1.35
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD2	5	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD1	5	1.35
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD2	5	1.35
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD1	5	1.35
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD2	5	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	3	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	3	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	3	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	3	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	3	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	3	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	3	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	3	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	3	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	4	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	4	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	4	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	4	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	4	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	4	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	4	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	4	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	4	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	6	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	6	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	6	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	6	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	6	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	6	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	6	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	6	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	6	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	8	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	8	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	8	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	8	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	8	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	8	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	8	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	8	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	8	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	9	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	9	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	9	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	9	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	9	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	9	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	9	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	9	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	9	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	12	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	12	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	12	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	12	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	12	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	12	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	12	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	12	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	12	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	14	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	14	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	14	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	14	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	14	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	14	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	14	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	14	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	14	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	15	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	15	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	15	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	15	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	15	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	15	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	15	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	15	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	15	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	16	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	16	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	16	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	16	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	16	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	16	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	16	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	16	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	16	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	17	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	17	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	17	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	17	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	17	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	17	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	17	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	17	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	17	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	19	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	19	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	19	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	19	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	19	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	19	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	19	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	19	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	19	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	20	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	20	1.35
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	20	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	20	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	20	1.35
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	20	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	20	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	20	1.35
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	20	1.35
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	11	1.35
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	11	1.35
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	11	1.35
(1,1898)	1:143:A:TYR:HD1	1:147:A:LEU:HD21	6	1.35
(1,1898)	1:143:A:TYR:HD1	1:147:A:LEU:HD22	6	1.35
(1,1898)	1:143:A:TYR:HD1	1:147:A:LEU:HD23	6	1.35
(1,1898)	1:143:A:TYR:HD2	1:147:A:LEU:HD21	6	1.35
(1,1898)	1:143:A:TYR:HD2	1:147:A:LEU:HD22	6	1.35
(1,1898)	1:143:A:TYR:HD2	1:147:A:LEU:HD23	6	1.35
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG11	9	1.35
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG12	9	1.35
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG13	9	1.35
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG11	18	1.35
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG12	18	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG13	18	1.35
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	19	1.35
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	19	1.35
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	19	1.35
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	1	1.35
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	1	1.35
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	1	1.35
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	5	1.35
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	5	1.35
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	5	1.35
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	5	1.35
(1,1020)	1:118:A:LEU:HD21	1:130:A:ALA:HA	17	1.35
(1,1020)	1:118:A:LEU:HD22	1:130:A:ALA:HA	17	1.35
(1,1020)	1:118:A:LEU:HD23	1:130:A:ALA:HA	17	1.35
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	13	1.35
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	13	1.35
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	13	1.35
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	13	1.34
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	13	1.34
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	13	1.34
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	13	1.34
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	13	1.34
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	13	1.34
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	13	1.34
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	13	1.34
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	13	1.34
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	5	1.34
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	5	1.34
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	5	1.34
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	5	1.34
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	5	1.34
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	5	1.34
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	5	1.34
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	5	1.34
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	5	1.34
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG11	2	1.34
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG12	2	1.34
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG13	2	1.34
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG11	7	1.34
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG12	7	1.34
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG13	7	1.34
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG11	11	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG12	11	1.34
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG13	11	1.34
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG11	20	1.34
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG12	20	1.34
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG13	20	1.34
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	7	1.34
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	7	1.34
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	7	1.34
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	14	1.34
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	14	1.34
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	14	1.34
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	11	1.34
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	11	1.34
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	11	1.34
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	13	1.34
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	13	1.34
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	13	1.34
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD1	10	1.33
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD2	10	1.33
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD1	10	1.33
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD2	10	1.33
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD1	10	1.33
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD2	10	1.33
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG11	15	1.33
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG12	15	1.33
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG13	15	1.33
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD11	2	1.33
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD12	2	1.33
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD13	2	1.33
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	1	1.33
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	1	1.33
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	1	1.33
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	3	1.33
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	3	1.33
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	3	1.33
(1,593)	1:131:A:LEU:HD21	1:135:A:GLY:H	18	1.33
(1,593)	1:131:A:LEU:HD22	1:135:A:GLY:H	18	1.33
(1,593)	1:131:A:LEU:HD23	1:135:A:GLY:H	18	1.33
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	11	1.32
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	11	1.32
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD1	12	1.32
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD2	12	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD1	12	1.32
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD2	12	1.32
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD1	12	1.32
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD2	12	1.32
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	3	1.32
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	3	1.32
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	3	1.32
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	3	1.32
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	3	1.32
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	3	1.32
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	3	1.32
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	3	1.32
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	3	1.32
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG11	4	1.32
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG12	4	1.32
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG13	4	1.32
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG11	13	1.32
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG12	13	1.32
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG13	13	1.32
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG11	19	1.32
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG12	19	1.32
(1,1891)	1:128:A:VAL:H	1:129:A:VAL:HG13	19	1.32
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD11	18	1.32
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD12	18	1.32
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD13	18	1.32
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	16	1.32
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	16	1.32
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	16	1.32
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	4	1.32
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	4	1.32
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	4	1.32
(1,1344)	1:34:A:VAL:HG21	1:38:A:TYR:HB3	15	1.32
(1,1344)	1:34:A:VAL:HG22	1:38:A:TYR:HB3	15	1.32
(1,1344)	1:34:A:VAL:HG23	1:38:A:TYR:HB3	15	1.32
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	12	1.32
(1,1020)	1:118:A:LEU:HD21	1:130:A:ALA:HA	3	1.32
(1,1020)	1:118:A:LEU:HD22	1:130:A:ALA:HA	3	1.32
(1,1020)	1:118:A:LEU:HD23	1:130:A:ALA:HA	3	1.32
(1,625)	1:118:A:LEU:HD21	1:128:A:VAL:HA	6	1.32
(1,625)	1:118:A:LEU:HD22	1:128:A:VAL:HA	6	1.32
(1,625)	1:118:A:LEU:HD23	1:128:A:VAL:HA	6	1.32
(1,593)	1:131:A:LEU:HD21	1:135:A:GLY:H	2	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:131:A:LEU:HD22	1:135:A:GLY:H	2	1.32
(1,593)	1:131:A:LEU:HD23	1:135:A:GLY:H	2	1.32
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	19	1.32
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	19	1.32
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	19	1.32
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD1	3	1.31
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD2	3	1.31
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD1	3	1.31
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD2	3	1.31
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD1	3	1.31
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD2	3	1.31
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD1	17	1.31
(1,2423)	1:131:A:LEU:HD21	1:134:A:PHE:HD2	17	1.31
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD1	17	1.31
(1,2423)	1:131:A:LEU:HD22	1:134:A:PHE:HD2	17	1.31
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD1	17	1.31
(1,2423)	1:131:A:LEU:HD23	1:134:A:PHE:HD2	17	1.31
(1,2365)	2:93:B:VAL:HG21	1:89:A:TYR:HD1	10	1.31
(1,2365)	2:93:B:VAL:HG21	1:89:A:TYR:HD2	10	1.31
(1,2365)	2:93:B:VAL:HG22	1:89:A:TYR:HD1	10	1.31
(1,2365)	2:93:B:VAL:HG22	1:89:A:TYR:HD2	10	1.31
(1,2365)	2:93:B:VAL:HG23	1:89:A:TYR:HD1	10	1.31
(1,2365)	2:93:B:VAL:HG23	1:89:A:TYR:HD2	10	1.31
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	12	1.31
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	12	1.31
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	12	1.31
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	12	1.31
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	12	1.31
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	12	1.31
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	12	1.31
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	12	1.31
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	12	1.31
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG11	11	1.31
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG12	11	1.31
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG13	11	1.31
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG11	11	1.31
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG12	11	1.31
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG13	11	1.31
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG11	11	1.31
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG12	11	1.31
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG13	11	1.31
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD11	15	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD12	15	1.31
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD13	15	1.31
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	18	1.31
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	11	1.31
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	11	1.31
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	11	1.31
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	13	1.31
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	13	1.31
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	13	1.31
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	10	1.31
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	3	1.31
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	3	1.31
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	3	1.31
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	11	1.31
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	11	1.31
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	11	1.31
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	8	1.3
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	8	1.3
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	8	1.3
(1,733)	1:26:A:GLN:HG3	1:23:A:SER:HB3	4	1.3
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	4	1.3
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	4	1.3
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	4	1.3
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	17	1.3
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	17	1.3
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	17	1.3
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	13	1.29
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	13	1.29
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	14	1.29
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	14	1.29
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	14	1.29
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	6	1.29
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	6	1.29
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	6	1.29
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	7	1.29
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	7	1.29
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	7	1.29
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	8	1.29
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	8	1.29
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	8	1.29
(1,1350)	1:179:A:ALA:HB1	1:182:A:ASN:HB3	12	1.29
(1,1350)	1:179:A:ALA:HB2	1:182:A:ASN:HB3	12	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1350)	1:179:A:ALA:HB3	1:182:A:ASN:HB3	12	1.29
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	6	1.29
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	17	1.29
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE1	14	1.28
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE2	14	1.28
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE1	14	1.28
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE2	14	1.28
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE1	14	1.28
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE2	14	1.28
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD1	17	1.28
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD2	17	1.28
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD1	17	1.28
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD2	17	1.28
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD1	17	1.28
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD2	17	1.28
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	1	1.28
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	1	1.28
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	1	1.28
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	1	1.28
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	1	1.28
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	1	1.28
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	1	1.28
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	1	1.28
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	1	1.28
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG21	11	1.28
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG22	11	1.28
(1,1957)	1:74:A:VAL:HG11	1:70:A:THR:HG23	11	1.28
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG21	11	1.28
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG22	11	1.28
(1,1957)	1:74:A:VAL:HG12	1:70:A:THR:HG23	11	1.28
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG21	11	1.28
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG22	11	1.28
(1,1957)	1:74:A:VAL:HG13	1:70:A:THR:HG23	11	1.28
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD21	3	1.28
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD22	3	1.28
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD23	3	1.28
(1,1867)	1:73:A:GLN:HG3	1:181:A:LEU:HD11	1	1.28
(1,1867)	1:73:A:GLN:HG3	1:181:A:LEU:HD12	1	1.28
(1,1867)	1:73:A:GLN:HG3	1:181:A:LEU:HD13	1	1.28
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	1	1.28
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	2	1.28
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	20	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1627)	1:129:A:VAL:HG11	1:125:A:TRP:HB3	13	1.28
(1,1627)	1:129:A:VAL:HG12	1:125:A:TRP:HB3	13	1.28
(1,1627)	1:129:A:VAL:HG13	1:125:A:TRP:HB3	13	1.28
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	8	1.28
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	1	1.28
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	9	1.28
(1,854)	1:159:A:VAL:HG11	1:32:A:GLU:HA	16	1.28
(1,854)	1:159:A:VAL:HG12	1:32:A:GLU:HA	16	1.28
(1,854)	1:159:A:VAL:HG13	1:32:A:GLU:HA	16	1.28
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	16	1.28
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	16	1.28
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	16	1.28
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	15	1.27
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	15	1.27
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD11	10	1.27
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD12	10	1.27
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD13	10	1.27
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD11	10	1.27
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD12	10	1.27
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD13	10	1.27
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD11	10	1.27
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD12	10	1.27
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD13	10	1.27
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD11	10	1.27
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD12	10	1.27
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD13	10	1.27
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD11	10	1.27
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD12	10	1.27
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD13	10	1.27
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD11	10	1.27
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD12	10	1.27
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD13	10	1.27
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	3	1.27
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	6	1.27
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	7	1.27
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	12	1.27
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	15	1.27
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	16	1.27
(1,1627)	1:129:A:VAL:HG11	1:125:A:TRP:HB3	20	1.27
(1,1627)	1:129:A:VAL:HG12	1:125:A:TRP:HB3	20	1.27
(1,1627)	1:129:A:VAL:HG13	1:125:A:TRP:HB3	20	1.27
(1,1087)	1:47:A:GLN:HE22	1:55:A:PRO:HD3	19	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1020)	1:118:A:LEU:HD21	1:130:A:ALA:HA	14	1.27
(1,1020)	1:118:A:LEU:HD22	1:130:A:ALA:HA	14	1.27
(1,1020)	1:118:A:LEU:HD23	1:130:A:ALA:HA	14	1.27
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	9	1.27
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	9	1.27
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	9	1.27
(1,625)	1:118:A:LEU:HD21	1:128:A:VAL:HA	12	1.27
(1,625)	1:118:A:LEU:HD22	1:128:A:VAL:HA	12	1.27
(1,625)	1:118:A:LEU:HD23	1:128:A:VAL:HA	12	1.27
(1,593)	1:131:A:LEU:HD21	1:135:A:GLY:H	19	1.27
(1,593)	1:131:A:LEU:HD22	1:135:A:GLY:H	19	1.27
(1,593)	1:131:A:LEU:HD23	1:135:A:GLY:H	19	1.27
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	3	1.27
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	3	1.27
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	3	1.27
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	5	1.27
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	5	1.27
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	5	1.27
(1,90)	1:97:A:LEU:HD21	1:138:A:LEU:H	14	1.27
(1,90)	1:97:A:LEU:HD22	1:138:A:LEU:H	14	1.27
(1,90)	1:97:A:LEU:HD23	1:138:A:LEU:H	14	1.27
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE1	9	1.26
(1,2439)	1:118:A:LEU:HD21	1:134:A:PHE:HE2	9	1.26
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE1	9	1.26
(1,2439)	1:118:A:LEU:HD22	1:134:A:PHE:HE2	9	1.26
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE1	9	1.26
(1,2439)	1:118:A:LEU:HD23	1:134:A:PHE:HE2	9	1.26
(1,2202)	1:97:A:LEU:HD11	1:96:A:MET:HE1	6	1.26
(1,2202)	1:97:A:LEU:HD11	1:96:A:MET:HE2	6	1.26
(1,2202)	1:97:A:LEU:HD11	1:96:A:MET:HE3	6	1.26
(1,2202)	1:97:A:LEU:HD12	1:96:A:MET:HE1	6	1.26
(1,2202)	1:97:A:LEU:HD12	1:96:A:MET:HE2	6	1.26
(1,2202)	1:97:A:LEU:HD12	1:96:A:MET:HE3	6	1.26
(1,2202)	1:97:A:LEU:HD13	1:96:A:MET:HE1	6	1.26
(1,2202)	1:97:A:LEU:HD13	1:96:A:MET:HE2	6	1.26
(1,2202)	1:97:A:LEU:HD13	1:96:A:MET:HE3	6	1.26
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	4	1.26
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	5	1.26
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	8	1.26
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	9	1.26
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	10	1.26
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	13	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	14	1.26
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	17	1.26
(1,1627)	1:129:A:VAL:HG11	1:125:A:TRP:HB3	19	1.26
(1,1627)	1:129:A:VAL:HG12	1:125:A:TRP:HB3	19	1.26
(1,1627)	1:129:A:VAL:HG13	1:125:A:TRP:HB3	19	1.26
(1,1570)	1:159:A:VAL:HG11	1:158:A:VAL:HB	1	1.26
(1,1570)	1:159:A:VAL:HG12	1:158:A:VAL:HB	1	1.26
(1,1570)	1:159:A:VAL:HG13	1:158:A:VAL:HB	1	1.26
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	13	1.26
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	13	1.26
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	13	1.26
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	10	1.26
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	16	1.26
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	16	1.26
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	16	1.26
(1,593)	1:131:A:LEU:HD21	1:135:A:GLY:H	7	1.26
(1,593)	1:131:A:LEU:HD22	1:135:A:GLY:H	7	1.26
(1,593)	1:131:A:LEU:HD23	1:135:A:GLY:H	7	1.26
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	7	1.26
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	11	1.26
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	12	1.25
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	12	1.25
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	12	1.25
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	10	1.25
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	10	1.25
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	10	1.25
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	11	1.25
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	11	1.25
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	11	1.25
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	11	1.25
(1,1783)	1:75:A:GLY:HA3	1:78:A:LEU:HG	19	1.25
(1,1570)	1:159:A:VAL:HG11	1:158:A:VAL:HB	18	1.25
(1,1570)	1:159:A:VAL:HG12	1:158:A:VAL:HB	18	1.25
(1,1570)	1:159:A:VAL:HG13	1:158:A:VAL:HB	18	1.25
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	9	1.25
(1,1350)	1:179:A:ALA:HB1	1:182:A:ASN:HB3	4	1.25
(1,1350)	1:179:A:ALA:HB2	1:182:A:ASN:HB3	4	1.25
(1,1350)	1:179:A:ALA:HB3	1:182:A:ASN:HB3	4	1.25
(1,1350)	1:179:A:ALA:HB1	1:182:A:ASN:HB3	6	1.25
(1,1350)	1:179:A:ALA:HB2	1:182:A:ASN:HB3	6	1.25
(1,1350)	1:179:A:ALA:HB3	1:182:A:ASN:HB3	6	1.25
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	7	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1033)	1:118:A:LEU:HD21	1:115:A:ALA:HA	19	1.25
(1,1033)	1:118:A:LEU:HD22	1:115:A:ALA:HA	19	1.25
(1,1033)	1:118:A:LEU:HD23	1:115:A:ALA:HA	19	1.25
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	17	1.25
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	17	1.25
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	17	1.25
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	1	1.25
(1,139)	1:131:A:LEU:HD21	1:115:A:ALA:H	19	1.25
(1,139)	1:131:A:LEU:HD22	1:115:A:ALA:H	19	1.25
(1,139)	1:131:A:LEU:HD23	1:115:A:ALA:H	19	1.25
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD1	3	1.24
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD2	3	1.24
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD1	3	1.24
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD2	3	1.24
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD1	3	1.24
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD2	3	1.24
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD21	3	1.24
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD22	3	1.24
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD23	3	1.24
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD21	3	1.24
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD22	3	1.24
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD23	3	1.24
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD21	3	1.24
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD22	3	1.24
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD23	3	1.24
(1,1329)	1:118:A:LEU:HD21	1:134:A:PHE:HB3	17	1.24
(1,1329)	1:118:A:LEU:HD22	1:134:A:PHE:HB3	17	1.24
(1,1329)	1:118:A:LEU:HD23	1:134:A:PHE:HB3	17	1.24
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	4	1.24
(1,1020)	1:118:A:LEU:HD21	1:130:A:ALA:HA	6	1.24
(1,1020)	1:118:A:LEU:HD22	1:130:A:ALA:HA	6	1.24
(1,1020)	1:118:A:LEU:HD23	1:130:A:ALA:HA	6	1.24
(1,921)	1:98:A:GLN:HE22	1:98:A:GLN:HA	7	1.24
(1,625)	1:118:A:LEU:HD21	1:128:A:VAL:HA	3	1.24
(1,625)	1:118:A:LEU:HD22	1:128:A:VAL:HA	3	1.24
(1,625)	1:118:A:LEU:HD23	1:128:A:VAL:HA	3	1.24
(1,528)	1:55:A:PRO:HD3	1:47:A:GLN:HE21	8	1.24
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	7	1.24
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	7	1.24
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	7	1.24
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	8	1.24
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	8	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	8	1.24
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	12	1.24
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	12	1.24
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	12	1.24
(1,90)	1:97:A:LEU:HD21	1:138:A:LEU:H	16	1.24
(1,90)	1:97:A:LEU:HD22	1:138:A:LEU:H	16	1.24
(1,90)	1:97:A:LEU:HD23	1:138:A:LEU:H	16	1.24
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD1	6	1.23
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD2	6	1.23
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD1	6	1.23
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD2	6	1.23
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD1	6	1.23
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD2	6	1.23
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD1	12	1.23
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD2	12	1.23
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD1	12	1.23
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD2	12	1.23
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD1	12	1.23
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD2	12	1.23
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	3	1.23
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	3	1.23
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	3	1.23
(1,1570)	1:159:A:VAL:HG11	1:158:A:VAL:HB	3	1.23
(1,1570)	1:159:A:VAL:HG12	1:158:A:VAL:HB	3	1.23
(1,1570)	1:159:A:VAL:HG13	1:158:A:VAL:HB	3	1.23
(1,1570)	1:159:A:VAL:HG11	1:158:A:VAL:HB	7	1.23
(1,1570)	1:159:A:VAL:HG12	1:158:A:VAL:HB	7	1.23
(1,1570)	1:159:A:VAL:HG13	1:158:A:VAL:HB	7	1.23
(1,1570)	1:159:A:VAL:HG11	1:158:A:VAL:HB	11	1.23
(1,1570)	1:159:A:VAL:HG12	1:158:A:VAL:HB	11	1.23
(1,1570)	1:159:A:VAL:HG13	1:158:A:VAL:HB	11	1.23
(1,593)	1:131:A:LEU:HD21	1:135:A:GLY:H	15	1.23
(1,593)	1:131:A:LEU:HD22	1:135:A:GLY:H	15	1.23
(1,593)	1:131:A:LEU:HD23	1:135:A:GLY:H	15	1.23
(1,543)	1:181:A:LEU:HD11	1:73:A:GLN:HE21	9	1.23
(1,543)	1:181:A:LEU:HD12	1:73:A:GLN:HE21	9	1.23
(1,543)	1:181:A:LEU:HD13	1:73:A:GLN:HE21	9	1.23
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	9	1.23
(1,74)	1:63:A:LEU:HD11	1:65:A:LEU:H	10	1.23
(1,74)	1:63:A:LEU:HD12	1:65:A:LEU:H	10	1.23
(1,74)	1:63:A:LEU:HD13	1:65:A:LEU:H	10	1.23
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE1	19	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE2	19	1.22
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE1	19	1.22
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE2	19	1.22
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE1	19	1.22
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE2	19	1.22
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	3	1.22
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	3	1.22
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	3	1.22
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE1	11	1.22
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE2	11	1.22
(1,2085)	1:34:A:VAL:HG11	1:71:A:MET:HE3	11	1.22
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE1	11	1.22
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE2	11	1.22
(1,2085)	1:34:A:VAL:HG12	1:71:A:MET:HE3	11	1.22
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE1	11	1.22
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE2	11	1.22
(1,2085)	1:34:A:VAL:HG13	1:71:A:MET:HE3	11	1.22
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD11	18	1.22
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD12	18	1.22
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD13	18	1.22
(1,1570)	1:159:A:VAL:HG11	1:158:A:VAL:HB	14	1.22
(1,1570)	1:159:A:VAL:HG12	1:158:A:VAL:HB	14	1.22
(1,1570)	1:159:A:VAL:HG13	1:158:A:VAL:HB	14	1.22
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	17	1.22
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	17	1.22
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	17	1.22
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	1	1.22
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	1	1.22
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	1	1.22
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	1	1.22
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	1	1.22
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	1	1.22
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD21	4	1.21
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD22	4	1.21
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD23	4	1.21
(1,1570)	1:159:A:VAL:HG11	1:158:A:VAL:HB	8	1.21
(1,1570)	1:159:A:VAL:HG12	1:158:A:VAL:HB	8	1.21
(1,1570)	1:159:A:VAL:HG13	1:158:A:VAL:HB	8	1.21
(1,1570)	1:159:A:VAL:HG11	1:158:A:VAL:HB	15	1.21
(1,1570)	1:159:A:VAL:HG12	1:158:A:VAL:HB	15	1.21
(1,1570)	1:159:A:VAL:HG13	1:158:A:VAL:HB	15	1.21
(1,1570)	1:159:A:VAL:HG11	1:158:A:VAL:HB	17	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1570)	1:159:A:VAL:HG12	1:158:A:VAL:HB	17	1.21
(1,1570)	1:159:A:VAL:HG13	1:158:A:VAL:HB	17	1.21
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	16	1.21
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	16	1.21
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	16	1.21
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	7	1.21
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	7	1.21
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	7	1.21
(1,1103)	1:39:A:VAL:HG11	1:133:A:GLY:HA2	2	1.21
(1,1103)	1:39:A:VAL:HG11	1:133:A:GLY:HA3	2	1.21
(1,1103)	1:39:A:VAL:HG12	1:133:A:GLY:HA2	2	1.21
(1,1103)	1:39:A:VAL:HG12	1:133:A:GLY:HA3	2	1.21
(1,1103)	1:39:A:VAL:HG13	1:133:A:GLY:HA2	2	1.21
(1,1103)	1:39:A:VAL:HG13	1:133:A:GLY:HA3	2	1.21
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	19	1.21
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	4	1.21
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	4	1.21
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	4	1.21
(1,921)	1:98:A:GLN:HE22	1:98:A:GLN:HA	20	1.21
(1,593)	1:131:A:LEU:HD21	1:135:A:GLY:H	5	1.21
(1,593)	1:131:A:LEU:HD22	1:135:A:GLY:H	5	1.21
(1,593)	1:131:A:LEU:HD23	1:135:A:GLY:H	5	1.21
(1,593)	1:131:A:LEU:HD21	1:135:A:GLY:H	12	1.21
(1,593)	1:131:A:LEU:HD22	1:135:A:GLY:H	12	1.21
(1,593)	1:131:A:LEU:HD23	1:135:A:GLY:H	12	1.21
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	9	1.21
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	9	1.21
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	9	1.21
(1,2483)	1:147:A:LEU:HD21	1:150:A:PHE:HZ	6	1.2
(1,2483)	1:147:A:LEU:HD22	1:150:A:PHE:HZ	6	1.2
(1,2483)	1:147:A:LEU:HD23	1:150:A:PHE:HZ	6	1.2
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	15	1.2
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	15	1.2
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	15	1.2
(1,1627)	1:129:A:VAL:HG11	1:125:A:TRP:HB3	9	1.2
(1,1627)	1:129:A:VAL:HG12	1:125:A:TRP:HB3	9	1.2
(1,1627)	1:129:A:VAL:HG13	1:125:A:TRP:HB3	9	1.2
(1,1570)	1:159:A:VAL:HG11	1:158:A:VAL:HB	19	1.2
(1,1570)	1:159:A:VAL:HG12	1:158:A:VAL:HB	19	1.2
(1,1570)	1:159:A:VAL:HG13	1:158:A:VAL:HB	19	1.2
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	19	1.2
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	19	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	19	1.2
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	8	1.2
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	12	1.2
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	2	1.2
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	2	1.2
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	2	1.2
(1,625)	1:118:A:LEU:HD21	1:128:A:VAL:HA	17	1.2
(1,625)	1:118:A:LEU:HD22	1:128:A:VAL:HA	17	1.2
(1,625)	1:118:A:LEU:HD23	1:128:A:VAL:HA	17	1.2
(1,593)	1:131:A:LEU:HD21	1:135:A:GLY:H	10	1.2
(1,593)	1:131:A:LEU:HD22	1:135:A:GLY:H	10	1.2
(1,593)	1:131:A:LEU:HD23	1:135:A:GLY:H	10	1.2
(1,543)	1:181:A:LEU:HD11	1:73:A:GLN:HE21	11	1.2
(1,543)	1:181:A:LEU:HD12	1:73:A:GLN:HE21	11	1.2
(1,543)	1:181:A:LEU:HD13	1:73:A:GLN:HE21	11	1.2
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	18	1.19
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	18	1.19
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	18	1.19
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	13	1.19
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	13	1.19
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	13	1.19
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	20	1.19
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	2	1.19
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	15	1.19
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	18	1.19
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	14	1.19
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	14	1.19
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	14	1.19
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	19	1.19
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	19	1.19
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	19	1.19
(1,921)	1:98:A:GLN:HE22	1:98:A:GLN:HA	6	1.19
(1,921)	1:98:A:GLN:HE22	1:98:A:GLN:HA	8	1.19
(1,593)	1:131:A:LEU:HD21	1:135:A:GLY:H	3	1.19
(1,593)	1:131:A:LEU:HD22	1:135:A:GLY:H	3	1.19
(1,593)	1:131:A:LEU:HD23	1:135:A:GLY:H	3	1.19
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	11	1.19
(1,90)	1:97:A:LEU:HD21	1:138:A:LEU:H	13	1.19
(1,90)	1:97:A:LEU:HD22	1:138:A:LEU:H	13	1.19
(1,90)	1:97:A:LEU:HD23	1:138:A:LEU:H	13	1.19
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	18	1.18
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	18	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	18	1.18
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD11	7	1.18
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD12	7	1.18
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD13	7	1.18
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	2	1.18
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	15	1.18
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	7	1.18
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	13	1.18
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	5	1.18
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	5	1.18
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	5	1.18
(1,921)	1:98:A:GLN:HE22	1:98:A:GLN:HA	16	1.18
(1,625)	1:118:A:LEU:HD21	1:128:A:VAL:HA	4	1.18
(1,625)	1:118:A:LEU:HD22	1:128:A:VAL:HA	4	1.18
(1,625)	1:118:A:LEU:HD23	1:128:A:VAL:HA	4	1.18
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	13	1.18
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	16	1.18
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	10	1.18
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	20	1.18
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	20	1.18
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	20	1.18
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	8	1.17
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	8	1.17
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	1	1.17
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	1	1.17
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	1	1.17
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD11	9	1.17
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD12	9	1.17
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD13	9	1.17
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	4	1.17
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	4	1.17
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	4	1.17
(1,1627)	1:129:A:VAL:HG11	1:125:A:TRP:HB3	5	1.17
(1,1627)	1:129:A:VAL:HG12	1:125:A:TRP:HB3	5	1.17
(1,1627)	1:129:A:VAL:HG13	1:125:A:TRP:HB3	5	1.17
(1,1103)	1:39:A:VAL:HG11	1:133:A:GLY:HA2	20	1.17
(1,1103)	1:39:A:VAL:HG11	1:133:A:GLY:HA3	20	1.17
(1,1103)	1:39:A:VAL:HG12	1:133:A:GLY:HA2	20	1.17
(1,1103)	1:39:A:VAL:HG12	1:133:A:GLY:HA3	20	1.17
(1,1103)	1:39:A:VAL:HG13	1:133:A:GLY:HA2	20	1.17
(1,1103)	1:39:A:VAL:HG13	1:133:A:GLY:HA3	20	1.17
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	8	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	8	1.17
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	8	1.17
(1,921)	1:98:A:GLN:HE22	1:98:A:GLN:HA	3	1.17
(1,854)	1:159:A:VAL:HG11	1:32:A:GLU:HA	9	1.17
(1,854)	1:159:A:VAL:HG12	1:32:A:GLU:HA	9	1.17
(1,854)	1:159:A:VAL:HG13	1:32:A:GLU:HA	9	1.17
(1,841)	1:97:A:LEU:HD11	1:93:A:PHE:HA	15	1.17
(1,841)	1:97:A:LEU:HD12	1:93:A:PHE:HA	15	1.17
(1,841)	1:97:A:LEU:HD13	1:93:A:PHE:HA	15	1.17
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	6	1.17
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	6	1.17
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	6	1.17
(1,3031)	1:118:A:LEU:HD11	2:91:B:ALA:HA	9	1.16
(1,3031)	1:118:A:LEU:HD12	2:91:B:ALA:HA	9	1.16
(1,3031)	1:118:A:LEU:HD13	2:91:B:ALA:HA	9	1.16
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	7	1.16
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	7	1.16
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	7	1.16
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	20	1.16
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	20	1.16
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	20	1.16
(1,1570)	1:159:A:VAL:HG11	1:158:A:VAL:HB	4	1.16
(1,1570)	1:159:A:VAL:HG12	1:158:A:VAL:HB	4	1.16
(1,1570)	1:159:A:VAL:HG13	1:158:A:VAL:HB	4	1.16
(1,1329)	1:118:A:LEU:HD21	1:134:A:PHE:HB3	3	1.16
(1,1329)	1:118:A:LEU:HD22	1:134:A:PHE:HB3	3	1.16
(1,1329)	1:118:A:LEU:HD23	1:134:A:PHE:HB3	3	1.16
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	17	1.16
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	5	1.16
(1,178)	1:118:A:LEU:HD21	1:131:A:LEU:H	4	1.16
(1,178)	1:118:A:LEU:HD22	1:131:A:LEU:H	4	1.16
(1,178)	1:118:A:LEU:HD23	1:131:A:LEU:H	4	1.16
(1,178)	1:118:A:LEU:HD21	1:131:A:LEU:H	6	1.16
(1,178)	1:118:A:LEU:HD22	1:131:A:LEU:H	6	1.16
(1,178)	1:118:A:LEU:HD23	1:131:A:LEU:H	6	1.16
(1,178)	1:118:A:LEU:HD21	1:131:A:LEU:H	19	1.16
(1,178)	1:118:A:LEU:HD22	1:131:A:LEU:H	19	1.16
(1,178)	1:118:A:LEU:HD23	1:131:A:LEU:H	19	1.16
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD1	16	1.15
(1,2395)	1:142:A:VAL:HG11	1:150:A:PHE:HD2	16	1.15
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD1	16	1.15
(1,2395)	1:142:A:VAL:HG12	1:150:A:PHE:HD2	16	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD1	16	1.15
(1,2395)	1:142:A:VAL:HG13	1:150:A:PHE:HD2	16	1.15
(1,1570)	1:159:A:VAL:HG11	1:158:A:VAL:HB	13	1.15
(1,1570)	1:159:A:VAL:HG12	1:158:A:VAL:HB	13	1.15
(1,1570)	1:159:A:VAL:HG13	1:158:A:VAL:HB	13	1.15
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	3	1.15
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	19	1.15
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	1	1.14
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	1	1.14
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	1	1.14
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	11	1.14
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	11	1.14
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	11	1.14
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	11	1.14
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	11	1.14
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	11	1.14
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	11	1.14
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	11	1.14
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	11	1.14
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	3	1.14
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	3	1.14
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	3	1.14
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	11	1.14
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	11	1.14
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	11	1.14
(1,1627)	1:129:A:VAL:HG11	1:125:A:TRP:HB3	18	1.14
(1,1627)	1:129:A:VAL:HG12	1:125:A:TRP:HB3	18	1.14
(1,1627)	1:129:A:VAL:HG13	1:125:A:TRP:HB3	18	1.14
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	15	1.14
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	15	1.14
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	15	1.14
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	3	1.14
(1,2556)	1:183:A:LEU:HD21	1:125:A:TRP:HE3	19	1.13
(1,2556)	1:183:A:LEU:HD22	1:125:A:TRP:HE3	19	1.13
(1,2556)	1:183:A:LEU:HD23	1:125:A:TRP:HE3	19	1.13
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD21	11	1.13
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD22	11	1.13
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD23	11	1.13
(1,1043)	1:182:A:ASN:HB3	1:179:A:ALA:HA	17	1.13
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	7	1.13
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	7	1.13
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	7	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	12	1.13
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	12	1.13
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	12	1.13
(1,921)	1:98:A:GLN:HE22	1:98:A:GLN:HA	12	1.13
(1,625)	1:118:A:LEU:HD21	1:128:A:VAL:HA	14	1.13
(1,625)	1:118:A:LEU:HD22	1:128:A:VAL:HA	14	1.13
(1,625)	1:118:A:LEU:HD23	1:128:A:VAL:HA	14	1.13
(1,410)	1:94:A:GLN:HE22	1:95:A:THR:H	6	1.13
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	12	1.13
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	15	1.13
(1,90)	1:97:A:LEU:HD21	1:138:A:LEU:H	15	1.13
(1,90)	1:97:A:LEU:HD22	1:138:A:LEU:H	15	1.13
(1,90)	1:97:A:LEU:HD23	1:138:A:LEU:H	15	1.13
(1,1570)	1:159:A:VAL:HG11	1:158:A:VAL:HB	9	1.12
(1,1570)	1:159:A:VAL:HG12	1:158:A:VAL:HB	9	1.12
(1,1570)	1:159:A:VAL:HG13	1:158:A:VAL:HB	9	1.12
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	1	1.12
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	7	1.12
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	5	1.12
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	5	1.12
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	5	1.12
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	10	1.12
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	10	1.12
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	10	1.12
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	20	1.12
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	20	1.12
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	20	1.12
(1,841)	1:97:A:LEU:HD11	1:93:A:PHE:HA	10	1.12
(1,841)	1:97:A:LEU:HD12	1:93:A:PHE:HA	10	1.12
(1,841)	1:97:A:LEU:HD13	1:93:A:PHE:HA	10	1.12
(1,593)	1:131:A:LEU:HD21	1:135:A:GLY:H	17	1.12
(1,593)	1:131:A:LEU:HD22	1:135:A:GLY:H	17	1.12
(1,593)	1:131:A:LEU:HD23	1:135:A:GLY:H	17	1.12
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	14	1.12
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	8	1.11
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	8	1.11
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	8	1.11
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	2	1.11
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	2	1.11
(1,2433)	1:97:A:LEU:HD11	1:93:A:PHE:HE1	1	1.11
(1,2433)	1:97:A:LEU:HD11	1:93:A:PHE:HE2	1	1.11
(1,2433)	1:97:A:LEU:HD12	1:93:A:PHE:HE1	1	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2433)	1:97:A:LEU:HD12	1:93:A:PHE:HE2	1	1.11
(1,2433)	1:97:A:LEU:HD13	1:93:A:PHE:HE1	1	1.11
(1,2433)	1:97:A:LEU:HD13	1:93:A:PHE:HE2	1	1.11
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD1	4	1.11
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD2	4	1.11
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD1	4	1.11
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD2	4	1.11
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD1	4	1.11
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD2	4	1.11
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD1	14	1.11
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD2	14	1.11
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD1	14	1.11
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD2	14	1.11
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD1	14	1.11
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD2	14	1.11
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	7	1.11
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	7	1.11
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	7	1.11
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	4	1.11
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	4	1.11
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	4	1.11
(1,1570)	1:159:A:VAL:HG11	1:158:A:VAL:HB	16	1.11
(1,1570)	1:159:A:VAL:HG12	1:158:A:VAL:HB	16	1.11
(1,1570)	1:159:A:VAL:HG13	1:158:A:VAL:HB	16	1.11
(1,1329)	1:118:A:LEU:HD21	1:134:A:PHE:HB3	14	1.11
(1,1329)	1:118:A:LEU:HD22	1:134:A:PHE:HB3	14	1.11
(1,1329)	1:118:A:LEU:HD23	1:134:A:PHE:HB3	14	1.11
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	7	1.11
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	7	1.11
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	7	1.11
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	9	1.11
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	9	1.11
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	9	1.11
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	18	1.11
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	18	1.11
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	18	1.11
(1,1033)	1:118:A:LEU:HD21	1:115:A:ALA:HA	14	1.11
(1,1033)	1:118:A:LEU:HD22	1:115:A:ALA:HA	14	1.11
(1,1033)	1:118:A:LEU:HD23	1:115:A:ALA:HA	14	1.11
(1,841)	1:97:A:LEU:HD11	1:93:A:PHE:HA	16	1.11
(1,841)	1:97:A:LEU:HD12	1:93:A:PHE:HA	16	1.11
(1,841)	1:97:A:LEU:HD13	1:93:A:PHE:HA	16	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	20	1.11
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	20	1.11
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	20	1.11
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	13	1.11
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	2	1.11
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	2	1.11
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	2	1.11
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	15	1.11
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	15	1.11
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	15	1.11
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	16	1.1
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	16	1.1
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	16	1.1
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG21	11	1.1
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG22	11	1.1
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG23	11	1.1
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG21	11	1.1
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG22	11	1.1
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG23	11	1.1
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG21	11	1.1
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG22	11	1.1
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG23	11	1.1
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG21	11	1.1
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG22	11	1.1
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG23	11	1.1
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG21	11	1.1
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG22	11	1.1
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG23	11	1.1
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG21	11	1.1
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG22	11	1.1
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG23	11	1.1
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	13	1.1
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	13	1.1
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	13	1.1
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD11	4	1.1
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD12	4	1.1
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD13	4	1.1
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD11	4	1.1
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD12	4	1.1
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD13	4	1.1
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD11	4	1.1
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD12	4	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD13	4	1.1
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD11	4	1.1
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD12	4	1.1
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD13	4	1.1
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD11	4	1.1
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD12	4	1.1
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD13	4	1.1
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD11	4	1.1
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD12	4	1.1
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD13	4	1.1
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	11	1.1
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	3	1.1
(1,90)	1:97:A:LEU:HD21	1:138:A:LEU:H	17	1.1
(1,90)	1:97:A:LEU:HD22	1:138:A:LEU:H	17	1.1
(1,90)	1:97:A:LEU:HD23	1:138:A:LEU:H	17	1.1
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	18	1.09
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	18	1.09
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	18	1.09
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	6	1.09
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	6	1.09
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	6	1.09
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	9	1.09
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	9	1.09
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	9	1.09
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	13	1.09
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	13	1.09
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	13	1.09
(1,1627)	1:129:A:VAL:HG11	1:125:A:TRP:HB3	4	1.09
(1,1627)	1:129:A:VAL:HG12	1:125:A:TRP:HB3	4	1.09
(1,1627)	1:129:A:VAL:HG13	1:125:A:TRP:HB3	4	1.09
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	19	1.09
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	15	1.09
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	15	1.09
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	15	1.09
(1,1329)	1:118:A:LEU:HD21	1:134:A:PHE:HB3	9	1.09
(1,1329)	1:118:A:LEU:HD22	1:134:A:PHE:HB3	9	1.09
(1,1329)	1:118:A:LEU:HD23	1:134:A:PHE:HB3	9	1.09
(1,1329)	1:118:A:LEU:HD21	1:134:A:PHE:HB3	12	1.09
(1,1329)	1:118:A:LEU:HD22	1:134:A:PHE:HB3	12	1.09
(1,1329)	1:118:A:LEU:HD23	1:134:A:PHE:HB3	12	1.09
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	18	1.09
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	18	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	18	1.09
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	3	1.09
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	5	1.09
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	5	1.09
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	5	1.09
(1,178)	1:118:A:LEU:HD21	1:131:A:LEU:H	12	1.09
(1,178)	1:118:A:LEU:HD22	1:131:A:LEU:H	12	1.09
(1,178)	1:118:A:LEU:HD23	1:131:A:LEU:H	12	1.09
(1,139)	1:131:A:LEU:HD21	1:115:A:ALA:H	7	1.09
(1,139)	1:131:A:LEU:HD22	1:115:A:ALA:H	7	1.09
(1,139)	1:131:A:LEU:HD23	1:115:A:ALA:H	7	1.09
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	13	1.09
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	13	1.09
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	13	1.09
(1,2454)	1:147:A:LEU:HD21	1:150:A:PHE:HE1	7	1.08
(1,2454)	1:147:A:LEU:HD21	1:150:A:PHE:HE2	7	1.08
(1,2454)	1:147:A:LEU:HD22	1:150:A:PHE:HE1	7	1.08
(1,2454)	1:147:A:LEU:HD22	1:150:A:PHE:HE2	7	1.08
(1,2454)	1:147:A:LEU:HD23	1:150:A:PHE:HE1	7	1.08
(1,2454)	1:147:A:LEU:HD23	1:150:A:PHE:HE2	7	1.08
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	13	1.08
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	13	1.08
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	13	1.08
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	9	1.08
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	9	1.08
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	9	1.08
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	8	1.08
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	8	1.08
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	8	1.08
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	20	1.08
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	20	1.08
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	20	1.08
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	12	1.08
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	14	1.07
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	14	1.07
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	14	1.07
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	16	1.07
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	16	1.07
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	16	1.07
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	4	1.07
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	4	1.07
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	4	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	17	1.07
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	17	1.07
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	17	1.07
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD11	6	1.07
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD12	6	1.07
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD13	6	1.07
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	3	1.07
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	3	1.07
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	3	1.07
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	15	1.07
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	15	1.07
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	15	1.07
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	20	1.07
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	20	1.07
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	20	1.07
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	17	1.07
(1,1103)	1:39:A:VAL:HG11	1:133:A:GLY:HA2	12	1.07
(1,1103)	1:39:A:VAL:HG11	1:133:A:GLY:HA3	12	1.07
(1,1103)	1:39:A:VAL:HG12	1:133:A:GLY:HA2	12	1.07
(1,1103)	1:39:A:VAL:HG12	1:133:A:GLY:HA3	12	1.07
(1,1103)	1:39:A:VAL:HG13	1:133:A:GLY:HA2	12	1.07
(1,1103)	1:39:A:VAL:HG13	1:133:A:GLY:HA3	12	1.07
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	10	1.07
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	10	1.07
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	10	1.07
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	12	1.07
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	12	1.07
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	12	1.07
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	18	1.07
(1,178)	1:118:A:LEU:HD21	1:131:A:LEU:H	14	1.07
(1,178)	1:118:A:LEU:HD22	1:131:A:LEU:H	14	1.07
(1,178)	1:118:A:LEU:HD23	1:131:A:LEU:H	14	1.07
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	15	1.06
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	15	1.06
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	15	1.06
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	17	1.06
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	17	1.06
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	17	1.06
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD1	9	1.06
(1,2430)	1:118:A:LEU:HD21	1:134:A:PHE:HD2	9	1.06
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD1	9	1.06
(1,2430)	1:118:A:LEU:HD22	1:134:A:PHE:HD2	9	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD1	9	1.06
(1,2430)	1:118:A:LEU:HD23	1:134:A:PHE:HD2	9	1.06
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	6	1.06
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	6	1.06
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG11	8	1.06
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG12	8	1.06
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG13	8	1.06
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG11	8	1.06
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG12	8	1.06
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG13	8	1.06
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG11	8	1.06
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG12	8	1.06
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG13	8	1.06
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	18	1.06
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	18	1.06
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	18	1.06
(1,178)	1:118:A:LEU:HD21	1:131:A:LEU:H	3	1.06
(1,178)	1:118:A:LEU:HD22	1:131:A:LEU:H	3	1.06
(1,178)	1:118:A:LEU:HD23	1:131:A:LEU:H	3	1.06
(1,139)	1:131:A:LEU:HD21	1:115:A:ALA:H	5	1.06
(1,139)	1:131:A:LEU:HD22	1:115:A:ALA:H	5	1.06
(1,139)	1:131:A:LEU:HD23	1:115:A:ALA:H	5	1.06
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	4	1.06
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	4	1.06
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	4	1.06
(1,100)	1:69:A:SER:HB3	1:70:A:THR:H	1	1.06
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	1	1.05
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	1	1.05
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	1	1.05
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	14	1.05
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	14	1.05
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	14	1.05
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	2	1.05
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	2	1.05
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	2	1.05
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG21	12	1.05
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG22	12	1.05
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG23	12	1.05
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	19	1.05
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	19	1.05
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	19	1.05
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	19	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	19	1.05
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	19	1.05
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	19	1.05
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	19	1.05
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	19	1.05
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG11	15	1.05
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG12	15	1.05
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG13	15	1.05
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	10	1.05
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	10	1.05
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	10	1.05
(1,1329)	1:118:A:LEU:HD21	1:134:A:PHE:HB3	19	1.05
(1,1329)	1:118:A:LEU:HD22	1:134:A:PHE:HB3	19	1.05
(1,1329)	1:118:A:LEU:HD23	1:134:A:PHE:HB3	19	1.05
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	15	1.05
(1,1020)	1:118:A:LEU:HD21	1:130:A:ALA:HA	9	1.05
(1,1020)	1:118:A:LEU:HD22	1:130:A:ALA:HA	9	1.05
(1,1020)	1:118:A:LEU:HD23	1:130:A:ALA:HA	9	1.05
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	6	1.05
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	6	1.05
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	6	1.05
(1,921)	1:98:A:GLN:HE22	1:98:A:GLN:HA	11	1.05
(1,854)	1:159:A:VAL:HG11	1:32:A:GLU:HA	3	1.05
(1,854)	1:159:A:VAL:HG12	1:32:A:GLU:HA	3	1.05
(1,854)	1:159:A:VAL:HG13	1:32:A:GLU:HA	3	1.05
(1,2493)	1:118:A:LEU:HD21	1:119:A:PHE:HZ	19	1.04
(1,2493)	1:118:A:LEU:HD22	1:119:A:PHE:HZ	19	1.04
(1,2493)	1:118:A:LEU:HD23	1:119:A:PHE:HZ	19	1.04
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	17	1.04
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	17	1.04
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	17	1.04
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG21	15	1.04
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG22	15	1.04
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG23	15	1.04
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG21	15	1.04
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG22	15	1.04
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG23	15	1.04
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG21	15	1.04
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG22	15	1.04
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG23	15	1.04
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG21	15	1.04
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG22	15	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG23	15	1.04
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG21	15	1.04
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG22	15	1.04
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG23	15	1.04
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG21	15	1.04
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG22	15	1.04
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG23	15	1.04
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG11	11	1.04
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG12	11	1.04
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG13	11	1.04
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	2	1.04
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	2	1.04
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	2	1.04
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	15	1.04
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	15	1.04
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	15	1.04
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	9	1.04
(1,528)	1:55:A:PRO:HD3	1:47:A:GLN:HE21	6	1.04
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	17	1.04
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	17	1.04
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	17	1.04
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	6	1.04
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	8	1.04
(1,190)	1:183:A:LEU:HD21	1:125:A:TRP:H	19	1.04
(1,190)	1:183:A:LEU:HD22	1:125:A:TRP:H	19	1.04
(1,190)	1:183:A:LEU:HD23	1:125:A:TRP:H	19	1.04
(1,178)	1:118:A:LEU:HD21	1:131:A:LEU:H	17	1.04
(1,178)	1:118:A:LEU:HD22	1:131:A:LEU:H	17	1.04
(1,178)	1:118:A:LEU:HD23	1:131:A:LEU:H	17	1.04
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	10	1.04
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	10	1.04
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	10	1.04
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	14	1.04
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	14	1.04
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	14	1.04
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	18	1.04
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	18	1.04
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	18	1.04
(1,108)	1:74:A:VAL:HG11	1:73:A:GLN:H	19	1.04
(1,108)	1:74:A:VAL:HG12	1:73:A:GLN:H	19	1.04
(1,108)	1:74:A:VAL:HG13	1:73:A:GLN:H	19	1.04
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	2	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	2	1.03
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	2	1.03
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	4	1.03
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	4	1.03
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	4	1.03
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	10	1.03
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	10	1.03
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	10	1.03
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	20	1.03
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	20	1.03
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	20	1.03
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	5	1.03
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	5	1.03
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	5	1.03
(1,2365)	2:93:B:VAL:HG21	1:89:A:TYR:HD1	2	1.03
(1,2365)	2:93:B:VAL:HG21	1:89:A:TYR:HD2	2	1.03
(1,2365)	2:93:B:VAL:HG22	1:89:A:TYR:HD1	2	1.03
(1,2365)	2:93:B:VAL:HG22	1:89:A:TYR:HD2	2	1.03
(1,2365)	2:93:B:VAL:HG23	1:89:A:TYR:HD1	2	1.03
(1,2365)	2:93:B:VAL:HG23	1:89:A:TYR:HD2	2	1.03
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG21	5	1.03
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG22	5	1.03
(1,1983)	1:36:A:ARG:HG3	1:39:A:VAL:HG23	5	1.03
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	5	1.03
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	5	1.03
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	5	1.03
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	1	1.03
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	1	1.03
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	1	1.03
(1,1103)	1:39:A:VAL:HG11	1:133:A:GLY:HA2	14	1.03
(1,1103)	1:39:A:VAL:HG11	1:133:A:GLY:HA3	14	1.03
(1,1103)	1:39:A:VAL:HG12	1:133:A:GLY:HA2	14	1.03
(1,1103)	1:39:A:VAL:HG12	1:133:A:GLY:HA3	14	1.03
(1,1103)	1:39:A:VAL:HG13	1:133:A:GLY:HA2	14	1.03
(1,1103)	1:39:A:VAL:HG13	1:133:A:GLY:HA3	14	1.03
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	20	1.03
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	10	1.02
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	10	1.02
(1,2556)	1:183:A:LEU:HD21	1:125:A:TRP:HE3	14	1.02
(1,2556)	1:183:A:LEU:HD22	1:125:A:TRP:HE3	14	1.02
(1,2556)	1:183:A:LEU:HD23	1:125:A:TRP:HE3	14	1.02
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	7	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	7	1.02
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	7	1.02
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	17	1.02
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	17	1.02
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	17	1.02
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	1	1.02
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	1	1.02
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	1	1.02
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	2	1.02
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	2	1.02
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	2	1.02
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	16	1.02
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	16	1.02
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	16	1.02
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD11	8	1.02
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD12	8	1.02
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD13	8	1.02
(1,1746)	1:86:A:ASN:HB3	1:87:A:ARG:HG3	18	1.02
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	17	1.02
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	17	1.02
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	17	1.02
(1,1329)	1:118:A:LEU:HD21	1:134:A:PHE:HB3	6	1.02
(1,1329)	1:118:A:LEU:HD22	1:134:A:PHE:HB3	6	1.02
(1,1329)	1:118:A:LEU:HD23	1:134:A:PHE:HB3	6	1.02
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	16	1.02
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	16	1.02
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	16	1.02
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	6	1.02
(1,1087)	1:47:A:GLN:HE22	1:55:A:PRO:HD3	12	1.02
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	5	1.02
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	2	1.02
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	3	1.02
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	3	1.02
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	3	1.02
(1,190)	1:183:A:LEU:HD21	1:125:A:TRP:H	14	1.02
(1,190)	1:183:A:LEU:HD22	1:125:A:TRP:H	14	1.02
(1,190)	1:183:A:LEU:HD23	1:125:A:TRP:H	14	1.02
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	3	1.01
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	3	1.01
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	3	1.01
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	6	1.01
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	6	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	6	1.01
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	11	1.01
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	11	1.01
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	11	1.01
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	14	1.01
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	14	1.01
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	14	1.01
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	18	1.01
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	18	1.01
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	18	1.01
(1,2344)	1:160:A:ASP:HB3	1:164:A:HIS:HE1	18	1.01
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	2	1.01
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	2	1.01
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	2	1.01
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG21	16	1.01
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG22	16	1.01
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG23	16	1.01
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG21	16	1.01
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG22	16	1.01
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG23	16	1.01
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG21	16	1.01
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG22	16	1.01
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG23	16	1.01
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG21	16	1.01
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG22	16	1.01
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG23	16	1.01
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG21	16	1.01
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG22	16	1.01
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG23	16	1.01
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG21	16	1.01
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG22	16	1.01
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG23	16	1.01
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	14	1.01
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	14	1.01
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	14	1.01
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	18	1.01
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	18	1.01
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	18	1.01
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	20	1.01
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	20	1.01
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	20	1.01
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	10	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	10	1.01
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	10	1.01
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	11	1.01
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	11	1.01
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	11	1.01
(1,1746)	1:86:A:ASN:HB3	1:87:A:ARG:HG3	12	1.01
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	3	1.01
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	3	1.01
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	3	1.01
(1,1033)	1:118:A:LEU:HD21	1:115:A:ALA:HA	17	1.01
(1,1033)	1:118:A:LEU:HD22	1:115:A:ALA:HA	17	1.01
(1,1033)	1:118:A:LEU:HD23	1:115:A:ALA:HA	17	1.01
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	7	1.01
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	12	1.01
(1,841)	1:97:A:LEU:HD11	1:93:A:PHE:HA	20	1.01
(1,841)	1:97:A:LEU:HD12	1:93:A:PHE:HA	20	1.01
(1,841)	1:97:A:LEU:HD13	1:93:A:PHE:HA	20	1.01
(1,528)	1:55:A:PRO:HD3	1:47:A:GLN:HE21	19	1.01
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	7	1.01
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	7	1.01
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	7	1.01
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG21	6	1.0
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG22	6	1.0
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG23	6	1.0
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG21	6	1.0
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG22	6	1.0
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG23	6	1.0
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG21	6	1.0
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG22	6	1.0
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG23	6	1.0
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	13	1.0
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	13	1.0
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	13	1.0
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	17	1.0
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	17	1.0
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	17	1.0
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD11	16	1.0
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD12	16	1.0
(1,1882)	1:101:A:GLN:HB3	1:100:A:LEU:HD13	16	1.0
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	4	1.0
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	4	1.0
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	4	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1033)	1:118:A:LEU:HD21	1:115:A:ALA:HA	3	1.0
(1,1033)	1:118:A:LEU:HD22	1:115:A:ALA:HA	3	1.0
(1,1033)	1:118:A:LEU:HD23	1:115:A:ALA:HA	3	1.0
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	19	0.99
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	19	0.99
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	19	0.99
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG21	17	0.99
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG22	17	0.99
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG23	17	0.99
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG21	17	0.99
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG22	17	0.99
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG23	17	0.99
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG21	17	0.99
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG22	17	0.99
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG23	17	0.99
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	8	0.99
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	8	0.99
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	8	0.99
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	10	0.99
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	10	0.99
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	10	0.99
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	7	0.99
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	7	0.99
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	7	0.99
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	19	0.99
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	19	0.99
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	19	0.99
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	10	0.99
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	10	0.99
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	10	0.99
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	19	0.99
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	19	0.99
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	19	0.99
(1,1746)	1:86:A:ASN:HB3	1:87:A:ARG:HG3	7	0.99
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	14	0.99
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	14	0.99
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	14	0.99
(1,1033)	1:118:A:LEU:HD21	1:115:A:ALA:HA	6	0.99
(1,1033)	1:118:A:LEU:HD22	1:115:A:ALA:HA	6	0.99
(1,1033)	1:118:A:LEU:HD23	1:115:A:ALA:HA	6	0.99
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	15	0.99
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	16	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:97:A:LEU:HD21	1:138:A:LEU:H	12	0.99
(1,90)	1:97:A:LEU:HD22	1:138:A:LEU:H	12	0.99
(1,90)	1:97:A:LEU:HD23	1:138:A:LEU:H	12	0.99
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	5	0.98
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	5	0.98
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	5	0.98
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	12	0.98
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	12	0.98
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	12	0.98
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	4	0.98
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	4	0.98
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	4	0.98
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	19	0.98
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	19	0.98
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	19	0.98
(1,2483)	1:147:A:LEU:HD21	1:150:A:PHE:HZ	13	0.98
(1,2483)	1:147:A:LEU:HD22	1:150:A:PHE:HZ	13	0.98
(1,2483)	1:147:A:LEU:HD23	1:150:A:PHE:HZ	13	0.98
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	10	0.98
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	10	0.98
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	10	0.98
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	8	0.98
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	8	0.98
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	8	0.98
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	8	0.98
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	8	0.98
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	8	0.98
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	8	0.98
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	8	0.98
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	8	0.98
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	9	0.98
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	9	0.98
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	9	0.98
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG21	13	0.98
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG22	13	0.98
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG23	13	0.98
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG21	13	0.98
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG22	13	0.98
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG23	13	0.98
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG21	13	0.98
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG22	13	0.98
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG23	13	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG21	13	0.98
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG22	13	0.98
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG23	13	0.98
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG21	13	0.98
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG22	13	0.98
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG23	13	0.98
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG21	13	0.98
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG22	13	0.98
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG23	13	0.98
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	14	0.98
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	14	0.98
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	14	0.98
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG11	2	0.98
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG12	2	0.98
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG13	2	0.98
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG11	13	0.98
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG12	13	0.98
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG13	13	0.98
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	16	0.98
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	16	0.98
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	16	0.98
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	8	0.98
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	8	0.98
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	8	0.98
(1,1020)	1:118:A:LEU:HD21	1:130:A:ALA:HA	19	0.98
(1,1020)	1:118:A:LEU:HD22	1:130:A:ALA:HA	19	0.98
(1,1020)	1:118:A:LEU:HD23	1:130:A:ALA:HA	19	0.98
(1,841)	1:97:A:LEU:HD11	1:93:A:PHE:HA	3	0.98
(1,841)	1:97:A:LEU:HD12	1:93:A:PHE:HA	3	0.98
(1,841)	1:97:A:LEU:HD13	1:93:A:PHE:HA	3	0.98
(1,139)	1:131:A:LEU:HD21	1:115:A:ALA:H	18	0.98
(1,139)	1:131:A:LEU:HD22	1:115:A:ALA:H	18	0.98
(1,139)	1:131:A:LEU:HD23	1:115:A:ALA:H	18	0.98
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	8	0.97
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	8	0.97
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	8	0.97
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	4	0.97
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	4	0.97
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	4	0.97
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	4	0.97
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	4	0.97
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	4	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	4	0.97
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	4	0.97
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	4	0.97
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	6	0.97
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	6	0.97
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	6	0.97
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	3	0.97
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	3	0.97
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	3	0.97
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	15	0.97
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	15	0.97
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	15	0.97
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD21	1	0.97
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD22	1	0.97
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD23	1	0.97
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	9	0.97
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	9	0.97
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	9	0.97
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	10	0.97
(1,1121)	1:158:A:VAL:HG21	1:135:A:GLY:HA3	10	0.97
(1,1121)	1:158:A:VAL:HG22	1:135:A:GLY:HA3	10	0.97
(1,1121)	1:158:A:VAL:HG23	1:135:A:GLY:HA3	10	0.97
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	3	0.97
(1,1012)	1:27:A:VAL:HG11	1:172:A:ALA:HA	1	0.97
(1,1012)	1:27:A:VAL:HG12	1:172:A:ALA:HA	1	0.97
(1,1012)	1:27:A:VAL:HG13	1:172:A:ALA:HA	1	0.97
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	8	0.97
(1,841)	1:97:A:LEU:HD11	1:93:A:PHE:HA	12	0.97
(1,841)	1:97:A:LEU:HD12	1:93:A:PHE:HA	12	0.97
(1,841)	1:97:A:LEU:HD13	1:93:A:PHE:HA	12	0.97
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	7	0.96
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	7	0.96
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	7	0.96
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	9	0.96
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	9	0.96
(1,2556)	1:183:A:LEU:HD21	1:125:A:TRP:HE3	10	0.96
(1,2556)	1:183:A:LEU:HD22	1:125:A:TRP:HE3	10	0.96
(1,2556)	1:183:A:LEU:HD23	1:125:A:TRP:HE3	10	0.96
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG21	4	0.96
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG22	4	0.96
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG23	4	0.96
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG21	4	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG22	4	0.96
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG23	4	0.96
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG21	4	0.96
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG22	4	0.96
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG23	4	0.96
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	16	0.96
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	16	0.96
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	16	0.96
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	6	0.96
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	6	0.96
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	6	0.96
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD21	12	0.96
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD22	12	0.96
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD23	12	0.96
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD21	12	0.96
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD22	12	0.96
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD23	12	0.96
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD21	12	0.96
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD22	12	0.96
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD23	12	0.96
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD21	14	0.96
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD22	14	0.96
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD23	14	0.96
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD21	14	0.96
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD22	14	0.96
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD23	14	0.96
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD21	14	0.96
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD22	14	0.96
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD23	14	0.96
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD11	5	0.96
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD12	5	0.96
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD13	5	0.96
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD11	5	0.96
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD12	5	0.96
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD13	5	0.96
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD11	5	0.96
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD12	5	0.96
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD13	5	0.96
(1,1746)	1:86:A:ASN:HB3	1:87:A:ARG:HG3	10	0.96
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	16	0.96
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	16	0.96
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	16	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	19	0.96
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	19	0.96
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	19	0.96
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	19	0.96
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	11	0.96
(1,841)	1:97:A:LEU:HD11	1:93:A:PHE:HA	7	0.96
(1,841)	1:97:A:LEU:HD12	1:93:A:PHE:HA	7	0.96
(1,841)	1:97:A:LEU:HD13	1:93:A:PHE:HA	7	0.96
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	4	0.96
(1,2454)	1:147:A:LEU:HD21	1:150:A:PHE:HE1	8	0.95
(1,2454)	1:147:A:LEU:HD21	1:150:A:PHE:HE2	8	0.95
(1,2454)	1:147:A:LEU:HD22	1:150:A:PHE:HE1	8	0.95
(1,2454)	1:147:A:LEU:HD22	1:150:A:PHE:HE2	8	0.95
(1,2454)	1:147:A:LEU:HD23	1:150:A:PHE:HE1	8	0.95
(1,2454)	1:147:A:LEU:HD23	1:150:A:PHE:HE2	8	0.95
(1,2365)	2:93:B:VAL:HG21	1:89:A:TYR:HD1	13	0.95
(1,2365)	2:93:B:VAL:HG21	1:89:A:TYR:HD2	13	0.95
(1,2365)	2:93:B:VAL:HG22	1:89:A:TYR:HD1	13	0.95
(1,2365)	2:93:B:VAL:HG22	1:89:A:TYR:HD2	13	0.95
(1,2365)	2:93:B:VAL:HG23	1:89:A:TYR:HD1	13	0.95
(1,2365)	2:93:B:VAL:HG23	1:89:A:TYR:HD2	13	0.95
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG21	3	0.95
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG22	3	0.95
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG23	3	0.95
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG21	3	0.95
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG22	3	0.95
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG23	3	0.95
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG21	3	0.95
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG22	3	0.95
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG23	3	0.95
(1,2163)	1:158:A:VAL:HG11	1:162:A:MET:HE1	10	0.95
(1,2163)	1:158:A:VAL:HG11	1:162:A:MET:HE2	10	0.95
(1,2163)	1:158:A:VAL:HG11	1:162:A:MET:HE3	10	0.95
(1,2163)	1:158:A:VAL:HG12	1:162:A:MET:HE1	10	0.95
(1,2163)	1:158:A:VAL:HG12	1:162:A:MET:HE2	10	0.95
(1,2163)	1:158:A:VAL:HG12	1:162:A:MET:HE3	10	0.95
(1,2163)	1:158:A:VAL:HG13	1:162:A:MET:HE1	10	0.95
(1,2163)	1:158:A:VAL:HG13	1:162:A:MET:HE2	10	0.95
(1,2163)	1:158:A:VAL:HG13	1:162:A:MET:HE3	10	0.95
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	1	0.95
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	1	0.95
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	1	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD21	9	0.95
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD22	9	0.95
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD23	9	0.95
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG11	19	0.95
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG12	19	0.95
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG13	19	0.95
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	18	0.95
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	13	0.95
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	13	0.95
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	13	0.95
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	14	0.95
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	14	0.95
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	14	0.95
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	4	0.95
(1,732)	1:66:A:GLN:HG3	1:69:A:SER:HB3	4	0.95
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	20	0.95
(1,90)	1:97:A:LEU:HD21	1:138:A:LEU:H	7	0.95
(1,90)	1:97:A:LEU:HD22	1:138:A:LEU:H	7	0.95
(1,90)	1:97:A:LEU:HD23	1:138:A:LEU:H	7	0.95
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	15	0.94
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	15	0.94
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	15	0.94
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	19	0.94
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	19	0.94
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG21	9	0.94
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG22	9	0.94
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG23	9	0.94
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG21	9	0.94
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG22	9	0.94
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG23	9	0.94
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG21	9	0.94
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG22	9	0.94
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG23	9	0.94
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	1	0.94
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	1	0.94
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	1	0.94
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	18	0.94
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	18	0.94
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	18	0.94
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	5	0.94
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	5	0.94
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	5	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	8	0.94
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	8	0.94
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	8	0.94
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD21	4	0.94
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD22	4	0.94
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD23	4	0.94
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD21	4	0.94
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD22	4	0.94
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD23	4	0.94
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD21	4	0.94
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD22	4	0.94
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD23	4	0.94
(1,1329)	1:118:A:LEU:HD21	1:134:A:PHE:HB3	4	0.94
(1,1329)	1:118:A:LEU:HD22	1:134:A:PHE:HB3	4	0.94
(1,1329)	1:118:A:LEU:HD23	1:134:A:PHE:HB3	4	0.94
(1,1103)	1:39:A:VAL:HG11	1:133:A:GLY:HA2	3	0.94
(1,1103)	1:39:A:VAL:HG11	1:133:A:GLY:HA3	3	0.94
(1,1103)	1:39:A:VAL:HG12	1:133:A:GLY:HA2	3	0.94
(1,1103)	1:39:A:VAL:HG12	1:133:A:GLY:HA3	3	0.94
(1,1103)	1:39:A:VAL:HG13	1:133:A:GLY:HA2	3	0.94
(1,1103)	1:39:A:VAL:HG13	1:133:A:GLY:HA3	3	0.94
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	9	0.94
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	18	0.94
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	12	0.93
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	12	0.93
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	12	0.93
(1,2382)	1:147:A:LEU:HD21	1:150:A:PHE:HD1	6	0.93
(1,2382)	1:147:A:LEU:HD21	1:150:A:PHE:HD2	6	0.93
(1,2382)	1:147:A:LEU:HD22	1:150:A:PHE:HD1	6	0.93
(1,2382)	1:147:A:LEU:HD22	1:150:A:PHE:HD2	6	0.93
(1,2382)	1:147:A:LEU:HD23	1:150:A:PHE:HD1	6	0.93
(1,2382)	1:147:A:LEU:HD23	1:150:A:PHE:HD2	6	0.93
(1,2382)	1:147:A:LEU:HD21	1:150:A:PHE:HD1	7	0.93
(1,2382)	1:147:A:LEU:HD21	1:150:A:PHE:HD2	7	0.93
(1,2382)	1:147:A:LEU:HD22	1:150:A:PHE:HD1	7	0.93
(1,2382)	1:147:A:LEU:HD22	1:150:A:PHE:HD2	7	0.93
(1,2382)	1:147:A:LEU:HD23	1:150:A:PHE:HD1	7	0.93
(1,2382)	1:147:A:LEU:HD23	1:150:A:PHE:HD2	7	0.93
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	15	0.93
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	15	0.93
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	15	0.93
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD11	17	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD12	17	0.93
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD13	17	0.93
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	5	0.93
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	5	0.93
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	5	0.93
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	8	0.93
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	8	0.93
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	8	0.93
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	14	0.93
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	14	0.93
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	14	0.93
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	19	0.93
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	19	0.93
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	19	0.93
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	1	0.93
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	1	0.93
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	1	0.93
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG11	7	0.93
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG12	7	0.93
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG13	7	0.93
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG11	9	0.93
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG12	9	0.93
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG13	9	0.93
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	6	0.93
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	6	0.93
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	6	0.93
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	10	0.93
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	10	0.93
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	10	0.93
(1,1103)	1:39:A:VAL:HG11	1:133:A:GLY:HA2	5	0.93
(1,1103)	1:39:A:VAL:HG11	1:133:A:GLY:HA3	5	0.93
(1,1103)	1:39:A:VAL:HG12	1:133:A:GLY:HA2	5	0.93
(1,1103)	1:39:A:VAL:HG12	1:133:A:GLY:HA3	5	0.93
(1,1103)	1:39:A:VAL:HG13	1:133:A:GLY:HA2	5	0.93
(1,1103)	1:39:A:VAL:HG13	1:133:A:GLY:HA3	5	0.93
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	6	0.93
(1,921)	1:98:A:GLN:HE22	1:98:A:GLN:HA	9	0.93
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	17	0.93
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	1	0.93
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	19	0.93
(1,74)	1:63:A:LEU:HD11	1:65:A:LEU:H	4	0.93
(1,74)	1:63:A:LEU:HD12	1:65:A:LEU:H	4	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:63:A:LEU:HD13	1:65:A:LEU:H	4	0.93
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	5	0.92
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	5	0.92
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	14	0.92
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	14	0.92
(1,2344)	1:160:A:ASP:HB3	1:164:A:HIS:HE1	11	0.92
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	11	0.92
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	11	0.92
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	11	0.92
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	11	0.92
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	11	0.92
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	11	0.92
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	11	0.92
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	11	0.92
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	11	0.92
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	4	0.92
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	4	0.92
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	4	0.92
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	10	0.92
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	10	0.92
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	10	0.92
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	10	0.92
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	10	0.92
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	10	0.92
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	7	0.92
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	5	0.92
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	12	0.92
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	12	0.92
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	12	0.92
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	2	0.92
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	2	0.92
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	2	0.92
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	6	0.92
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	6	0.92
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	6	0.92
(1,841)	1:97:A:LEU:HD11	1:93:A:PHE:HA	1	0.92
(1,841)	1:97:A:LEU:HD12	1:93:A:PHE:HA	1	0.92
(1,841)	1:97:A:LEU:HD13	1:93:A:PHE:HA	1	0.92
(1,298)	1:88:A:ARG:HD3	1:88:A:ARG:H	18	0.92
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG21	12	0.91
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG22	12	0.91
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG23	12	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG21	12	0.91
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG22	12	0.91
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG23	12	0.91
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG21	12	0.91
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG22	12	0.91
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG23	12	0.91
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB1	7	0.91
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB2	7	0.91
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB3	7	0.91
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB1	7	0.91
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB2	7	0.91
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB3	7	0.91
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB1	7	0.91
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB2	7	0.91
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB3	7	0.91
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG21	17	0.91
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG22	17	0.91
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG23	17	0.91
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG21	17	0.91
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG22	17	0.91
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG23	17	0.91
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG21	17	0.91
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG22	17	0.91
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG23	17	0.91
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG21	17	0.91
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG22	17	0.91
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG23	17	0.91
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG21	17	0.91
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG22	17	0.91
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG23	17	0.91
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG21	17	0.91
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG22	17	0.91
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG23	17	0.91
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	13	0.91
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	13	0.91
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	13	0.91
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	5	0.91
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	5	0.91
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	5	0.91
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	7	0.91
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	7	0.91
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	7	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	20	0.91
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	20	0.91
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	20	0.91
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	1	0.91
(1,921)	1:98:A:GLN:HE22	1:98:A:GLN:HA	15	0.91
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	1	0.91
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	1	0.91
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	1	0.91
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	3	0.91
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	3	0.91
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	3	0.91
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	4	0.91
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	4	0.91
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	4	0.91
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	5	0.91
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	5	0.91
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	5	0.91
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	9	0.91
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	9	0.91
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	9	0.91
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	11	0.91
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	11	0.91
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	11	0.91
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	14	0.91
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	14	0.91
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	14	0.91
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	15	0.91
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	15	0.91
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	15	0.91
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	19	0.91
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	19	0.91
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	19	0.91
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	14	0.91
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	14	0.91
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	14	0.91
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	18	0.9
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	18	0.9
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	18	0.9
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	20	0.9
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	20	0.9
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	13	0.9
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	13	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	13	0.9
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB1	20	0.9
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB2	20	0.9
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB3	20	0.9
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB1	20	0.9
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB2	20	0.9
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB3	20	0.9
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB1	20	0.9
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB2	20	0.9
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB3	20	0.9
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	7	0.9
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	7	0.9
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	7	0.9
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	4	0.9
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	4	0.9
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	4	0.9
(1,1746)	1:86:A:ASN:HB3	1:87:A:ARG:HG3	4	0.9
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	9	0.9
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	18	0.9
(1,883)	1:39:A:VAL:HG21	1:36:A:ARG:HA	2	0.9
(1,883)	1:39:A:VAL:HG22	1:36:A:ARG:HA	2	0.9
(1,883)	1:39:A:VAL:HG23	1:36:A:ARG:HA	2	0.9
(1,841)	1:97:A:LEU:HD11	1:93:A:PHE:HA	13	0.9
(1,841)	1:97:A:LEU:HD12	1:93:A:PHE:HA	13	0.9
(1,841)	1:97:A:LEU:HD13	1:93:A:PHE:HA	13	0.9
(1,841)	1:97:A:LEU:HD11	1:93:A:PHE:HA	17	0.9
(1,841)	1:97:A:LEU:HD12	1:93:A:PHE:HA	17	0.9
(1,841)	1:97:A:LEU:HD13	1:93:A:PHE:HA	17	0.9
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	2	0.9
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	2	0.9
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	2	0.9
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	6	0.9
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	6	0.9
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	6	0.9
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	7	0.9
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	7	0.9
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	7	0.9
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	8	0.9
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	8	0.9
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	8	0.9
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	10	0.9
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	10	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	10	0.9
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	12	0.9
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	12	0.9
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	12	0.9
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	13	0.9
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	13	0.9
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	13	0.9
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	16	0.9
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	16	0.9
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	16	0.9
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	17	0.9
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	17	0.9
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	17	0.9
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	18	0.9
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	18	0.9
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	18	0.9
(1,801)	1:34:A:VAL:HG21	1:35:A:PHE:HA	20	0.9
(1,801)	1:34:A:VAL:HG22	1:35:A:PHE:HA	20	0.9
(1,801)	1:34:A:VAL:HG23	1:35:A:PHE:HA	20	0.9
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	4	0.9
(1,139)	1:131:A:LEU:HD21	1:115:A:ALA:H	15	0.9
(1,139)	1:131:A:LEU:HD22	1:115:A:ALA:H	15	0.9
(1,139)	1:131:A:LEU:HD23	1:115:A:ALA:H	15	0.9
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	19	0.89
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	19	0.89
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	19	0.89
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	11	0.89
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	11	0.89
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	11	0.89
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB1	5	0.89
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB2	5	0.89
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB3	5	0.89
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB1	5	0.89
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB2	5	0.89
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB3	5	0.89
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB1	5	0.89
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB2	5	0.89
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB3	5	0.89
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG21	16	0.89
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG22	16	0.89
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG23	16	0.89
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	2	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	2	0.89
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	2	0.89
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	9	0.89
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	9	0.89
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	9	0.89
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	14	0.89
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	14	0.89
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	14	0.89
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	14	0.89
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	14	0.89
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	14	0.89
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	14	0.89
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	14	0.89
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	14	0.89
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	20	0.89
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	20	0.89
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	20	0.89
(1,1898)	1:143:A:TYR:HD1	1:147:A:LEU:HD21	20	0.89
(1,1898)	1:143:A:TYR:HD1	1:147:A:LEU:HD22	20	0.89
(1,1898)	1:143:A:TYR:HD1	1:147:A:LEU:HD23	20	0.89
(1,1898)	1:143:A:TYR:HD2	1:147:A:LEU:HD21	20	0.89
(1,1898)	1:143:A:TYR:HD2	1:147:A:LEU:HD22	20	0.89
(1,1898)	1:143:A:TYR:HD2	1:147:A:LEU:HD23	20	0.89
(1,1746)	1:86:A:ASN:HB3	1:87:A:ARG:HG3	15	0.89
(1,1588)	1:129:A:VAL:HG11	1:128:A:VAL:HB	11	0.89
(1,1588)	1:129:A:VAL:HG12	1:128:A:VAL:HB	11	0.89
(1,1588)	1:129:A:VAL:HG13	1:128:A:VAL:HB	11	0.89
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	16	0.89
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	5	0.89
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	8	0.89
(1,404)	1:34:A:VAL:HG21	1:78:A:LEU:H	2	0.89
(1,404)	1:34:A:VAL:HG22	1:78:A:LEU:H	2	0.89
(1,404)	1:34:A:VAL:HG23	1:78:A:LEU:H	2	0.89
(1,139)	1:131:A:LEU:HD21	1:115:A:ALA:H	12	0.89
(1,139)	1:131:A:LEU:HD22	1:115:A:ALA:H	12	0.89
(1,139)	1:131:A:LEU:HD23	1:115:A:ALA:H	12	0.89
(1,2604)	1:88:A:ARG:HD3	1:89:A:TYR:HE1	18	0.88
(1,2604)	1:88:A:ARG:HD3	1:89:A:TYR:HE2	18	0.88
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	7	0.88
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	7	0.88
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	7	0.88
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG21	14	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG22	14	0.88
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG23	14	0.88
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG21	14	0.88
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG22	14	0.88
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG23	14	0.88
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG21	14	0.88
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG22	14	0.88
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG23	14	0.88
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	20	0.88
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	20	0.88
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	20	0.88
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	20	0.88
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	20	0.88
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	20	0.88
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	20	0.88
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	20	0.88
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	20	0.88
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	18	0.88
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	18	0.88
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	18	0.88
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	18	0.88
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	18	0.88
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	18	0.88
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	18	0.88
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	18	0.88
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	18	0.88
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	18	0.88
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	18	0.88
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	18	0.88
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	18	0.88
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	18	0.88
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	18	0.88
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	18	0.88
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	18	0.88
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	18	0.88
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	6	0.88
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	6	0.88
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	6	0.88
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	11	0.88
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	11	0.88
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	11	0.88
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	15	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	15	0.88
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	15	0.88
(1,1588)	1:129:A:VAL:HG11	1:128:A:VAL:HB	4	0.88
(1,1588)	1:129:A:VAL:HG12	1:128:A:VAL:HB	4	0.88
(1,1588)	1:129:A:VAL:HG13	1:128:A:VAL:HB	4	0.88
(1,1588)	1:129:A:VAL:HG11	1:128:A:VAL:HB	15	0.88
(1,1588)	1:129:A:VAL:HG12	1:128:A:VAL:HB	15	0.88
(1,1588)	1:129:A:VAL:HG13	1:128:A:VAL:HB	15	0.88
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	4	0.88
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	10	0.88
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	10	0.88
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	2	0.88
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	2	0.87
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	2	0.87
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	10	0.87
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	10	0.87
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE1	3	0.87
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE2	3	0.87
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE1	3	0.87
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE2	3	0.87
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE1	3	0.87
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE2	3	0.87
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE1	12	0.87
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE2	12	0.87
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE1	12	0.87
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE2	12	0.87
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE1	12	0.87
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE2	12	0.87
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	20	0.87
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	20	0.87
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	20	0.87
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	6	0.87
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	6	0.87
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	6	0.87
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG21	12	0.87
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG22	12	0.87
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG23	12	0.87
(1,1588)	1:129:A:VAL:HG11	1:128:A:VAL:HB	9	0.87
(1,1588)	1:129:A:VAL:HG12	1:128:A:VAL:HB	9	0.87
(1,1588)	1:129:A:VAL:HG13	1:128:A:VAL:HB	9	0.87
(1,1588)	1:129:A:VAL:HG11	1:128:A:VAL:HB	13	0.87
(1,1588)	1:129:A:VAL:HG12	1:128:A:VAL:HB	13	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1588)	1:129:A:VAL:HG13	1:128:A:VAL:HB	13	0.87
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	20	0.87
(1,1033)	1:118:A:LEU:HD21	1:115:A:ALA:HA	12	0.87
(1,1033)	1:118:A:LEU:HD22	1:115:A:ALA:HA	12	0.87
(1,1033)	1:118:A:LEU:HD23	1:115:A:ALA:HA	12	0.87
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	9	0.87
(1,841)	1:97:A:LEU:HD11	1:93:A:PHE:HA	14	0.87
(1,841)	1:97:A:LEU:HD12	1:93:A:PHE:HA	14	0.87
(1,841)	1:97:A:LEU:HD13	1:93:A:PHE:HA	14	0.87
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	6	0.86
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	6	0.86
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	6	0.86
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	10	0.86
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	10	0.86
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	10	0.86
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	17	0.86
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	17	0.86
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	17	0.86
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	4	0.86
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	4	0.86
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	4	0.86
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	18	0.86
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	18	0.86
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	18	0.86
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	18	0.86
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	18	0.86
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	18	0.86
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	18	0.86
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	18	0.86
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	18	0.86
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG11	20	0.86
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG12	20	0.86
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG13	20	0.86
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD21	18	0.86
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD22	18	0.86
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD23	18	0.86
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD21	18	0.86
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD22	18	0.86
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD23	18	0.86
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD21	18	0.86
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD22	18	0.86
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD23	18	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1588)	1:129:A:VAL:HG11	1:128:A:VAL:HB	7	0.86
(1,1588)	1:129:A:VAL:HG12	1:128:A:VAL:HB	7	0.86
(1,1588)	1:129:A:VAL:HG13	1:128:A:VAL:HB	7	0.86
(1,1535)	1:156:A:ARG:HA	1:159:A:VAL:HB	5	0.86
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	7	0.86
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	18	0.86
(1,410)	1:94:A:GLN:HE22	1:95:A:THR:H	13	0.86
(1,298)	1:88:A:ARG:HD3	1:88:A:ARG:H	3	0.86
(1,139)	1:131:A:LEU:HD21	1:115:A:ALA:H	2	0.86
(1,139)	1:131:A:LEU:HD22	1:115:A:ALA:H	2	0.86
(1,139)	1:131:A:LEU:HD23	1:115:A:ALA:H	2	0.86
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	10	0.85
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	10	0.85
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	3	0.85
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	3	0.85
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	3	0.85
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	16	0.85
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	16	0.85
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	16	0.85
(1,2483)	1:147:A:LEU:HD21	1:150:A:PHE:HZ	4	0.85
(1,2483)	1:147:A:LEU:HD22	1:150:A:PHE:HZ	4	0.85
(1,2483)	1:147:A:LEU:HD23	1:150:A:PHE:HZ	4	0.85
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE1	6	0.85
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE2	6	0.85
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE1	6	0.85
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE2	6	0.85
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE1	6	0.85
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE2	6	0.85
(1,2454)	1:147:A:LEU:HD21	1:150:A:PHE:HE1	6	0.85
(1,2454)	1:147:A:LEU:HD21	1:150:A:PHE:HE2	6	0.85
(1,2454)	1:147:A:LEU:HD22	1:150:A:PHE:HE1	6	0.85
(1,2454)	1:147:A:LEU:HD22	1:150:A:PHE:HE2	6	0.85
(1,2454)	1:147:A:LEU:HD23	1:150:A:PHE:HE1	6	0.85
(1,2454)	1:147:A:LEU:HD23	1:150:A:PHE:HE2	6	0.85
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	7	0.85
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	7	0.85
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	7	0.85
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	7	0.85
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	7	0.85
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	7	0.85
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	7	0.85
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	7	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	7	0.85
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG21	14	0.85
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG22	14	0.85
(1,2099)	1:75:A:GLY:HA3	1:34:A:VAL:HG23	14	0.85
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	19	0.85
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	19	0.85
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	19	0.85
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG11	10	0.85
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG12	10	0.85
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG13	10	0.85
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	4	0.85
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	4	0.85
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	4	0.85
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	2	0.85
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	2	0.85
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	2	0.85
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	18	0.85
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	18	0.85
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	18	0.85
(1,1746)	1:86:A:ASN:HB3	1:87:A:ARG:HG3	14	0.85
(1,1746)	1:86:A:ASN:HB3	1:87:A:ARG:HG3	17	0.85
(1,1588)	1:129:A:VAL:HG11	1:128:A:VAL:HB	2	0.85
(1,1588)	1:129:A:VAL:HG12	1:128:A:VAL:HB	2	0.85
(1,1588)	1:129:A:VAL:HG13	1:128:A:VAL:HB	2	0.85
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	1	0.85
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	1	0.85
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	1	0.85
(1,921)	1:98:A:GLN:HE22	1:98:A:GLN:HA	14	0.85
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	19	0.85
(1,883)	1:39:A:VAL:HG21	1:36:A:ARG:HA	20	0.85
(1,883)	1:39:A:VAL:HG22	1:36:A:ARG:HA	20	0.85
(1,883)	1:39:A:VAL:HG23	1:36:A:ARG:HA	20	0.85
(1,854)	1:159:A:VAL:HG11	1:32:A:GLU:HA	4	0.85
(1,854)	1:159:A:VAL:HG12	1:32:A:GLU:HA	4	0.85
(1,854)	1:159:A:VAL:HG13	1:32:A:GLU:HA	4	0.85
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	19	0.84
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	19	0.84
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB1	15	0.84
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB2	15	0.84
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB3	15	0.84
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB1	15	0.84
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB2	15	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB3	15	0.84
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB1	15	0.84
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB2	15	0.84
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB3	15	0.84
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	12	0.84
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	12	0.84
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	12	0.84
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	20	0.84
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	20	0.84
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	20	0.84
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG21	3	0.84
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG22	3	0.84
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG23	3	0.84
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	14	0.84
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	14	0.84
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	14	0.84
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD21	2	0.84
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD22	2	0.84
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD23	2	0.84
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD21	2	0.84
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD22	2	0.84
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD23	2	0.84
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD21	2	0.84
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD22	2	0.84
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD23	2	0.84
(1,1746)	1:86:A:ASN:HB3	1:87:A:ARG:HG3	13	0.84
(1,1588)	1:129:A:VAL:HG11	1:128:A:VAL:HB	20	0.84
(1,1588)	1:129:A:VAL:HG12	1:128:A:VAL:HB	20	0.84
(1,1588)	1:129:A:VAL:HG13	1:128:A:VAL:HB	20	0.84
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	16	0.84
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	9	0.84
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	9	0.84
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	9	0.84
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	1	0.84
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	2	0.84
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	6	0.84
(1,390)	1:63:A:LEU:HD11	1:36:A:ARG:H	10	0.84
(1,390)	1:63:A:LEU:HD12	1:36:A:ARG:H	10	0.84
(1,390)	1:63:A:LEU:HD13	1:36:A:ARG:H	10	0.84
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE1	17	0.83
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE2	17	0.83
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE1	17	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE2	17	0.83
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE1	17	0.83
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE2	17	0.83
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	13	0.83
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	13	0.83
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	13	0.83
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG21	19	0.83
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG22	19	0.83
(1,2196)	1:118:A:LEU:HD21	1:114:A:ILE:HG23	19	0.83
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG21	19	0.83
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG22	19	0.83
(1,2196)	1:118:A:LEU:HD22	1:114:A:ILE:HG23	19	0.83
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG21	19	0.83
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG22	19	0.83
(1,2196)	1:118:A:LEU:HD23	1:114:A:ILE:HG23	19	0.83
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG11	18	0.83
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG12	18	0.83
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG13	18	0.83
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG11	18	0.83
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG12	18	0.83
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG13	18	0.83
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	8	0.83
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	8	0.83
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	8	0.83
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	3	0.83
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	3	0.83
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	3	0.83
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	14	0.83
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	14	0.83
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	14	0.83
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	19	0.83
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	19	0.83
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	19	0.83
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	7	0.83
(1,1746)	1:86:A:ASN:HB3	1:87:A:ARG:HG3	2	0.83
(1,1746)	1:86:A:ASN:HB3	1:87:A:ARG:HG3	9	0.83
(1,1033)	1:118:A:LEU:HD21	1:115:A:ALA:HA	4	0.83
(1,1033)	1:118:A:LEU:HD22	1:115:A:ALA:HA	4	0.83
(1,1033)	1:118:A:LEU:HD23	1:115:A:ALA:HA	4	0.83
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	4	0.83
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	7	0.83
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	13	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	13	0.82
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	13	0.82
(1,2556)	1:183:A:LEU:HD21	1:125:A:TRP:HE3	12	0.82
(1,2556)	1:183:A:LEU:HD22	1:125:A:TRP:HE3	12	0.82
(1,2556)	1:183:A:LEU:HD23	1:125:A:TRP:HE3	12	0.82
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	10	0.82
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	10	0.82
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	10	0.82
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	10	0.82
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	10	0.82
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	10	0.82
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	10	0.82
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	10	0.82
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	10	0.82
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG21	14	0.82
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG22	14	0.82
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG23	14	0.82
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG21	14	0.82
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG22	14	0.82
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG23	14	0.82
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG21	14	0.82
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG22	14	0.82
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG23	14	0.82
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG21	14	0.82
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG22	14	0.82
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG23	14	0.82
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG21	14	0.82
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG22	14	0.82
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG23	14	0.82
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG21	14	0.82
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG22	14	0.82
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG23	14	0.82
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	10	0.82
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	10	0.82
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	10	0.82
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG21	17	0.82
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG22	17	0.82
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG23	17	0.82
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	6	0.82
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	6	0.82
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	6	0.82
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	10	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1151)	1:27:A:VAL:HG11	1:176:A:GLY:HA3	1	0.82
(1,1151)	1:27:A:VAL:HG12	1:176:A:GLY:HA3	1	0.82
(1,1151)	1:27:A:VAL:HG13	1:176:A:GLY:HA3	1	0.82
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	14	0.82
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	16	0.82
(1,934)	1:159:A:VAL:HG11	1:156:A:ARG:HA	4	0.82
(1,934)	1:159:A:VAL:HG12	1:156:A:ARG:HA	4	0.82
(1,934)	1:159:A:VAL:HG13	1:156:A:ARG:HA	4	0.82
(1,190)	1:183:A:LEU:HD21	1:125:A:TRP:H	20	0.82
(1,190)	1:183:A:LEU:HD22	1:125:A:TRP:H	20	0.82
(1,190)	1:183:A:LEU:HD23	1:125:A:TRP:H	20	0.82
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	19	0.81
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	19	0.81
(1,2556)	1:183:A:LEU:HD21	1:125:A:TRP:HE3	20	0.81
(1,2556)	1:183:A:LEU:HD22	1:125:A:TRP:HE3	20	0.81
(1,2556)	1:183:A:LEU:HD23	1:125:A:TRP:HE3	20	0.81
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	9	0.81
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	9	0.81
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	9	0.81
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	4	0.81
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	4	0.81
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	4	0.81
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG21	9	0.81
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG22	9	0.81
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG23	9	0.81
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG21	9	0.81
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG22	9	0.81
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG23	9	0.81
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG21	9	0.81
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG22	9	0.81
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG23	9	0.81
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG21	9	0.81
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG22	9	0.81
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG23	9	0.81
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG21	9	0.81
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG22	9	0.81
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG23	9	0.81
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG21	9	0.81
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG22	9	0.81
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG23	9	0.81
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	12	0.81
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	12	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	12	0.81
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	15	0.81
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	15	0.81
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	15	0.81
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	7	0.81
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	7	0.81
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	7	0.81
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	12	0.81
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	12	0.81
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	12	0.81
(1,1043)	1:182:A:ASN:HB3	1:179:A:ALA:HA	18	0.81
(1,883)	1:39:A:VAL:HG21	1:36:A:ARG:HA	12	0.81
(1,883)	1:39:A:VAL:HG22	1:36:A:ARG:HA	12	0.81
(1,883)	1:39:A:VAL:HG23	1:36:A:ARG:HA	12	0.81
(1,90)	1:97:A:LEU:HD21	1:138:A:LEU:H	10	0.81
(1,90)	1:97:A:LEU:HD22	1:138:A:LEU:H	10	0.81
(1,90)	1:97:A:LEU:HD23	1:138:A:LEU:H	10	0.81
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	15	0.8
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	15	0.8
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	1	0.8
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	1	0.8
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	1	0.8
(1,2365)	2:93:B:VAL:HG21	1:89:A:TYR:HD1	4	0.8
(1,2365)	2:93:B:VAL:HG21	1:89:A:TYR:HD2	4	0.8
(1,2365)	2:93:B:VAL:HG22	1:89:A:TYR:HD1	4	0.8
(1,2365)	2:93:B:VAL:HG22	1:89:A:TYR:HD2	4	0.8
(1,2365)	2:93:B:VAL:HG23	1:89:A:TYR:HD1	4	0.8
(1,2365)	2:93:B:VAL:HG23	1:89:A:TYR:HD2	4	0.8
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	4	0.8
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	4	0.8
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	4	0.8
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	13	0.8
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	13	0.8
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	13	0.8
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	5	0.8
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	5	0.8
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	5	0.8
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	20	0.8
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	20	0.8
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	20	0.8
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG21	7	0.8
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG22	7	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG23	7	0.8
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG21	7	0.8
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG22	7	0.8
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG23	7	0.8
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG21	7	0.8
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG22	7	0.8
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG23	7	0.8
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG21	7	0.8
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG22	7	0.8
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG23	7	0.8
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG21	7	0.8
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG22	7	0.8
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG23	7	0.8
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG21	7	0.8
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG22	7	0.8
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG23	7	0.8
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	5	0.8
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	5	0.8
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	5	0.8
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	5	0.8
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	5	0.8
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	5	0.8
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	5	0.8
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	5	0.8
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	5	0.8
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	5	0.8
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	5	0.8
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	5	0.8
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	5	0.8
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	5	0.8
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	5	0.8
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	5	0.8
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	5	0.8
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	5	0.8
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	19	0.8
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	19	0.8
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	19	0.8
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	19	0.8
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	19	0.8
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	19	0.8
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	19	0.8
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	19	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	19	0.8
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	19	0.8
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	19	0.8
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	19	0.8
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	19	0.8
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	19	0.8
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	19	0.8
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	19	0.8
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	19	0.8
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	19	0.8
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG11	9	0.8
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG12	9	0.8
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG13	9	0.8
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG11	15	0.8
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG12	15	0.8
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG13	15	0.8
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	17	0.8
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	17	0.8
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	17	0.8
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	17	0.8
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	17	0.8
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	17	0.8
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	17	0.8
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	17	0.8
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	17	0.8
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD21	6	0.8
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD22	6	0.8
(1,1854)	1:141:A:HIS:HB3	1:97:A:LEU:HD23	6	0.8
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD21	20	0.8
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD22	20	0.8
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD23	20	0.8
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD21	20	0.8
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD22	20	0.8
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD23	20	0.8
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD21	20	0.8
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD22	20	0.8
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD23	20	0.8
(1,1588)	1:129:A:VAL:HG11	1:128:A:VAL:HB	19	0.8
(1,1588)	1:129:A:VAL:HG12	1:128:A:VAL:HB	19	0.8
(1,1588)	1:129:A:VAL:HG13	1:128:A:VAL:HB	19	0.8
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	1	0.8
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	1	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	1	0.8
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	11	0.8
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	11	0.8
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	11	0.8
(1,239)	1:98:A:GLN:HB3	1:97:A:LEU:H	20	0.8
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	3	0.79
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	3	0.79
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	5	0.79
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	5	0.79
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	5	0.79
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	5	0.79
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	5	0.79
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	5	0.79
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	5	0.79
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	5	0.79
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	5	0.79
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	20	0.79
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	20	0.79
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	20	0.79
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	9	0.79
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	9	0.79
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	9	0.79
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG21	8	0.79
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG22	8	0.79
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG23	8	0.79
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG21	8	0.79
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG22	8	0.79
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG23	8	0.79
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG21	8	0.79
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG22	8	0.79
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG23	8	0.79
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG21	8	0.79
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG22	8	0.79
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG23	8	0.79
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG21	8	0.79
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG22	8	0.79
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG23	8	0.79
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG21	8	0.79
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG22	8	0.79
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG23	8	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG11	1	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG12	1	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG13	1	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG11	3	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG12	3	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG13	3	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG11	4	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG12	4	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG13	4	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG11	7	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG12	7	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG13	7	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG11	8	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG12	8	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG13	8	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG11	11	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG12	11	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG13	11	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG11	13	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG12	13	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG13	13	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG11	14	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG12	14	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG13	14	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG11	16	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG12	16	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG13	16	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG11	17	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG12	17	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG13	17	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG11	18	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG12	18	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG13	18	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG11	19	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG12	19	0.79
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG13	19	0.79
(1,1746)	1:86:A:ASN:HB3	1:87:A:ARG:HG3	8	0.79
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	4	0.79
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	4	0.79
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	4	0.79
(1,883)	1:39:A:VAL:HG21	1:36:A:ARG:HA	14	0.79
(1,883)	1:39:A:VAL:HG22	1:36:A:ARG:HA	14	0.79
(1,883)	1:39:A:VAL:HG23	1:36:A:ARG:HA	14	0.79
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	8	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	3	0.79
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	1	0.78
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	1	0.78
(1,2497)	1:39:A:VAL:HG21	1:35:A:PHE:HZ	12	0.78
(1,2497)	1:39:A:VAL:HG22	1:35:A:PHE:HZ	12	0.78
(1,2497)	1:39:A:VAL:HG23	1:35:A:PHE:HZ	12	0.78
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG11	11	0.78
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG12	11	0.78
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG13	11	0.78
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	10	0.78
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	10	0.78
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	10	0.78
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	14	0.78
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	14	0.78
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	14	0.78
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	14	0.78
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	14	0.78
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	14	0.78
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	14	0.78
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	14	0.78
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	14	0.78
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	14	0.78
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	14	0.78
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	14	0.78
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	14	0.78
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	14	0.78
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	14	0.78
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	14	0.78
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	14	0.78
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	14	0.78
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	15	0.78
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	15	0.78
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	15	0.78
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	15	0.78
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	15	0.78
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	15	0.78
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	15	0.78
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	15	0.78
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	15	0.78
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	15	0.78
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	15	0.78
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	15	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	15	0.78
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	15	0.78
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	15	0.78
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	15	0.78
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	15	0.78
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	15	0.78
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG11	10	0.78
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG12	10	0.78
(1,2012)	1:159:A:VAL:H	1:159:A:VAL:HG13	10	0.78
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	13	0.78
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	13	0.78
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	13	0.78
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD11	10	0.78
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD12	10	0.78
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD13	10	0.78
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	10	0.77
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	10	0.77
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	12	0.77
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	12	0.77
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	12	0.77
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG11	6	0.77
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG12	6	0.77
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG13	6	0.77
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG11	6	0.77
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG12	6	0.77
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG13	6	0.77
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG11	6	0.77
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG12	6	0.77
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG13	6	0.77
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	1	0.77
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	1	0.77
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	1	0.77
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	17	0.77
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	17	0.77
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	17	0.77
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	12	0.77
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	12	0.77
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	12	0.77
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	6	0.77
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	19	0.76
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	19	0.76
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	19	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	19	0.76
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	19	0.76
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	19	0.76
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	19	0.76
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	19	0.76
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	19	0.76
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	5	0.76
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	5	0.76
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	5	0.76
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	6	0.76
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	6	0.76
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	6	0.76
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	15	0.76
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	15	0.76
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	15	0.76
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	18	0.76
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	18	0.76
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	18	0.76
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	12	0.76
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	12	0.76
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	12	0.76
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	12	0.76
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	12	0.76
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	12	0.76
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	12	0.76
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	12	0.76
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	12	0.76
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	12	0.76
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	12	0.76
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	12	0.76
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	12	0.76
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	12	0.76
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	12	0.76
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	12	0.76
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	12	0.76
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	12	0.76
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	11	0.76
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	11	0.76
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	11	0.76
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	15	0.76
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	15	0.76
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	15	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD11	3	0.76
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD12	3	0.76
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD13	3	0.76
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	6	0.76
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	17	0.76
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	11	0.76
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	11	0.76
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	11	0.76
(1,1029)	1:147:A:LEU:HD21	1:104:A:ALA:HA	7	0.76
(1,1029)	1:147:A:LEU:HD22	1:104:A:ALA:HA	7	0.76
(1,1029)	1:147:A:LEU:HD23	1:104:A:ALA:HA	7	0.76
(1,542)	1:172:A:ALA:HB1	1:173:A:GLN:HE22	4	0.76
(1,542)	1:172:A:ALA:HB2	1:173:A:GLN:HE22	4	0.76
(1,542)	1:172:A:ALA:HB3	1:173:A:GLN:HE22	4	0.76
(1,298)	1:88:A:ARG:HD3	1:88:A:ARG:H	9	0.76
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	5	0.75
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	5	0.75
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	16	0.75
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	16	0.75
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE1	14	0.75
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE2	14	0.75
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE1	14	0.75
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE2	14	0.75
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE1	14	0.75
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE2	14	0.75
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	7	0.75
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	7	0.75
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	6	0.75
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	6	0.75
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	6	0.75
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	3	0.75
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	3	0.75
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	3	0.75
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	7	0.75
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	7	0.75
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	7	0.75
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	8	0.75
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	8	0.75
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	8	0.75
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	19	0.75
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	19	0.75
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	19	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	10	0.75
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	10	0.75
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	10	0.75
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	10	0.75
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	10	0.75
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	10	0.75
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	10	0.75
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	10	0.75
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	10	0.75
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	10	0.75
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	10	0.75
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	10	0.75
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	10	0.75
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	10	0.75
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	10	0.75
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	10	0.75
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	10	0.75
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	10	0.75
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD11	12	0.75
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD12	12	0.75
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD13	12	0.75
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	8	0.75
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	14	0.75
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	20	0.75
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	13	0.75
(1,410)	1:94:A:GLN:HE22	1:95:A:THR:H	15	0.75
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	2	0.75
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	5	0.75
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	8	0.75
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	10	0.75
(1,190)	1:183:A:LEU:HD21	1:125:A:TRP:H	10	0.75
(1,190)	1:183:A:LEU:HD22	1:125:A:TRP:H	10	0.75
(1,190)	1:183:A:LEU:HD23	1:125:A:TRP:H	10	0.75
(1,123)	1:34:A:VAL:HG11	1:74:A:VAL:H	3	0.75
(1,123)	1:34:A:VAL:HG12	1:74:A:VAL:H	3	0.75
(1,123)	1:34:A:VAL:HG13	1:74:A:VAL:H	3	0.75
(1,2493)	1:118:A:LEU:HD21	1:119:A:PHE:HZ	6	0.74
(1,2493)	1:118:A:LEU:HD22	1:119:A:PHE:HZ	6	0.74
(1,2493)	1:118:A:LEU:HD23	1:119:A:PHE:HZ	6	0.74
(1,2354)	1:76:A:ARG:HB3	1:41:A:TYR:HD1	14	0.74
(1,2354)	1:76:A:ARG:HB3	1:41:A:TYR:HD2	14	0.74
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB1	8	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB2	8	0.74
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB3	8	0.74
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB1	8	0.74
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB2	8	0.74
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB3	8	0.74
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB1	8	0.74
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB2	8	0.74
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB3	8	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	2	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	2	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	2	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	11	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	11	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	11	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	12	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	12	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	12	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	13	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	13	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	13	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	14	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	14	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	14	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	16	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	16	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	16	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG11	17	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG12	17	0.74
(1,2077)	1:61:A:VAL:H	1:61:A:VAL:HG13	17	0.74
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	1	0.74
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	1	0.74
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	1	0.74
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	1	0.74
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	1	0.74
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	1	0.74
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	1	0.74
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	1	0.74
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	1	0.74
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	1	0.74
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	1	0.74
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	1	0.74
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	1	0.74
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	1	0.74
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	1	0.74
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	1	0.74
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	1	0.74
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	4	0.74
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	4	0.74
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	4	0.74
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	4	0.74
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	4	0.74
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	4	0.74
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	4	0.74
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	4	0.74
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	4	0.74
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	4	0.74
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	4	0.74
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	4	0.74
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	4	0.74
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	4	0.74
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	4	0.74
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	4	0.74
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	4	0.74
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	4	0.74
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	19	0.74
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	19	0.74
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	19	0.74
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	5	0.74
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	13	0.74
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	15	0.74
(1,1350)	1:179:A:ALA:HB1	1:182:A:ASN:HB3	19	0.74
(1,1350)	1:179:A:ALA:HB2	1:182:A:ASN:HB3	19	0.74
(1,1350)	1:179:A:ALA:HB3	1:182:A:ASN:HB3	19	0.74
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	12	0.74
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	12	0.74
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	12	0.74
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	10	0.74
(1,298)	1:88:A:ARG:HD3	1:88:A:ARG:H	12	0.74
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	6	0.74
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	14	0.74
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	20	0.74
(1,139)	1:131:A:LEU:HD21	1:115:A:ALA:H	17	0.74
(1,139)	1:131:A:LEU:HD22	1:115:A:ALA:H	17	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,139)	1:131:A:LEU:HD23	1:115:A:ALA:H	17	0.74
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE1	4	0.73
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE2	4	0.73
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE1	4	0.73
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE2	4	0.73
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE1	4	0.73
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE2	4	0.73
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG11	9	0.73
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG12	9	0.73
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG13	9	0.73
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG11	9	0.73
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG12	9	0.73
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG13	9	0.73
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG11	9	0.73
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG12	9	0.73
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG13	9	0.73
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	7	0.73
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	7	0.73
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	7	0.73
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	8	0.73
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	8	0.73
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	8	0.73
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	18	0.73
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	18	0.73
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	18	0.73
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD21	15	0.73
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD22	15	0.73
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD23	15	0.73
(1,1842)	1:165:A:HIS:HA	1:166:A:CYS:HB3	3	0.73
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD11	17	0.73
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD12	17	0.73
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD13	17	0.73
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	18	0.73
(1,1033)	1:118:A:LEU:HD21	1:115:A:ALA:HA	9	0.73
(1,1033)	1:118:A:LEU:HD22	1:115:A:ALA:HA	9	0.73
(1,1033)	1:118:A:LEU:HD23	1:115:A:ALA:HA	9	0.73
(1,883)	1:39:A:VAL:HG21	1:36:A:ARG:HA	3	0.73
(1,883)	1:39:A:VAL:HG22	1:36:A:ARG:HA	3	0.73
(1,883)	1:39:A:VAL:HG23	1:36:A:ARG:HA	3	0.73
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	4	0.73
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	12	0.73
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	15	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	6	0.72
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	6	0.72
(1,2497)	1:39:A:VAL:HG21	1:35:A:PHE:HZ	20	0.72
(1,2497)	1:39:A:VAL:HG22	1:35:A:PHE:HZ	20	0.72
(1,2497)	1:39:A:VAL:HG23	1:35:A:PHE:HZ	20	0.72
(1,2443)	1:153:A:GLN:HB3	1:150:A:PHE:HE1	3	0.72
(1,2443)	1:153:A:GLN:HB3	1:150:A:PHE:HE2	3	0.72
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	2	0.72
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	2	0.72
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	2	0.72
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	6	0.72
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	6	0.72
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	6	0.72
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	6	0.72
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	6	0.72
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	6	0.72
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	6	0.72
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	6	0.72
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	6	0.72
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	6	0.72
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	6	0.72
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	6	0.72
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	6	0.72
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	6	0.72
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	6	0.72
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	6	0.72
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	6	0.72
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	6	0.72
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	19	0.72
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	19	0.72
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	19	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	1	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	1	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	1	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	2	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	2	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	2	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	3	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	3	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	3	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	6	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	6	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	6	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	7	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	7	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	7	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	8	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	8	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	8	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	9	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	9	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	9	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	10	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	10	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	10	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	11	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	11	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	11	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	12	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	12	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	12	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	13	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	13	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	13	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	15	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	15	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	15	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	18	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	18	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	18	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	20	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	20	0.72
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	20	0.72
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG11	4	0.72
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG12	4	0.72
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG13	4	0.72
(1,1867)	1:73:A:GLN:HG3	1:181:A:LEU:HD11	11	0.72
(1,1867)	1:73:A:GLN:HG3	1:181:A:LEU:HD12	11	0.72
(1,1867)	1:73:A:GLN:HG3	1:181:A:LEU:HD13	11	0.72
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	16	0.72
(1,410)	1:94:A:GLN:HE22	1:95:A:THR:H	19	0.72
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	17	0.72
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	18	0.72
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	5	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	5	0.71
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	11	0.71
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	11	0.71
(1,2483)	1:147:A:LEU:HD21	1:150:A:PHE:HZ	9	0.71
(1,2483)	1:147:A:LEU:HD22	1:150:A:PHE:HZ	9	0.71
(1,2483)	1:147:A:LEU:HD23	1:150:A:PHE:HZ	9	0.71
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	16	0.71
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	16	0.71
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	16	0.71
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG21	8	0.71
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG22	8	0.71
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG23	8	0.71
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	5	0.71
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	5	0.71
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	5	0.71
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	3	0.71
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	3	0.71
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	3	0.71
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	3	0.71
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	3	0.71
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	3	0.71
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	3	0.71
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	3	0.71
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	3	0.71
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	3	0.71
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	3	0.71
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	3	0.71
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	3	0.71
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	3	0.71
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	3	0.71
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	3	0.71
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	3	0.71
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	3	0.71
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	7	0.71
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	7	0.71
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	7	0.71
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	7	0.71
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	7	0.71
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	7	0.71
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	7	0.71
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	7	0.71
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	7	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	7	0.71
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	7	0.71
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	7	0.71
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	7	0.71
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	7	0.71
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	7	0.71
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	7	0.71
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	7	0.71
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	7	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	4	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	4	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	4	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	5	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	5	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	5	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	14	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	14	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	14	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	16	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	16	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	16	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	17	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	17	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	17	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG11	19	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG12	19	0.71
(1,1908)	1:27:A:VAL:H	1:27:A:VAL:HG13	19	0.71
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD21	15	0.71
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD22	15	0.71
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD23	15	0.71
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD21	15	0.71
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD22	15	0.71
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD23	15	0.71
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD21	15	0.71
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD22	15	0.71
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD23	15	0.71
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	12	0.71
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	12	0.71
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	12	0.71
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	13	0.71
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	13	0.71
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	13	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	17	0.71
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	1	0.71
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	7	0.71
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	11	0.71
(1,139)	1:131:A:LEU:HD21	1:115:A:ALA:H	3	0.71
(1,139)	1:131:A:LEU:HD22	1:115:A:ALA:H	3	0.71
(1,139)	1:131:A:LEU:HD23	1:115:A:ALA:H	3	0.71
(1,2556)	1:183:A:LEU:HD21	1:125:A:TRP:HE3	5	0.7
(1,2556)	1:183:A:LEU:HD22	1:125:A:TRP:HE3	5	0.7
(1,2556)	1:183:A:LEU:HD23	1:125:A:TRP:HE3	5	0.7
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB1	19	0.7
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB2	19	0.7
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB3	19	0.7
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB1	19	0.7
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB2	19	0.7
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB3	19	0.7
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB1	19	0.7
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB2	19	0.7
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB3	19	0.7
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	17	0.7
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	17	0.7
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	17	0.7
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	17	0.7
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	17	0.7
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	17	0.7
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	17	0.7
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	17	0.7
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	17	0.7
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	17	0.7
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	17	0.7
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	17	0.7
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	17	0.7
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	17	0.7
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	17	0.7
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	17	0.7
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	17	0.7
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	17	0.7
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG11	11	0.7
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG12	11	0.7
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG13	11	0.7
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	9	0.7
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	9	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	9	0.7
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	14	0.7
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	14	0.7
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	14	0.7
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD21	18	0.7
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD22	18	0.7
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD23	18	0.7
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	11	0.7
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	19	0.7
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	13	0.7
(1,934)	1:159:A:VAL:HG11	1:156:A:ARG:HA	15	0.7
(1,934)	1:159:A:VAL:HG12	1:156:A:ARG:HA	15	0.7
(1,934)	1:159:A:VAL:HG13	1:156:A:ARG:HA	15	0.7
(1,920)	1:20:A:PRO:HB3	1:21:A:SER:HA	14	0.7
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	9	0.7
(1,190)	1:183:A:LEU:HD21	1:125:A:TRP:H	5	0.7
(1,190)	1:183:A:LEU:HD22	1:125:A:TRP:H	5	0.7
(1,190)	1:183:A:LEU:HD23	1:125:A:TRP:H	5	0.7
(1,123)	1:34:A:VAL:HG11	1:74:A:VAL:H	12	0.7
(1,123)	1:34:A:VAL:HG12	1:74:A:VAL:H	12	0.7
(1,123)	1:34:A:VAL:HG13	1:74:A:VAL:H	12	0.7
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	7	0.69
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	7	0.69
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	13	0.69
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	13	0.69
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG11	8	0.69
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG12	8	0.69
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG13	8	0.69
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG11	8	0.69
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG12	8	0.69
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG13	8	0.69
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	8	0.69
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	8	0.69
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	8	0.69
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	8	0.69
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	8	0.69
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	8	0.69
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	8	0.69
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	8	0.69
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	8	0.69
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	16	0.69
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	16	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	16	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	3	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	3	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	3	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	4	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	4	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	4	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	5	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	5	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	5	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	6	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	6	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	6	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	8	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	8	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	8	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	9	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	9	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	9	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	12	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	12	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	12	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	14	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	14	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	14	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	15	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	15	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	15	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	16	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	16	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	16	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	17	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	17	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	17	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	19	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	19	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	19	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	20	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	20	0.69
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	20	0.69
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	17	0.69
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	17	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	17	0.69
(1,1842)	1:165:A:HIS:HA	1:166:A:CYS:HB3	4	0.69
(1,1842)	1:165:A:HIS:HA	1:166:A:CYS:HB3	5	0.69
(1,1842)	1:165:A:HIS:HA	1:166:A:CYS:HB3	20	0.69
(1,1746)	1:86:A:ASN:HB3	1:87:A:ARG:HG3	20	0.69
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	11	0.69
(1,1350)	1:179:A:ALA:HB1	1:182:A:ASN:HB3	17	0.69
(1,1350)	1:179:A:ALA:HB2	1:182:A:ASN:HB3	17	0.69
(1,1350)	1:179:A:ALA:HB3	1:182:A:ASN:HB3	17	0.69
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	17	0.69
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	17	0.69
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	17	0.69
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	20	0.69
(1,883)	1:39:A:VAL:HG21	1:36:A:ARG:HA	5	0.69
(1,883)	1:39:A:VAL:HG22	1:36:A:ARG:HA	5	0.69
(1,883)	1:39:A:VAL:HG23	1:36:A:ARG:HA	5	0.69
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	19	0.69
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	2	0.68
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	2	0.68
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	2	0.68
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	8	0.68
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	8	0.68
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	8	0.68
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	2	0.68
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	2	0.68
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	2	0.68
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	10	0.68
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	10	0.68
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	10	0.68
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	8	0.68
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	8	0.68
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	8	0.68
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	9	0.68
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	9	0.68
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	9	0.68
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	8	0.68
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	15	0.68
(1,934)	1:159:A:VAL:HG11	1:156:A:ARG:HA	9	0.68
(1,934)	1:159:A:VAL:HG12	1:156:A:ARG:HA	9	0.68
(1,934)	1:159:A:VAL:HG13	1:156:A:ARG:HA	9	0.68
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	13	0.68
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	2	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	2	0.67
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	2	0.67
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	2	0.67
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	2	0.67
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	2	0.67
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	2	0.67
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	2	0.67
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	2	0.67
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	2	0.67
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	2	0.67
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	2	0.67
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	2	0.67
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	2	0.67
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	2	0.67
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	2	0.67
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	2	0.67
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	2	0.67
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	3	0.67
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	3	0.67
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	3	0.67
(1,1905)	1:26:A:GLN:HG3	1:27:A:VAL:HG11	4	0.67
(1,1905)	1:26:A:GLN:HG3	1:27:A:VAL:HG12	4	0.67
(1,1905)	1:26:A:GLN:HG3	1:27:A:VAL:HG13	4	0.67
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD11	18	0.67
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD12	18	0.67
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD13	18	0.67
(1,670)	1:158:A:VAL:HB	1:155:A:THR:HA	10	0.67
(1,410)	1:94:A:GLN:HE22	1:95:A:THR:H	1	0.67
(1,204)	1:152:A:GLY:HA3	1:156:A:ARG:H	16	0.67
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	11	0.66
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	11	0.66
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE1	13	0.66
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE2	13	0.66
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE1	13	0.66
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE2	13	0.66
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE1	13	0.66
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE2	13	0.66
(1,2493)	1:118:A:LEU:HD21	1:119:A:PHE:HZ	3	0.66
(1,2493)	1:118:A:LEU:HD22	1:119:A:PHE:HZ	3	0.66
(1,2493)	1:118:A:LEU:HD23	1:119:A:PHE:HZ	3	0.66
(1,2493)	1:118:A:LEU:HD21	1:119:A:PHE:HZ	12	0.66
(1,2493)	1:118:A:LEU:HD22	1:119:A:PHE:HZ	12	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2493)	1:118:A:LEU:HD23	1:119:A:PHE:HZ	12	0.66
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	9	0.66
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	9	0.66
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	20	0.66
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	20	0.66
(1,2354)	1:76:A:ARG:HB3	1:41:A:TYR:HD1	17	0.66
(1,2354)	1:76:A:ARG:HB3	1:41:A:TYR:HD2	17	0.66
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG21	6	0.66
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG22	6	0.66
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG23	6	0.66
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	13	0.66
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	13	0.66
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	13	0.66
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	13	0.66
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	13	0.66
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	13	0.66
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	13	0.66
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	13	0.66
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	13	0.66
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	13	0.66
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	13	0.66
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	13	0.66
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	13	0.66
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	13	0.66
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	13	0.66
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	13	0.66
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	13	0.66
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	13	0.66
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	16	0.66
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	16	0.66
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	16	0.66
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	16	0.66
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	16	0.66
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	16	0.66
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	16	0.66
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	16	0.66
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	16	0.66
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	16	0.66
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	16	0.66
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	16	0.66
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	16	0.66
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	16	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	16	0.66
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	16	0.66
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	16	0.66
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	16	0.66
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	17	0.66
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	17	0.66
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	17	0.66
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	10	0.66
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	10	0.66
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	10	0.66
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	10	0.66
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	10	0.66
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	10	0.66
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	10	0.66
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	10	0.66
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	10	0.66
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	4	0.66
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	4	0.66
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	4	0.66
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG11	1	0.66
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG12	1	0.66
(1,1910)	1:176:A:GLY:HA2	1:27:A:VAL:HG13	1	0.66
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD11	5	0.66
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD12	5	0.66
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD13	5	0.66
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD11	15	0.66
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD12	15	0.66
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD13	15	0.66
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	3	0.66
(1,1588)	1:129:A:VAL:HG11	1:128:A:VAL:HB	5	0.66
(1,1588)	1:129:A:VAL:HG12	1:128:A:VAL:HB	5	0.66
(1,1588)	1:129:A:VAL:HG13	1:128:A:VAL:HB	5	0.66
(1,1588)	1:129:A:VAL:HG11	1:128:A:VAL:HB	18	0.66
(1,1588)	1:129:A:VAL:HG12	1:128:A:VAL:HB	18	0.66
(1,1588)	1:129:A:VAL:HG13	1:128:A:VAL:HB	18	0.66
(1,934)	1:159:A:VAL:HG11	1:156:A:ARG:HA	1	0.66
(1,934)	1:159:A:VAL:HG12	1:156:A:ARG:HA	1	0.66
(1,934)	1:159:A:VAL:HG13	1:156:A:ARG:HA	1	0.66
(1,608)	1:106:A:ASN:H	1:103:A:THR:HB	12	0.66
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	17	0.66
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE1	16	0.65
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE2	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE1	16	0.65
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE2	16	0.65
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE1	16	0.65
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE2	16	0.65
(1,2556)	1:183:A:LEU:HD21	1:125:A:TRP:HE3	7	0.65
(1,2556)	1:183:A:LEU:HD22	1:125:A:TRP:HE3	7	0.65
(1,2556)	1:183:A:LEU:HD23	1:125:A:TRP:HE3	7	0.65
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	9	0.65
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	9	0.65
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	9	0.65
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	9	0.65
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	9	0.65
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	9	0.65
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	9	0.65
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	9	0.65
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	9	0.65
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	9	0.65
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	9	0.65
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	9	0.65
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	9	0.65
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	9	0.65
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	9	0.65
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	9	0.65
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	9	0.65
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	9	0.65
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG21	10	0.65
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG22	10	0.65
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG23	10	0.65
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG11	5	0.65
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG12	5	0.65
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG13	5	0.65
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	2	0.65
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	2	0.65
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	2	0.65
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG11	19	0.65
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG12	19	0.65
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG13	19	0.65
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD11	2	0.65
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD12	2	0.65
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD13	2	0.65
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	12	0.65
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	3	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	4	0.65
(1,921)	1:98:A:GLN:HE22	1:98:A:GLN:HA	1	0.65
(1,298)	1:88:A:ARG:HD3	1:88:A:ARG:H	20	0.65
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	19	0.64
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	19	0.64
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE1	15	0.64
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE2	15	0.64
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE1	15	0.64
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE2	15	0.64
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE1	15	0.64
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE2	15	0.64
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	3	0.64
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	3	0.64
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	3	0.64
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG11	11	0.64
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG12	11	0.64
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG13	11	0.64
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	12	0.64
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	12	0.64
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	12	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG11	2	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG12	2	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG13	2	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG11	4	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG12	4	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG13	4	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG11	5	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG12	5	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG13	5	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG11	7	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG12	7	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG13	7	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG11	9	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG12	9	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG13	9	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG11	11	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG12	11	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG13	11	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG11	13	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG12	13	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG13	13	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG11	15	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG12	15	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG13	15	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG11	18	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG12	18	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG13	18	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG11	20	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG12	20	0.64
(1,1863)	1:129:A:VAL:H	1:129:A:VAL:HG13	20	0.64
(1,1746)	1:86:A:ASN:HB3	1:87:A:ARG:HG3	1	0.64
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	2	0.64
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	5	0.64
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	6	0.64
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	7	0.64
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	8	0.64
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	9	0.64
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	10	0.64
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	12	0.64
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	13	0.64
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	14	0.64
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	15	0.64
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	16	0.64
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	17	0.64
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	19	0.64
(1,1129)	1:155:A:THR:HG21	1:152:A:GLY:HA3	5	0.64
(1,1129)	1:155:A:THR:HG22	1:152:A:GLY:HA3	5	0.64
(1,1129)	1:155:A:THR:HG23	1:152:A:GLY:HA3	5	0.64
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	8	0.64
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	12	0.64
(1,1029)	1:147:A:LEU:HD21	1:104:A:ALA:HA	8	0.64
(1,1029)	1:147:A:LEU:HD22	1:104:A:ALA:HA	8	0.64
(1,1029)	1:147:A:LEU:HD23	1:104:A:ALA:HA	8	0.64
(1,896)	1:142:A:VAL:HG21	1:103:A:THR:HA	16	0.64
(1,896)	1:142:A:VAL:HG22	1:103:A:THR:HA	16	0.64
(1,896)	1:142:A:VAL:HG23	1:103:A:THR:HA	16	0.64
(1,298)	1:88:A:ARG:HD3	1:88:A:ARG:H	11	0.64
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	1	0.63
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	1	0.63
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	18	0.63
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	18	0.63
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE1	6	0.63
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE2	6	0.63
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE1	6	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE2	6	0.63
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE1	6	0.63
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE2	6	0.63
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE1	7	0.63
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE2	7	0.63
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE1	7	0.63
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE2	7	0.63
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE1	7	0.63
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE2	7	0.63
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	15	0.63
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	15	0.63
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	9	0.63
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	9	0.63
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	9	0.63
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	18	0.63
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	18	0.63
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	18	0.63
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG11	2	0.63
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG12	2	0.63
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG13	2	0.63
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	15	0.63
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	15	0.63
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	15	0.63
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	16	0.63
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	16	0.63
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	16	0.63
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	16	0.63
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	16	0.63
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	16	0.63
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	16	0.63
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	16	0.63
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	16	0.63
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	16	0.63
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	16	0.63
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	16	0.63
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	6	0.63
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	6	0.63
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	6	0.63
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	9	0.63
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	9	0.63
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	9	0.63
(1,1898)	1:143:A:TYR:HD1	1:147:A:LEU:HD21	7	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1898)	1:143:A:TYR:HD1	1:147:A:LEU:HD22	7	0.63
(1,1898)	1:143:A:TYR:HD1	1:147:A:LEU:HD23	7	0.63
(1,1898)	1:143:A:TYR:HD2	1:147:A:LEU:HD21	7	0.63
(1,1898)	1:143:A:TYR:HD2	1:147:A:LEU:HD22	7	0.63
(1,1898)	1:143:A:TYR:HD2	1:147:A:LEU:HD23	7	0.63
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD11	1	0.63
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD12	1	0.63
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD13	1	0.63
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD11	1	0.63
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD12	1	0.63
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD13	1	0.63
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD11	1	0.63
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD12	1	0.63
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD13	1	0.63
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD11	1	0.63
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD12	1	0.63
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD13	1	0.63
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD11	1	0.63
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD12	1	0.63
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD13	1	0.63
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD11	1	0.63
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD12	1	0.63
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD13	1	0.63
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD21	7	0.63
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD22	7	0.63
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD23	7	0.63
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD21	7	0.63
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD22	7	0.63
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD23	7	0.63
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD21	7	0.63
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD22	7	0.63
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD23	7	0.63
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD21	7	0.63
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD22	7	0.63
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD23	7	0.63
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD21	7	0.63
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD22	7	0.63
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD23	7	0.63
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD21	7	0.63
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD22	7	0.63
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD23	7	0.63
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	1	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	11	0.63
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	18	0.63
(1,1545)	1:103:A:THR:HA	1:102:A:PRO:HB3	20	0.63
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	13	0.63
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	13	0.63
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	13	0.63
(1,542)	1:172:A:ALA:HB1	1:173:A:GLN:HE22	8	0.63
(1,542)	1:172:A:ALA:HB2	1:173:A:GLN:HE22	8	0.63
(1,542)	1:172:A:ALA:HB3	1:173:A:GLN:HE22	8	0.63
(1,298)	1:88:A:ARG:HD3	1:88:A:ARG:H	4	0.63
(1,171)	1:162:A:MET:HB3	1:161:A:PHE:H	18	0.63
(1,106)	1:162:A:MET:HG3	1:168:A:ALA:H	10	0.63
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	7	0.62
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	7	0.62
(1,2497)	1:39:A:VAL:HG21	1:35:A:PHE:HZ	2	0.62
(1,2497)	1:39:A:VAL:HG22	1:35:A:PHE:HZ	2	0.62
(1,2497)	1:39:A:VAL:HG23	1:35:A:PHE:HZ	2	0.62
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	14	0.62
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	14	0.62
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	14	0.62
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	14	0.62
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	14	0.62
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	14	0.62
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	14	0.62
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	14	0.62
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	14	0.62
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	11	0.62
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	11	0.62
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	11	0.62
(1,2058)	1:111:A:PHE:HZ	1:158:A:VAL:HG21	10	0.62
(1,2058)	1:111:A:PHE:HZ	1:158:A:VAL:HG22	10	0.62
(1,2058)	1:111:A:PHE:HZ	1:158:A:VAL:HG23	10	0.62
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	8	0.62
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	8	0.62
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	8	0.62
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	8	0.62
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	8	0.62
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	8	0.62
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	8	0.62
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	8	0.62
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	8	0.62
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	8	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	8	0.62
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	8	0.62
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	8	0.62
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	8	0.62
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	8	0.62
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	8	0.62
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	8	0.62
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	8	0.62
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	11	0.62
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	11	0.62
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	11	0.62
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	11	0.62
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	11	0.62
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	11	0.62
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	11	0.62
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	11	0.62
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	11	0.62
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	11	0.62
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	11	0.62
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	11	0.62
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	11	0.62
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	11	0.62
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	11	0.62
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	11	0.62
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	11	0.62
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	11	0.62
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	8	0.62
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	8	0.62
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	8	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	1	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	1	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	1	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	2	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	2	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	2	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	3	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	3	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	3	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	4	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	4	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	4	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	5	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	5	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	5	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	7	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	7	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	7	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	10	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	10	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	10	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	11	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	11	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	11	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	12	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	12	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	12	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	13	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	13	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	13	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	14	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	14	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	14	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	15	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	15	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	15	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	16	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	16	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	16	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	17	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	17	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	17	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	18	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	18	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	18	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	19	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	19	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	19	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	20	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	20	0.62
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	20	0.62
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	1	0.62
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	1	0.62
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	1	0.62
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	15	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	15	0.62
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	15	0.62
(1,178)	1:118:A:LEU:HD21	1:131:A:LEU:H	9	0.62
(1,178)	1:118:A:LEU:HD22	1:131:A:LEU:H	9	0.62
(1,178)	1:118:A:LEU:HD23	1:131:A:LEU:H	9	0.62
(1,139)	1:131:A:LEU:HD21	1:115:A:ALA:H	10	0.62
(1,139)	1:131:A:LEU:HD22	1:115:A:ALA:H	10	0.62
(1,139)	1:131:A:LEU:HD23	1:115:A:ALA:H	10	0.62
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	2	0.61
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	2	0.61
(1,2382)	1:147:A:LEU:HD21	1:150:A:PHE:HD1	8	0.61
(1,2382)	1:147:A:LEU:HD21	1:150:A:PHE:HD2	8	0.61
(1,2382)	1:147:A:LEU:HD22	1:150:A:PHE:HD1	8	0.61
(1,2382)	1:147:A:LEU:HD22	1:150:A:PHE:HD2	8	0.61
(1,2382)	1:147:A:LEU:HD23	1:150:A:PHE:HD1	8	0.61
(1,2382)	1:147:A:LEU:HD23	1:150:A:PHE:HD2	8	0.61
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	9	0.61
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	9	0.61
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	9	0.61
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	9	0.61
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	9	0.61
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	9	0.61
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	9	0.61
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	9	0.61
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	9	0.61
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG21	14	0.61
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG22	14	0.61
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG23	14	0.61
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	20	0.61
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	20	0.61
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	20	0.61
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD11	7	0.61
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD12	7	0.61
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD13	7	0.61
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	4	0.61
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	16	0.61
(1,934)	1:159:A:VAL:HG11	1:156:A:ARG:HA	13	0.61
(1,934)	1:159:A:VAL:HG12	1:156:A:ARG:HA	13	0.61
(1,934)	1:159:A:VAL:HG13	1:156:A:ARG:HA	13	0.61
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	16	0.61
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	16	0.61
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	16	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:172:A:ALA:HB1	1:173:A:GLN:HE22	14	0.61
(1,542)	1:172:A:ALA:HB2	1:173:A:GLN:HE22	14	0.61
(1,542)	1:172:A:ALA:HB3	1:173:A:GLN:HE22	14	0.61
(1,410)	1:94:A:GLN:HE22	1:95:A:THR:H	11	0.61
(1,390)	1:63:A:LEU:HD11	1:36:A:ARG:H	9	0.61
(1,390)	1:63:A:LEU:HD12	1:36:A:ARG:H	9	0.61
(1,390)	1:63:A:LEU:HD13	1:36:A:ARG:H	9	0.61
(1,90)	1:97:A:LEU:HD21	1:138:A:LEU:H	1	0.61
(1,90)	1:97:A:LEU:HD22	1:138:A:LEU:H	1	0.61
(1,90)	1:97:A:LEU:HD23	1:138:A:LEU:H	1	0.61
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	13	0.6
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	13	0.6
(1,2497)	1:39:A:VAL:HG21	1:35:A:PHE:HZ	14	0.6
(1,2497)	1:39:A:VAL:HG22	1:35:A:PHE:HZ	14	0.6
(1,2497)	1:39:A:VAL:HG23	1:35:A:PHE:HZ	14	0.6
(1,2483)	1:147:A:LEU:HD21	1:150:A:PHE:HZ	20	0.6
(1,2483)	1:147:A:LEU:HD22	1:150:A:PHE:HZ	20	0.6
(1,2483)	1:147:A:LEU:HD23	1:150:A:PHE:HZ	20	0.6
(1,2433)	1:97:A:LEU:HD11	1:93:A:PHE:HE1	12	0.6
(1,2433)	1:97:A:LEU:HD11	1:93:A:PHE:HE2	12	0.6
(1,2433)	1:97:A:LEU:HD12	1:93:A:PHE:HE1	12	0.6
(1,2433)	1:97:A:LEU:HD12	1:93:A:PHE:HE2	12	0.6
(1,2433)	1:97:A:LEU:HD13	1:93:A:PHE:HE1	12	0.6
(1,2433)	1:97:A:LEU:HD13	1:93:A:PHE:HE2	12	0.6
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB1	3	0.6
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB2	3	0.6
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB3	3	0.6
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB1	3	0.6
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB2	3	0.6
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB3	3	0.6
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB1	3	0.6
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB2	3	0.6
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB3	3	0.6
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG11	7	0.6
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG12	7	0.6
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG13	7	0.6
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG11	7	0.6
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG12	7	0.6
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG13	7	0.6
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG11	7	0.6
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG12	7	0.6
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG13	7	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG11	19	0.6
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG12	19	0.6
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG13	19	0.6
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	17	0.6
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	17	0.6
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	17	0.6
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG11	8	0.6
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG12	8	0.6
(1,1929)	1:74:A:VAL:H	1:74:A:VAL:HG13	8	0.6
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG11	18	0.6
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG12	18	0.6
(1,1886)	1:125:A:TRP:HE3	1:129:A:VAL:HG13	18	0.6
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD11	9	0.6
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD12	9	0.6
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD13	9	0.6
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD11	19	0.6
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD12	19	0.6
(1,1826)	1:128:A:VAL:HA	1:131:A:LEU:HD13	19	0.6
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	12	0.6
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	12	0.6
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	12	0.6
(1,190)	1:183:A:LEU:HD21	1:125:A:TRP:H	6	0.6
(1,190)	1:183:A:LEU:HD22	1:125:A:TRP:H	6	0.6
(1,190)	1:183:A:LEU:HD23	1:125:A:TRP:H	6	0.6
(1,190)	1:183:A:LEU:HD21	1:125:A:TRP:H	7	0.6
(1,190)	1:183:A:LEU:HD22	1:125:A:TRP:H	7	0.6
(1,190)	1:183:A:LEU:HD23	1:125:A:TRP:H	7	0.6
(1,190)	1:183:A:LEU:HD21	1:125:A:TRP:H	8	0.6
(1,190)	1:183:A:LEU:HD22	1:125:A:TRP:H	8	0.6
(1,190)	1:183:A:LEU:HD23	1:125:A:TRP:H	8	0.6
(1,2493)	1:118:A:LEU:HD21	1:119:A:PHE:HZ	17	0.59
(1,2493)	1:118:A:LEU:HD22	1:119:A:PHE:HZ	17	0.59
(1,2493)	1:118:A:LEU:HD23	1:119:A:PHE:HZ	17	0.59
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	11	0.59
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	11	0.59
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	11	0.59
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	11	0.59
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	11	0.59
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	11	0.59
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	11	0.59
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	11	0.59
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	11	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG21	10	0.59
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG22	10	0.59
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG23	10	0.59
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG21	10	0.59
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG22	10	0.59
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG23	10	0.59
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG21	10	0.59
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG22	10	0.59
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG23	10	0.59
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG21	10	0.59
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG22	10	0.59
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG23	10	0.59
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG21	10	0.59
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG22	10	0.59
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG23	10	0.59
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG21	10	0.59
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG22	10	0.59
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG23	10	0.59
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD11	20	0.59
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD12	20	0.59
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD13	20	0.59
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD21	20	0.59
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD22	20	0.59
(1,2022)	1:34:A:VAL:HG21	1:132:A:LEU:HD23	20	0.59
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD11	20	0.59
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD12	20	0.59
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD13	20	0.59
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD21	20	0.59
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD22	20	0.59
(1,2022)	1:34:A:VAL:HG22	1:132:A:LEU:HD23	20	0.59
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD11	20	0.59
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD12	20	0.59
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD13	20	0.59
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD21	20	0.59
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD22	20	0.59
(1,2022)	1:34:A:VAL:HG23	1:132:A:LEU:HD23	20	0.59
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG11	10	0.59
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG12	10	0.59
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG13	10	0.59
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	16	0.59
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	16	0.59
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	16	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	2	0.59
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	2	0.59
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	2	0.59
(1,1842)	1:165:A:HIS:HA	1:166:A:CYS:HB3	16	0.59
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD11	17	0.59
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD12	17	0.59
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD13	17	0.59
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD11	17	0.59
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD12	17	0.59
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD13	17	0.59
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD11	17	0.59
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD12	17	0.59
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD13	17	0.59
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	2	0.59
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	13	0.59
(1,934)	1:159:A:VAL:HG11	1:156:A:ARG:HA	16	0.59
(1,934)	1:159:A:VAL:HG12	1:156:A:ARG:HA	16	0.59
(1,934)	1:159:A:VAL:HG13	1:156:A:ARG:HA	16	0.59
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	1	0.59
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	3	0.59
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	4	0.59
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	14	0.59
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	15	0.59
(1,2532)	1:34:A:VAL:HG21	1:177:A:TRP:HH2	20	0.58
(1,2532)	1:34:A:VAL:HG22	1:177:A:TRP:HH2	20	0.58
(1,2532)	1:34:A:VAL:HG23	1:177:A:TRP:HH2	20	0.58
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG11	16	0.58
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG12	16	0.58
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG13	16	0.58
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG11	16	0.58
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG12	16	0.58
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG13	16	0.58
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG11	16	0.58
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG12	16	0.58
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG13	16	0.58
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG21	3	0.58
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG22	3	0.58
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG23	3	0.58
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG21	3	0.58
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG22	3	0.58
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG23	3	0.58
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG21	3	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG22	3	0.58
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG23	3	0.58
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	1	0.58
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	1	0.58
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	1	0.58
(1,1682)	1:163:A:LEU:HB3	1:164:A:HIS:HB3	20	0.58
(1,1663)	1:27:A:VAL:HG11	1:24:A:GLU:HB3	4	0.58
(1,1663)	1:27:A:VAL:HG12	1:24:A:GLU:HB3	4	0.58
(1,1663)	1:27:A:VAL:HG13	1:24:A:GLU:HB3	4	0.58
(1,1349)	1:181:A:LEU:HD11	1:182:A:ASN:HB3	15	0.58
(1,1349)	1:181:A:LEU:HD12	1:182:A:ASN:HB3	15	0.58
(1,1349)	1:181:A:LEU:HD13	1:182:A:ASN:HB3	15	0.58
(1,1349)	1:181:A:LEU:HD11	1:182:A:ASN:HB3	17	0.58
(1,1349)	1:181:A:LEU:HD12	1:182:A:ASN:HB3	17	0.58
(1,1349)	1:181:A:LEU:HD13	1:182:A:ASN:HB3	17	0.58
(1,1043)	1:182:A:ASN:HB3	1:179:A:ALA:HA	19	0.58
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	2	0.58
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	6	0.58
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	7	0.58
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	8	0.58
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	9	0.58
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	10	0.58
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	11	0.58
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	12	0.58
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	13	0.58
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	15	0.58
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	16	0.58
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	17	0.58
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	19	0.58
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	20	0.58
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	3	0.57
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	3	0.57
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	4	0.57
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	4	0.57
(1,2556)	1:183:A:LEU:HD21	1:125:A:TRP:HE3	8	0.57
(1,2556)	1:183:A:LEU:HD22	1:125:A:TRP:HE3	8	0.57
(1,2556)	1:183:A:LEU:HD23	1:125:A:TRP:HE3	8	0.57
(1,2497)	1:39:A:VAL:HG21	1:35:A:PHE:HZ	3	0.57
(1,2497)	1:39:A:VAL:HG22	1:35:A:PHE:HZ	3	0.57
(1,2497)	1:39:A:VAL:HG23	1:35:A:PHE:HZ	3	0.57
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	4	0.57
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	4	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	5	0.57
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	5	0.57
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	5	0.57
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	20	0.57
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	20	0.57
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	20	0.57
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	6	0.57
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	6	0.57
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	6	0.57
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	6	0.57
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	6	0.57
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	6	0.57
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	6	0.57
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	6	0.57
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	6	0.57
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG11	18	0.57
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG12	18	0.57
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG13	18	0.57
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG11	18	0.57
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG12	18	0.57
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG13	18	0.57
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG11	18	0.57
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG12	18	0.57
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG13	18	0.57
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	6	0.57
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	6	0.57
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	6	0.57
(1,1349)	1:181:A:LEU:HD11	1:182:A:ASN:HB3	16	0.57
(1,1349)	1:181:A:LEU:HD12	1:182:A:ASN:HB3	16	0.57
(1,1349)	1:181:A:LEU:HD13	1:182:A:ASN:HB3	16	0.57
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	3	0.57
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	19	0.57
(1,921)	1:98:A:GLN:HE22	1:98:A:GLN:HA	17	0.57
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	11	0.57
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	11	0.57
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	11	0.57
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	17	0.57
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	17	0.57
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	17	0.57
(1,542)	1:172:A:ALA:HB1	1:173:A:GLN:HE22	17	0.57
(1,542)	1:172:A:ALA:HB2	1:173:A:GLN:HE22	17	0.57
(1,542)	1:172:A:ALA:HB3	1:173:A:GLN:HE22	17	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:94:A:GLN:HE22	1:95:A:THR:H	9	0.57
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	5	0.56
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	5	0.56
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	8	0.56
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	8	0.56
(1,2556)	1:183:A:LEU:HD21	1:125:A:TRP:HE3	6	0.56
(1,2556)	1:183:A:LEU:HD22	1:125:A:TRP:HE3	6	0.56
(1,2556)	1:183:A:LEU:HD23	1:125:A:TRP:HE3	6	0.56
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	9	0.56
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	9	0.56
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	9	0.56
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG11	12	0.56
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG12	12	0.56
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG13	12	0.56
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	1	0.56
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	1	0.56
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	1	0.56
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	1	0.56
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	1	0.56
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	1	0.56
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	1	0.56
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	1	0.56
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	1	0.56
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD21	12	0.56
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD22	12	0.56
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD23	12	0.56
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD21	8	0.56
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD22	8	0.56
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD23	8	0.56
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD11	7	0.56
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD12	7	0.56
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD13	7	0.56
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD11	7	0.56
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD12	7	0.56
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD13	7	0.56
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD11	7	0.56
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD12	7	0.56
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD13	7	0.56
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	2	0.56
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	2	0.56
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	2	0.56
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	13	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	8	0.56
(1,542)	1:172:A:ALA:HB1	1:173:A:GLN:HE22	9	0.56
(1,542)	1:172:A:ALA:HB2	1:173:A:GLN:HE22	9	0.56
(1,542)	1:172:A:ALA:HB3	1:173:A:GLN:HE22	9	0.56
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	18	0.56
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	14	0.55
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	14	0.55
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	15	0.55
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	15	0.55
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG11	6	0.55
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG12	6	0.55
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG13	6	0.55
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG11	6	0.55
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG12	6	0.55
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG13	6	0.55
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG11	18	0.55
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG12	18	0.55
(1,1996)	1:177:A:TRP:HE1	1:34:A:VAL:HG13	18	0.55
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD11	1	0.55
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD12	1	0.55
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD13	1	0.55
(1,1730)	1:144:A:GLN:H	1:145:A:HIS:HB3	15	0.55
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	2	0.55
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	5	0.55
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	5	0.55
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	5	0.55
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	19	0.55
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	19	0.55
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	19	0.55
(1,625)	1:118:A:LEU:HD21	1:128:A:VAL:HA	9	0.55
(1,625)	1:118:A:LEU:HD22	1:128:A:VAL:HA	9	0.55
(1,625)	1:118:A:LEU:HD23	1:128:A:VAL:HA	9	0.55
(1,542)	1:172:A:ALA:HB1	1:173:A:GLN:HE22	19	0.55
(1,542)	1:172:A:ALA:HB2	1:173:A:GLN:HE22	19	0.55
(1,542)	1:172:A:ALA:HB3	1:173:A:GLN:HE22	19	0.55
(1,523)	1:185:A:ASN:HB3	1:77:A:GLN:HE22	2	0.55
(1,410)	1:94:A:GLN:HE22	1:95:A:THR:H	12	0.55
(1,171)	1:162:A:MET:HB3	1:161:A:PHE:H	4	0.55
(1,171)	1:162:A:MET:HB3	1:161:A:PHE:H	8	0.55
(1,171)	1:162:A:MET:HB3	1:161:A:PHE:H	20	0.55
(1,74)	1:63:A:LEU:HD11	1:65:A:LEU:H	13	0.55
(1,74)	1:63:A:LEU:HD12	1:65:A:LEU:H	13	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:63:A:LEU:HD13	1:65:A:LEU:H	13	0.55
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	7	0.54
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	7	0.54
(1,2556)	1:183:A:LEU:HD21	1:125:A:TRP:HE3	15	0.54
(1,2556)	1:183:A:LEU:HD22	1:125:A:TRP:HE3	15	0.54
(1,2556)	1:183:A:LEU:HD23	1:125:A:TRP:HE3	15	0.54
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE1	4	0.54
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE2	4	0.54
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	16	0.54
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	16	0.54
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	16	0.54
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	16	0.54
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	16	0.54
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	16	0.54
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	16	0.54
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	16	0.54
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	16	0.54
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	11	0.54
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	11	0.54
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	11	0.54
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	7	0.54
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	7	0.54
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	7	0.54
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	7	0.54
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	7	0.54
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	7	0.54
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	7	0.54
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	7	0.54
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	7	0.54
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	2	0.54
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	2	0.54
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	2	0.54
(1,1349)	1:181:A:LEU:HD11	1:182:A:ASN:HB3	12	0.54
(1,1349)	1:181:A:LEU:HD12	1:182:A:ASN:HB3	12	0.54
(1,1349)	1:181:A:LEU:HD13	1:182:A:ASN:HB3	12	0.54
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	7	0.54
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	7	0.54
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	7	0.54
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	7	0.54
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	5	0.54
(1,536)	1:67:A:PRO:HB3	1:68:A:SER:H	18	0.54
(1,410)	1:94:A:GLN:HE22	1:95:A:THR:H	20	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	6	0.53
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	20	0.53
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	11	0.53
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	11	0.53
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	15	0.53
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	15	0.53
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	6	0.53
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	6	0.53
(1,2493)	1:118:A:LEU:HD21	1:119:A:PHE:HZ	4	0.53
(1,2493)	1:118:A:LEU:HD22	1:119:A:PHE:HZ	4	0.53
(1,2493)	1:118:A:LEU:HD23	1:119:A:PHE:HZ	4	0.53
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE1	9	0.53
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE2	9	0.53
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	18	0.53
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	18	0.53
(1,2382)	1:147:A:LEU:HD21	1:150:A:PHE:HD1	4	0.53
(1,2382)	1:147:A:LEU:HD21	1:150:A:PHE:HD2	4	0.53
(1,2382)	1:147:A:LEU:HD22	1:150:A:PHE:HD1	4	0.53
(1,2382)	1:147:A:LEU:HD22	1:150:A:PHE:HD2	4	0.53
(1,2382)	1:147:A:LEU:HD23	1:150:A:PHE:HD1	4	0.53
(1,2382)	1:147:A:LEU:HD23	1:150:A:PHE:HD2	4	0.53
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	17	0.53
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	17	0.53
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	17	0.53
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	17	0.53
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	17	0.53
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	17	0.53
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	17	0.53
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	17	0.53
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	17	0.53
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	19	0.53
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	19	0.53
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	19	0.53
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	19	0.53
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	19	0.53
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	19	0.53
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	19	0.53
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	19	0.53
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	19	0.53
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	1	0.53
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	1	0.53
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	1	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	13	0.53
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	13	0.53
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	13	0.53
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	16	0.53
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	16	0.53
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	16	0.53
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG11	12	0.53
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG12	12	0.53
(1,1933)	1:178:A:VAL:HA	1:74:A:VAL:HG13	12	0.53
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD11	18	0.53
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD12	18	0.53
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD13	18	0.53
(1,1495)	1:153:A:GLN:H	1:153:A:GLN:HG3	16	0.53
(1,1350)	1:179:A:ALA:HB1	1:182:A:ASN:HB3	11	0.53
(1,1350)	1:179:A:ALA:HB2	1:182:A:ASN:HB3	11	0.53
(1,1350)	1:179:A:ALA:HB3	1:182:A:ASN:HB3	11	0.53
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	11	0.53
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	15	0.53
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	15	0.53
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	15	0.53
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	9	0.53
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	9	0.53
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	9	0.53
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	5	0.53
(1,410)	1:94:A:GLN:HE22	1:95:A:THR:H	3	0.53
(1,396)	1:158:A:VAL:HG11	1:162:A:MET:H	10	0.53
(1,396)	1:158:A:VAL:HG12	1:162:A:MET:H	10	0.53
(1,396)	1:158:A:VAL:HG13	1:162:A:MET:H	10	0.53
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	12	0.53
(1,2497)	1:39:A:VAL:HG21	1:35:A:PHE:HZ	5	0.52
(1,2497)	1:39:A:VAL:HG22	1:35:A:PHE:HZ	5	0.52
(1,2497)	1:39:A:VAL:HG23	1:35:A:PHE:HZ	5	0.52
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	12	0.52
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	12	0.52
(1,2354)	1:76:A:ARG:HB3	1:41:A:TYR:HD1	1	0.52
(1,2354)	1:76:A:ARG:HB3	1:41:A:TYR:HD2	1	0.52
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	1	0.52
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	1	0.52
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	1	0.52
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG11	10	0.52
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG12	10	0.52
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG13	10	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG11	10	0.52
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG12	10	0.52
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG13	10	0.52
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG11	10	0.52
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG12	10	0.52
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG13	10	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	5	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	5	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	5	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	7	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	7	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	7	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	8	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	8	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	8	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	9	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	9	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	9	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	10	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	10	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	10	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	11	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	11	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	11	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	14	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	14	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	14	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	15	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	15	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	15	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	17	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	17	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	17	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	19	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	19	0.52
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	19	0.52
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD21	9	0.52
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD22	9	0.52
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD23	9	0.52
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	11	0.52
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	11	0.52
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	11	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1535)	1:156:A:ARG:HA	1:159:A:VAL:HB	2	0.52
(1,1535)	1:156:A:ARG:HA	1:159:A:VAL:HB	6	0.52
(1,934)	1:159:A:VAL:HG11	1:156:A:ARG:HA	18	0.52
(1,934)	1:159:A:VAL:HG12	1:156:A:ARG:HA	18	0.52
(1,934)	1:159:A:VAL:HG13	1:156:A:ARG:HA	18	0.52
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	8	0.52
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	8	0.52
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	8	0.52
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	2	0.52
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	3	0.52
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	20	0.52
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	3	0.51
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	3	0.51
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	13	0.51
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	13	0.51
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	13	0.51
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	13	0.51
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	13	0.51
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	13	0.51
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	13	0.51
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	13	0.51
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	13	0.51
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG11	18	0.51
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG12	18	0.51
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG13	18	0.51
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG11	19	0.51
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG12	19	0.51
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG13	19	0.51
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	2	0.51
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	2	0.51
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	2	0.51
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	3	0.51
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	3	0.51
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	3	0.51
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	4	0.51
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	4	0.51
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	4	0.51
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	6	0.51
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	6	0.51
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	6	0.51
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	12	0.51
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	12	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	12	0.51
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	20	0.51
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	20	0.51
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	20	0.51
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD11	15	0.51
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD12	15	0.51
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD13	15	0.51
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD21	9	0.51
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD22	9	0.51
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD23	9	0.51
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD21	9	0.51
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD22	9	0.51
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD23	9	0.51
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD21	9	0.51
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD22	9	0.51
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD23	9	0.51
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD11	11	0.51
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD12	11	0.51
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD13	11	0.51
(1,1842)	1:165:A:HIS:HA	1:166:A:CYS:HB3	18	0.51
(1,1535)	1:156:A:ARG:HA	1:159:A:VAL:HB	12	0.51
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	9	0.51
(1,1032)	1:131:A:LEU:HD21	1:115:A:ALA:HA	19	0.51
(1,1032)	1:131:A:LEU:HD22	1:115:A:ALA:HA	19	0.51
(1,1032)	1:131:A:LEU:HD23	1:115:A:ALA:HA	19	0.51
(1,1027)	1:27:A:VAL:HG21	1:168:A:ALA:HA	20	0.51
(1,1027)	1:27:A:VAL:HG22	1:168:A:ALA:HA	20	0.51
(1,1027)	1:27:A:VAL:HG23	1:168:A:ALA:HA	20	0.51
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	7	0.51
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	7	0.51
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	7	0.51
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	10	0.51
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	10	0.51
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	10	0.51
(1,298)	1:88:A:ARG:HD3	1:88:A:ARG:H	14	0.51
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	5	0.51
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	6	0.51
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	15	0.51
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	17	0.51
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	18	0.51
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	12	0.5
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	12	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	17	0.5
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	17	0.5
(1,2433)	1:97:A:LEU:HD11	1:93:A:PHE:HE1	17	0.5
(1,2433)	1:97:A:LEU:HD11	1:93:A:PHE:HE2	17	0.5
(1,2433)	1:97:A:LEU:HD12	1:93:A:PHE:HE1	17	0.5
(1,2433)	1:97:A:LEU:HD12	1:93:A:PHE:HE2	17	0.5
(1,2433)	1:97:A:LEU:HD13	1:93:A:PHE:HE1	17	0.5
(1,2433)	1:97:A:LEU:HD13	1:93:A:PHE:HE2	17	0.5
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	16	0.5
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	16	0.5
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	16	0.5
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE1	9	0.5
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE2	9	0.5
(1,2123)	1:61:A:VAL:HG11	1:60:A:MET:HE3	9	0.5
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE1	9	0.5
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE2	9	0.5
(1,2123)	1:61:A:VAL:HG12	1:60:A:MET:HE3	9	0.5
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE1	9	0.5
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE2	9	0.5
(1,2123)	1:61:A:VAL:HG13	1:60:A:MET:HE3	9	0.5
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG21	19	0.5
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG22	19	0.5
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG23	19	0.5
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG21	19	0.5
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG22	19	0.5
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG23	19	0.5
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG21	19	0.5
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG22	19	0.5
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG23	19	0.5
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG21	19	0.5
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG22	19	0.5
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG23	19	0.5
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG21	19	0.5
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG22	19	0.5
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG23	19	0.5
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG21	19	0.5
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG22	19	0.5
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG23	19	0.5
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG21	7	0.5
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG22	7	0.5
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG23	7	0.5
(1,1740)	1:63:A:LEU:HD11	1:64:A:PRO:HG3	10	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1740)	1:63:A:LEU:HD12	1:64:A:PRO:HG3	10	0.5
(1,1740)	1:63:A:LEU:HD13	1:64:A:PRO:HG3	10	0.5
(1,1730)	1:144:A:GLN:H	1:145:A:HIS:HB3	1	0.5
(1,1349)	1:181:A:LEU:HD11	1:182:A:ASN:HB3	4	0.5
(1,1349)	1:181:A:LEU:HD12	1:182:A:ASN:HB3	4	0.5
(1,1349)	1:181:A:LEU:HD13	1:182:A:ASN:HB3	4	0.5
(1,1349)	1:181:A:LEU:HD11	1:182:A:ASN:HB3	18	0.5
(1,1349)	1:181:A:LEU:HD12	1:182:A:ASN:HB3	18	0.5
(1,1349)	1:181:A:LEU:HD13	1:182:A:ASN:HB3	18	0.5
(1,1027)	1:27:A:VAL:HG21	1:168:A:ALA:HA	1	0.5
(1,1027)	1:27:A:VAL:HG22	1:168:A:ALA:HA	1	0.5
(1,1027)	1:27:A:VAL:HG23	1:168:A:ALA:HA	1	0.5
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	5	0.5
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	5	0.5
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	5	0.5
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	2	0.5
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	9	0.5
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	14	0.5
(1,171)	1:162:A:MET:HB3	1:161:A:PHE:H	14	0.5
(1,171)	1:162:A:MET:HB3	1:161:A:PHE:H	17	0.5
(1,171)	1:162:A:MET:HB3	1:161:A:PHE:H	19	0.5
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	12	0.49
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	2	0.49
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	2	0.49
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	7	0.49
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	7	0.49
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	7	0.49
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG21	18	0.49
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG22	18	0.49
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG23	18	0.49
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG21	18	0.49
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG22	18	0.49
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG23	18	0.49
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG21	18	0.49
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG22	18	0.49
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG23	18	0.49
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG21	18	0.49
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG22	18	0.49
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG23	18	0.49
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG21	18	0.49
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG22	18	0.49
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG23	18	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG21	18	0.49
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG22	18	0.49
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG23	18	0.49
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG11	18	0.49
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG12	18	0.49
(1,1998)	1:34:A:VAL:H	1:34:A:VAL:HG13	18	0.49
(1,1867)	1:73:A:GLN:HG3	1:181:A:LEU:HD11	19	0.49
(1,1867)	1:73:A:GLN:HG3	1:181:A:LEU:HD12	19	0.49
(1,1867)	1:73:A:GLN:HG3	1:181:A:LEU:HD13	19	0.49
(1,1842)	1:165:A:HIS:HA	1:166:A:CYS:HB3	2	0.49
(1,1535)	1:156:A:ARG:HA	1:159:A:VAL:HB	20	0.49
(1,1429)	1:159:A:VAL:HG11	1:32:A:GLU:HG3	20	0.49
(1,1429)	1:159:A:VAL:HG12	1:32:A:GLU:HG3	20	0.49
(1,1429)	1:159:A:VAL:HG13	1:32:A:GLU:HG3	20	0.49
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	2	0.49
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	2	0.49
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	2	0.49
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	14	0.49
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	14	0.49
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	14	0.49
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	1	0.49
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	4	0.49
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	10	0.49
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	11	0.49
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	13	0.49
(1,123)	1:34:A:VAL:HG11	1:74:A:VAL:H	7	0.49
(1,123)	1:34:A:VAL:HG12	1:74:A:VAL:H	7	0.49
(1,123)	1:34:A:VAL:HG13	1:74:A:VAL:H	7	0.49
(1,90)	1:97:A:LEU:HD21	1:138:A:LEU:H	20	0.49
(1,90)	1:97:A:LEU:HD22	1:138:A:LEU:H	20	0.49
(1,90)	1:97:A:LEU:HD23	1:138:A:LEU:H	20	0.49
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	2	0.48
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	15	0.48
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	15	0.48
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	15	0.48
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB1	10	0.48
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB2	10	0.48
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB3	10	0.48
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB1	10	0.48
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB2	10	0.48
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB3	10	0.48
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB1	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB2	10	0.48
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB3	10	0.48
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG11	9	0.48
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG12	9	0.48
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG13	9	0.48
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD21	11	0.48
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD22	11	0.48
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD23	11	0.48
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG21	17	0.48
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG22	17	0.48
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG23	17	0.48
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG21	17	0.48
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG22	17	0.48
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG23	17	0.48
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG21	17	0.48
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG22	17	0.48
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG23	17	0.48
(1,1730)	1:144:A:GLN:H	1:145:A:HIS:HB3	19	0.48
(1,1495)	1:153:A:GLN:H	1:153:A:GLN:HG3	18	0.48
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	6	0.48
(1,934)	1:159:A:VAL:HG11	1:156:A:ARG:HA	17	0.48
(1,934)	1:159:A:VAL:HG12	1:156:A:ARG:HA	17	0.48
(1,934)	1:159:A:VAL:HG13	1:156:A:ARG:HA	17	0.48
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	3	0.48
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	16	0.48
(1,877)	1:46:A:GLU:HG3	1:43:A:HIS:HA	11	0.48
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	6	0.48
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	6	0.48
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	6	0.48
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	17	0.48
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	17	0.48
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	17	0.48
(1,268)	1:50:A:GLU:HB3	1:52:A:VAL:H	3	0.48
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	7	0.48
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	16	0.48
(1,205)	1:156:A:ARG:HB3	1:156:A:ARG:H	19	0.48
(1,123)	1:34:A:VAL:HG11	1:74:A:VAL:H	17	0.48
(1,123)	1:34:A:VAL:HG12	1:74:A:VAL:H	17	0.48
(1,123)	1:34:A:VAL:HG13	1:74:A:VAL:H	17	0.48
(1,2760)	2:87:B:ALA:HA	2:90:B:LEU:HG	9	0.47
(1,2354)	1:76:A:ARG:HB3	1:41:A:TYR:HD1	10	0.47
(1,2354)	1:76:A:ARG:HB3	1:41:A:TYR:HD2	10	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG11	17	0.47
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG12	17	0.47
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG13	17	0.47
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	9	0.47
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	9	0.47
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	9	0.47
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	11	0.47
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	11	0.47
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	11	0.47
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	13	0.47
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	13	0.47
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	13	0.47
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	15	0.47
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	20	0.47
(1,2493)	1:118:A:LEU:HD21	1:119:A:PHE:HZ	14	0.46
(1,2493)	1:118:A:LEU:HD22	1:119:A:PHE:HZ	14	0.46
(1,2493)	1:118:A:LEU:HD23	1:119:A:PHE:HZ	14	0.46
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE1	9	0.46
(1,2462)	1:118:A:LEU:HD21	1:119:A:PHE:HE2	9	0.46
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE1	9	0.46
(1,2462)	1:118:A:LEU:HD22	1:119:A:PHE:HE2	9	0.46
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE1	9	0.46
(1,2462)	1:118:A:LEU:HD23	1:119:A:PHE:HE2	9	0.46
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	3	0.46
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	3	0.46
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	3	0.46
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	3	0.46
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	3	0.46
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	3	0.46
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	3	0.46
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	3	0.46
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	3	0.46
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	14	0.46
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	14	0.46
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	14	0.46
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	14	0.46
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	14	0.46
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	14	0.46
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	14	0.46
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	14	0.46
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	14	0.46
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB1	4	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB2	4	0.46
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB3	4	0.46
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB1	4	0.46
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB2	4	0.46
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB3	4	0.46
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB1	4	0.46
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB2	4	0.46
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB3	4	0.46
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG11	18	0.46
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG12	18	0.46
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG13	18	0.46
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	15	0.46
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	15	0.46
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	15	0.46
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	15	0.46
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	15	0.46
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	15	0.46
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	15	0.46
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	15	0.46
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	15	0.46
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD21	10	0.46
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD22	10	0.46
(1,1918)	1:20:A:PRO:HD3	1:19:A:LEU:HD23	10	0.46
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD21	13	0.46
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD22	13	0.46
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD23	13	0.46
(1,1495)	1:153:A:GLN:H	1:153:A:GLN:HG3	8	0.46
(1,1349)	1:181:A:LEU:HD11	1:182:A:ASN:HB3	6	0.46
(1,1349)	1:181:A:LEU:HD12	1:182:A:ASN:HB3	6	0.46
(1,1349)	1:181:A:LEU:HD13	1:182:A:ASN:HB3	6	0.46
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	1	0.46
(1,1043)	1:182:A:ASN:HB3	1:179:A:ALA:HA	11	0.46
(1,874)	1:63:A:LEU:HD21	1:36:A:ARG:HA	18	0.46
(1,874)	1:63:A:LEU:HD22	1:36:A:ARG:HA	18	0.46
(1,874)	1:63:A:LEU:HD23	1:36:A:ARG:HA	18	0.46
(1,849)	1:158:A:VAL:HG11	1:32:A:GLU:HA	10	0.46
(1,849)	1:158:A:VAL:HG12	1:32:A:GLU:HA	10	0.46
(1,849)	1:158:A:VAL:HG13	1:32:A:GLU:HA	10	0.46
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	2	0.46
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	2	0.46
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	2	0.46
(1,542)	1:172:A:ALA:HB1	1:173:A:GLN:HE22	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:172:A:ALA:HB2	1:173:A:GLN:HE22	5	0.46
(1,542)	1:172:A:ALA:HB3	1:173:A:GLN:HE22	5	0.46
(1,410)	1:94:A:GLN:HE22	1:95:A:THR:H	16	0.46
(1,190)	1:183:A:LEU:HD21	1:125:A:TRP:H	12	0.46
(1,190)	1:183:A:LEU:HD22	1:125:A:TRP:H	12	0.46
(1,190)	1:183:A:LEU:HD23	1:125:A:TRP:H	12	0.46
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	6	0.46
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	6	0.46
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	6	0.46
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	18	0.45
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	18	0.45
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE1	8	0.45
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE2	8	0.45
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE1	8	0.45
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE2	8	0.45
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE1	8	0.45
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE2	8	0.45
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	16	0.45
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	16	0.45
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	4	0.45
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	4	0.45
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	4	0.45
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	4	0.45
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	4	0.45
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	4	0.45
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	4	0.45
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	4	0.45
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	4	0.45
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	15	0.45
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	15	0.45
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	15	0.45
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG21	14	0.45
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG22	14	0.45
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG23	14	0.45
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG21	14	0.45
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG22	14	0.45
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG23	14	0.45
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	13	0.45
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	13	0.45
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	13	0.45
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	13	0.45
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	13	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	13	0.45
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	13	0.45
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	13	0.45
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	13	0.45
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD21	2	0.45
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD22	2	0.45
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD23	2	0.45
(1,1349)	1:181:A:LEU:HD11	1:182:A:ASN:HB3	3	0.45
(1,1349)	1:181:A:LEU:HD12	1:182:A:ASN:HB3	3	0.45
(1,1349)	1:181:A:LEU:HD13	1:182:A:ASN:HB3	3	0.45
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	17	0.45
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	12	0.45
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	12	0.45
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	12	0.45
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	20	0.45
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	20	0.45
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	20	0.45
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	1	0.45
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	13	0.45
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	11	0.45
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	11	0.45
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	11	0.45
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	16	0.45
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	16	0.45
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	16	0.45
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	16	0.45
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	16	0.45
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	16	0.45
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	1	0.44
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	1	0.44
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB1	11	0.44
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB2	11	0.44
(1,2246)	1:162:A:MET:HG3	1:168:A:ALA:HB3	11	0.44
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	5	0.44
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	5	0.44
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	5	0.44
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	5	0.44
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	5	0.44
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	5	0.44
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	5	0.44
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	5	0.44
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB1	14	0.44
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB2	14	0.44
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB3	14	0.44
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB1	14	0.44
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB2	14	0.44
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB3	14	0.44
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB1	14	0.44
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB2	14	0.44
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB3	14	0.44
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	12	0.44
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	12	0.44
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	12	0.44
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD21	15	0.44
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD22	15	0.44
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD23	15	0.44
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD21	15	0.44
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD22	15	0.44
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD23	15	0.44
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD21	15	0.44
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD22	15	0.44
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD23	15	0.44
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD21	15	0.44
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD22	15	0.44
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD23	15	0.44
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD21	15	0.44
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD22	15	0.44
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD23	15	0.44
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD21	15	0.44
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD22	15	0.44
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD23	15	0.44
(1,1842)	1:165:A:HIS:HA	1:166:A:CYS:HB3	11	0.44
(1,1750)	1:142:A:VAL:HG21	1:102:A:PRO:HG3	16	0.44
(1,1750)	1:142:A:VAL:HG22	1:102:A:PRO:HG3	16	0.44
(1,1750)	1:142:A:VAL:HG23	1:102:A:PRO:HG3	16	0.44
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	5	0.44
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	5	0.44
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	5	0.44
(1,1350)	1:179:A:ALA:HB1	1:182:A:ASN:HB3	18	0.44
(1,1350)	1:179:A:ALA:HB2	1:182:A:ASN:HB3	18	0.44
(1,1350)	1:179:A:ALA:HB3	1:182:A:ASN:HB3	18	0.44
(1,1032)	1:131:A:LEU:HD21	1:115:A:ALA:HA	7	0.44
(1,1032)	1:131:A:LEU:HD22	1:115:A:ALA:HA	7	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1032)	1:131:A:LEU:HD23	1:115:A:ALA:HA	7	0.44
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	18	0.44
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	18	0.44
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	18	0.44
(1,542)	1:172:A:ALA:HB1	1:173:A:GLN:HE22	18	0.44
(1,542)	1:172:A:ALA:HB2	1:173:A:GLN:HE22	18	0.44
(1,542)	1:172:A:ALA:HB3	1:173:A:GLN:HE22	18	0.44
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	9	0.44
(1,390)	1:63:A:LEU:HD11	1:36:A:ARG:H	15	0.44
(1,390)	1:63:A:LEU:HD12	1:36:A:ARG:H	15	0.44
(1,390)	1:63:A:LEU:HD13	1:36:A:ARG:H	15	0.44
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	3	0.44
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	3	0.44
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	3	0.44
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	6	0.44
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	13	0.44
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	18	0.44
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	8	0.43
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	8	0.43
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	2	0.43
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	2	0.43
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	2	0.43
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	2	0.43
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	2	0.43
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	2	0.43
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	2	0.43
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	2	0.43
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	2	0.43
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	19	0.43
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	19	0.43
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	19	0.43
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG11	2	0.43
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG12	2	0.43
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG13	2	0.43
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG11	2	0.43
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG12	2	0.43
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG13	2	0.43
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	1	0.43
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	1	0.43
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	1	0.43
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG21	14	0.43
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG22	14	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG23	14	0.43
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG21	14	0.43
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG22	14	0.43
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG23	14	0.43
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD21	14	0.43
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD22	14	0.43
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD23	14	0.43
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	3	0.43
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	3	0.43
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	3	0.43
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	3	0.43
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	3	0.43
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	3	0.43
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	3	0.43
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	3	0.43
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	3	0.43
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	5	0.43
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	5	0.43
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	5	0.43
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	17	0.43
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	17	0.43
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	17	0.43
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD21	6	0.43
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD22	6	0.43
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD23	6	0.43
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD11	20	0.43
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD12	20	0.43
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD13	20	0.43
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD21	16	0.43
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD22	16	0.43
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD23	16	0.43
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD21	16	0.43
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD22	16	0.43
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD23	16	0.43
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD21	16	0.43
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD22	16	0.43
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD23	16	0.43
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD21	16	0.43
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD22	16	0.43
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD23	16	0.43
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD21	16	0.43
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD22	16	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD23	16	0.43
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD21	16	0.43
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD22	16	0.43
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD23	16	0.43
(1,1730)	1:144:A:GLN:H	1:145:A:HIS:HB3	14	0.43
(1,1495)	1:153:A:GLN:H	1:153:A:GLN:HG3	20	0.43
(1,1050)	1:19:A:LEU:HD21	1:19:A:LEU:HA	10	0.43
(1,1050)	1:19:A:LEU:HD22	1:19:A:LEU:HA	10	0.43
(1,1050)	1:19:A:LEU:HD23	1:19:A:LEU:HA	10	0.43
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	4	0.43
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	4	0.43
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	4	0.43
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	18	0.43
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	12	0.43
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	5	0.43
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	5	0.43
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	5	0.43
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	19	0.43
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	19	0.43
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	19	0.43
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	8	0.43
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	9	0.43
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	10	0.43
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	12	0.43
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	20	0.43
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	10	0.42
(1,2683)	2:84:B:ARG:HA	2:84:B:ARG:HD3	8	0.42
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	1	0.42
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	1	0.42
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	17	0.42
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	17	0.42
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG21	1	0.42
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG22	1	0.42
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG23	1	0.42
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG21	1	0.42
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG22	1	0.42
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG23	1	0.42
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG21	1	0.42
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG22	1	0.42
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG23	1	0.42
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG21	1	0.42
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG22	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG23	1	0.42
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG21	1	0.42
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG22	1	0.42
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG23	1	0.42
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG21	1	0.42
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG22	1	0.42
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG23	1	0.42
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	1	0.42
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	1	0.42
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	1	0.42
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG11	14	0.42
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG12	14	0.42
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG13	14	0.42
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD21	19	0.42
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD22	19	0.42
(1,1968)	1:180:A:ALA:H	1:181:A:LEU:HD23	19	0.42
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	14	0.42
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	14	0.42
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	14	0.42
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	17	0.42
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	4	0.42
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	4	0.42
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	4	0.42
(1,1126)	1:153:A:GLN:HG3	1:152:A:GLY:HA2	3	0.42
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	3	0.42
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	3	0.42
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	3	0.42
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	6	0.42
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	6	0.42
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	6	0.42
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	10	0.42
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	10	0.42
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	10	0.42
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	11	0.42
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	11	0.42
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	11	0.42
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	12	0.42
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	12	0.42
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	12	0.42
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	14	0.42
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	14	0.42
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	14	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	16	0.42
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	16	0.42
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	16	0.42
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	17	0.42
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	17	0.42
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	17	0.42
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	19	0.42
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	19	0.42
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	19	0.42
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	20	0.42
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	20	0.42
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	20	0.42
(1,1002)	1:181:A:LEU:HD21	1:181:A:LEU:HA	1	0.42
(1,1002)	1:181:A:LEU:HD22	1:181:A:LEU:HA	1	0.42
(1,1002)	1:181:A:LEU:HD23	1:181:A:LEU:HA	1	0.42
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	11	0.42
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	4	0.42
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	4	0.42
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	4	0.42
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	20	0.42
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	18	0.42
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	18	0.42
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	18	0.42
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	14	0.42
(2,157)	1:153:A:GLN:O	1:157:A:PHE:N	3	0.41
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	4	0.41
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	3	0.41
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	20	0.41
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	20	0.41
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	4	0.41
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	4	0.41
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	12	0.41
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	12	0.41
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	15	0.41
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	15	0.41
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	15	0.41
(1,2115)	1:50:A:GLU:HG3	1:49:A:ALA:HB1	19	0.41
(1,2115)	1:50:A:GLU:HG3	1:49:A:ALA:HB2	19	0.41
(1,2115)	1:50:A:GLU:HG3	1:49:A:ALA:HB3	19	0.41
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	1	0.41
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	1	0.41
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG21	18	0.41
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG22	18	0.41
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG23	18	0.41
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG11	1	0.41
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG12	1	0.41
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG13	1	0.41
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG21	12	0.41
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG22	12	0.41
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG23	12	0.41
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG21	12	0.41
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG22	12	0.41
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG23	12	0.41
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG21	12	0.41
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG22	12	0.41
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG23	12	0.41
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD21	7	0.41
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD22	7	0.41
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD23	7	0.41
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD11	18	0.41
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD12	18	0.41
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD13	18	0.41
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD11	18	0.41
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD12	18	0.41
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD13	18	0.41
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD11	18	0.41
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD12	18	0.41
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD13	18	0.41
(1,1495)	1:153:A:GLN:H	1:153:A:GLN:HG3	19	0.41
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	8	0.41
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	8	0.41
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	8	0.41
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	12	0.41
(1,542)	1:172:A:ALA:HB1	1:173:A:GLN:HE22	2	0.41
(1,542)	1:172:A:ALA:HB2	1:173:A:GLN:HE22	2	0.41
(1,542)	1:172:A:ALA:HB3	1:173:A:GLN:HE22	2	0.41
(1,542)	1:172:A:ALA:HB1	1:173:A:GLN:HE22	11	0.41
(1,542)	1:172:A:ALA:HB2	1:173:A:GLN:HE22	11	0.41
(1,542)	1:172:A:ALA:HB3	1:173:A:GLN:HE22	11	0.41
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	9	0.41
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	16	0.41
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	4	0.41
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	4	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	4	0.41
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	7	0.41
(1,171)	1:162:A:MET:HB3	1:161:A:PHE:H	7	0.41
(1,74)	1:63:A:LEU:HD11	1:65:A:LEU:H	9	0.41
(1,74)	1:63:A:LEU:HD12	1:65:A:LEU:H	9	0.41
(1,74)	1:63:A:LEU:HD13	1:65:A:LEU:H	9	0.41
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	4	0.4
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	12	0.4
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD21	1	0.4
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD22	1	0.4
(1,2674)	2:87:B:ALA:HA	2:90:B:LEU:HD23	1	0.4
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE1	20	0.4
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE2	20	0.4
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE1	20	0.4
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE2	20	0.4
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE1	20	0.4
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE2	20	0.4
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	5	0.4
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	5	0.4
(1,2354)	1:76:A:ARG:HB3	1:41:A:TYR:HD1	2	0.4
(1,2354)	1:76:A:ARG:HB3	1:41:A:TYR:HD2	2	0.4
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG11	8	0.4
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG12	8	0.4
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG13	8	0.4
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG11	12	0.4
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG12	12	0.4
(1,2003)	1:71:A:MET:HB3	1:34:A:VAL:HG13	12	0.4
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG11	11	0.4
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG12	11	0.4
(1,2000)	1:71:A:MET:HA	1:34:A:VAL:HG13	11	0.4
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG21	3	0.4
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG22	3	0.4
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG23	3	0.4
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG21	3	0.4
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG22	3	0.4
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG23	3	0.4
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	6	0.4
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	6	0.4
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	6	0.4
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD21	13	0.4
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD22	13	0.4
(1,1850)	1:39:A:VAL:HG21	1:63:A:LEU:HD23	13	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD21	13	0.4
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD22	13	0.4
(1,1850)	1:39:A:VAL:HG22	1:63:A:LEU:HD23	13	0.4
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD21	13	0.4
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD22	13	0.4
(1,1850)	1:39:A:VAL:HG23	1:63:A:LEU:HD23	13	0.4
(1,1730)	1:144:A:GLN:H	1:145:A:HIS:HB3	17	0.4
(1,1495)	1:153:A:GLN:H	1:153:A:GLN:HG3	7	0.4
(1,1495)	1:153:A:GLN:H	1:153:A:GLN:HG3	9	0.4
(1,1495)	1:153:A:GLN:H	1:153:A:GLN:HG3	10	0.4
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	20	0.4
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	20	0.4
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	20	0.4
(1,1032)	1:131:A:LEU:HD21	1:115:A:ALA:HA	5	0.4
(1,1032)	1:131:A:LEU:HD22	1:115:A:ALA:HA	5	0.4
(1,1032)	1:131:A:LEU:HD23	1:115:A:ALA:HA	5	0.4
(1,1002)	1:181:A:LEU:HD21	1:181:A:LEU:HA	14	0.4
(1,1002)	1:181:A:LEU:HD22	1:181:A:LEU:HA	14	0.4
(1,1002)	1:181:A:LEU:HD23	1:181:A:LEU:HA	14	0.4
(1,1002)	1:181:A:LEU:HD21	1:181:A:LEU:HA	19	0.4
(1,1002)	1:181:A:LEU:HD22	1:181:A:LEU:HA	19	0.4
(1,1002)	1:181:A:LEU:HD23	1:181:A:LEU:HA	19	0.4
(1,934)	1:159:A:VAL:HG11	1:156:A:ARG:HA	7	0.4
(1,934)	1:159:A:VAL:HG12	1:156:A:ARG:HA	7	0.4
(1,934)	1:159:A:VAL:HG13	1:156:A:ARG:HA	7	0.4
(1,934)	1:159:A:VAL:HG11	1:156:A:ARG:HA	10	0.4
(1,934)	1:159:A:VAL:HG12	1:156:A:ARG:HA	10	0.4
(1,934)	1:159:A:VAL:HG13	1:156:A:ARG:HA	10	0.4
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	7	0.4
(1,874)	1:63:A:LEU:HD21	1:36:A:ARG:HA	9	0.4
(1,874)	1:63:A:LEU:HD22	1:36:A:ARG:HA	9	0.4
(1,874)	1:63:A:LEU:HD23	1:36:A:ARG:HA	9	0.4
(1,797)	1:147:A:LEU:H	1:143:A:TYR:HA	5	0.4
(1,661)	1:34:A:VAL:HG11	1:31:A:THR:HA	3	0.4
(1,661)	1:34:A:VAL:HG12	1:31:A:THR:HA	3	0.4
(1,661)	1:34:A:VAL:HG13	1:31:A:THR:HA	3	0.4
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	4	0.4
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	11	0.4
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	4	0.39
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	14	0.39
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	18	0.39
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	1	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	4	0.39
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	19	0.39
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	14	0.39
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	14	0.39
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE1	4	0.39
(1,2582)	1:140:A:LEU:HB3	1:136:A:TYR:HE2	4	0.39
(1,2443)	1:153:A:GLN:HB3	1:150:A:PHE:HE1	15	0.39
(1,2443)	1:153:A:GLN:HB3	1:150:A:PHE:HE2	15	0.39
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	7	0.39
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	7	0.39
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	7	0.39
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	7	0.39
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	7	0.39
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	7	0.39
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	7	0.39
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	7	0.39
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	7	0.39
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG11	20	0.39
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG12	20	0.39
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG13	20	0.39
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG21	2	0.39
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG22	2	0.39
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG23	2	0.39
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	3	0.39
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	3	0.39
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	3	0.39
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	11	0.39
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	11	0.39
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	11	0.39
(1,1877)	1:101:A:GLN:H	1:100:A:LEU:HD11	8	0.39
(1,1877)	1:101:A:GLN:H	1:100:A:LEU:HD12	8	0.39
(1,1877)	1:101:A:GLN:H	1:100:A:LEU:HD13	8	0.39
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD11	13	0.39
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD12	13	0.39
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD13	13	0.39
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD11	3	0.39
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD12	3	0.39
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD13	3	0.39
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD11	13	0.39
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD12	13	0.39
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD13	13	0.39
(1,1807)	1:139:A:ALA:H	1:138:A:LEU:HG	15	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1709)	1:98:A:GLN:HE22	1:98:A:GLN:HB3	18	0.39
(1,1554)	1:33:A:GLU:HB3	1:34:A:VAL:HB	18	0.39
(1,1495)	1:153:A:GLN:H	1:153:A:GLN:HG3	1	0.39
(1,1495)	1:153:A:GLN:H	1:153:A:GLN:HG3	2	0.39
(1,1495)	1:153:A:GLN:H	1:153:A:GLN:HG3	4	0.39
(1,1495)	1:153:A:GLN:H	1:153:A:GLN:HG3	5	0.39
(1,1002)	1:181:A:LEU:HD21	1:181:A:LEU:HA	9	0.39
(1,1002)	1:181:A:LEU:HD22	1:181:A:LEU:HA	9	0.39
(1,1002)	1:181:A:LEU:HD23	1:181:A:LEU:HA	9	0.39
(1,543)	1:181:A:LEU:HD11	1:73:A:GLN:HE21	19	0.39
(1,543)	1:181:A:LEU:HD12	1:73:A:GLN:HE21	19	0.39
(1,543)	1:181:A:LEU:HD13	1:73:A:GLN:HE21	19	0.39
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	5	0.38
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	9	0.38
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	5	0.38
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	6	0.38
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	16	0.38
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	19	0.38
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	9	0.38
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	11	0.38
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	8	0.38
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	8	0.38
(1,2556)	1:183:A:LEU:HD21	1:125:A:TRP:HE3	4	0.38
(1,2556)	1:183:A:LEU:HD22	1:125:A:TRP:HE3	4	0.38
(1,2556)	1:183:A:LEU:HD23	1:125:A:TRP:HE3	4	0.38
(1,2454)	1:147:A:LEU:HD21	1:150:A:PHE:HE1	13	0.38
(1,2454)	1:147:A:LEU:HD21	1:150:A:PHE:HE2	13	0.38
(1,2454)	1:147:A:LEU:HD22	1:150:A:PHE:HE1	13	0.38
(1,2454)	1:147:A:LEU:HD22	1:150:A:PHE:HE2	13	0.38
(1,2454)	1:147:A:LEU:HD23	1:150:A:PHE:HE1	13	0.38
(1,2454)	1:147:A:LEU:HD23	1:150:A:PHE:HE2	13	0.38
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	12	0.38
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	12	0.38
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	12	0.38
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	12	0.38
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	12	0.38
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	12	0.38
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	12	0.38
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	12	0.38
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	12	0.38
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG11	12	0.38
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG12	12	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG13	12	0.38
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG11	12	0.38
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG12	12	0.38
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG13	12	0.38
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD11	7	0.38
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD12	7	0.38
(1,2055)	1:182:A:ASN:HB3	1:183:A:LEU:HD13	7	0.38
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	14	0.38
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	14	0.38
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	14	0.38
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG11	2	0.38
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG12	2	0.38
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG13	2	0.38
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD11	19	0.38
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD12	19	0.38
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD13	19	0.38
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG21	3	0.38
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG22	3	0.38
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG23	3	0.38
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG21	5	0.38
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG22	5	0.38
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG23	5	0.38
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG21	12	0.38
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG22	12	0.38
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG23	12	0.38
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG21	14	0.38
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG22	14	0.38
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG23	14	0.38
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG21	20	0.38
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG22	20	0.38
(1,1977)	1:39:A:VAL:H	1:39:A:VAL:HG23	20	0.38
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG21	7	0.38
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG22	7	0.38
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG23	7	0.38
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG21	7	0.38
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG22	7	0.38
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG23	7	0.38
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG21	7	0.38
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG22	7	0.38
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG23	7	0.38
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD21	19	0.38
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD22	19	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD23	19	0.38
(1,1877)	1:101:A:GLN:H	1:100:A:LEU:HD11	6	0.38
(1,1877)	1:101:A:GLN:H	1:100:A:LEU:HD12	6	0.38
(1,1877)	1:101:A:GLN:H	1:100:A:LEU:HD13	6	0.38
(1,1877)	1:101:A:GLN:H	1:100:A:LEU:HD11	16	0.38
(1,1877)	1:101:A:GLN:H	1:100:A:LEU:HD12	16	0.38
(1,1877)	1:101:A:GLN:H	1:100:A:LEU:HD13	16	0.38
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	7	0.38
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	7	0.38
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	7	0.38
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	19	0.38
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	19	0.38
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	19	0.38
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD11	1	0.38
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD12	1	0.38
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD13	1	0.38
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD11	9	0.38
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD12	9	0.38
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD13	9	0.38
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD21	9	0.38
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD22	9	0.38
(1,1847)	1:40:A:PHE:H	1:63:A:LEU:HD23	9	0.38
(1,1189)	1:159:A:VAL:HG11	1:156:A:ARG:HD3	4	0.38
(1,1189)	1:159:A:VAL:HG12	1:156:A:ARG:HD3	4	0.38
(1,1189)	1:159:A:VAL:HG13	1:156:A:ARG:HD3	4	0.38
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	9	0.38
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	9	0.38
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	9	0.38
(1,1002)	1:181:A:LEU:HD21	1:181:A:LEU:HA	11	0.38
(1,1002)	1:181:A:LEU:HD22	1:181:A:LEU:HA	11	0.38
(1,1002)	1:181:A:LEU:HD23	1:181:A:LEU:HA	11	0.38
(1,839)	1:63:A:LEU:HB3	1:62:A:THR:HA	17	0.38
(1,528)	1:55:A:PRO:HD3	1:47:A:GLN:HE21	3	0.38
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	18	0.38
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	19	0.38
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	15	0.38
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	10	0.37
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	2	0.37
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	12	0.37
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	10	0.37
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	3	0.37
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	14	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	1	0.37
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	3	0.37
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	14	0.37
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	20	0.37
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	16	0.37
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	17	0.37
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	9	0.37
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	9	0.37
(1,2556)	1:183:A:LEU:HD21	1:125:A:TRP:HE3	2	0.37
(1,2556)	1:183:A:LEU:HD22	1:125:A:TRP:HE3	2	0.37
(1,2556)	1:183:A:LEU:HD23	1:125:A:TRP:HE3	2	0.37
(1,2556)	1:183:A:LEU:HD21	1:125:A:TRP:HE3	3	0.37
(1,2556)	1:183:A:LEU:HD22	1:125:A:TRP:HE3	3	0.37
(1,2556)	1:183:A:LEU:HD23	1:125:A:TRP:HE3	3	0.37
(1,2454)	1:147:A:LEU:HD21	1:150:A:PHE:HE1	4	0.37
(1,2454)	1:147:A:LEU:HD21	1:150:A:PHE:HE2	4	0.37
(1,2454)	1:147:A:LEU:HD22	1:150:A:PHE:HE1	4	0.37
(1,2454)	1:147:A:LEU:HD22	1:150:A:PHE:HE2	4	0.37
(1,2454)	1:147:A:LEU:HD23	1:150:A:PHE:HE1	4	0.37
(1,2454)	1:147:A:LEU:HD23	1:150:A:PHE:HE2	4	0.37
(1,2433)	1:97:A:LEU:HD11	1:93:A:PHE:HE1	3	0.37
(1,2433)	1:97:A:LEU:HD11	1:93:A:PHE:HE2	3	0.37
(1,2433)	1:97:A:LEU:HD12	1:93:A:PHE:HE1	3	0.37
(1,2433)	1:97:A:LEU:HD12	1:93:A:PHE:HE2	3	0.37
(1,2433)	1:97:A:LEU:HD13	1:93:A:PHE:HE1	3	0.37
(1,2433)	1:97:A:LEU:HD13	1:93:A:PHE:HE2	3	0.37
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB1	11	0.37
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB2	11	0.37
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB3	11	0.37
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB1	11	0.37
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB2	11	0.37
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB3	11	0.37
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB1	11	0.37
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB2	11	0.37
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB3	11	0.37
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	12	0.37
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	12	0.37
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	12	0.37
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	5	0.37
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	5	0.37
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	5	0.37
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	9	0.37
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	9	0.37
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD11	9	0.37
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD12	9	0.37
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD13	9	0.37
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD11	14	0.37
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD12	14	0.37
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD13	14	0.37
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG21	1	0.37
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG22	1	0.37
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG23	1	0.37
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	15	0.37
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	15	0.37
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	15	0.37
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	18	0.37
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	18	0.37
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	18	0.37
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD11	4	0.37
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD12	4	0.37
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD13	4	0.37
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD11	10	0.37
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD12	10	0.37
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD13	10	0.37
(1,1730)	1:144:A:GLN:H	1:145:A:HIS:HB3	5	0.37
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	15	0.37
(1,1032)	1:131:A:LEU:HD21	1:115:A:ALA:HA	18	0.37
(1,1032)	1:131:A:LEU:HD22	1:115:A:ALA:HA	18	0.37
(1,1032)	1:131:A:LEU:HD23	1:115:A:ALA:HA	18	0.37
(1,1029)	1:147:A:LEU:HD21	1:104:A:ALA:HA	13	0.37
(1,1029)	1:147:A:LEU:HD22	1:104:A:ALA:HA	13	0.37
(1,1029)	1:147:A:LEU:HD23	1:104:A:ALA:HA	13	0.37
(1,874)	1:63:A:LEU:HD21	1:36:A:ARG:HA	15	0.37
(1,874)	1:63:A:LEU:HD22	1:36:A:ARG:HA	15	0.37
(1,874)	1:63:A:LEU:HD23	1:36:A:ARG:HA	15	0.37
(1,839)	1:63:A:LEU:HB3	1:62:A:THR:HA	9	0.37
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	5	0.37
(1,190)	1:183:A:LEU:HD21	1:125:A:TRP:H	3	0.37
(1,190)	1:183:A:LEU:HD22	1:125:A:TRP:H	3	0.37
(1,190)	1:183:A:LEU:HD23	1:125:A:TRP:H	3	0.37
(1,171)	1:162:A:MET:HB3	1:161:A:PHE:H	1	0.37
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	20	0.37
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	20	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	20	0.37
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	20	0.36
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	20	0.36
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	8	0.36
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	14	0.36
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	18	0.36
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	6	0.36
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	2	0.36
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	12	0.36
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	20	0.36
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	11	0.36
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	9	0.36
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	11	0.36
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	15	0.36
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	13	0.36
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	15	0.36
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	18	0.36
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	1	0.36
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	1	0.36
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	1	0.36
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	1	0.36
(1,3021)	1:114:A:ILE:HG21	2:86:B:ILE:HB	1	0.36
(1,3021)	1:114:A:ILE:HG22	2:86:B:ILE:HB	1	0.36
(1,3021)	1:114:A:ILE:HG23	2:86:B:ILE:HB	1	0.36
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	5	0.36
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	5	0.36
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	20	0.36
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	20	0.36
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	16	0.36
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	16	0.36
(1,2443)	1:153:A:GLN:HB3	1:150:A:PHE:HE1	2	0.36
(1,2443)	1:153:A:GLN:HB3	1:150:A:PHE:HE2	2	0.36
(1,2433)	1:97:A:LEU:HD11	1:93:A:PHE:HE1	20	0.36
(1,2433)	1:97:A:LEU:HD11	1:93:A:PHE:HE2	20	0.36
(1,2433)	1:97:A:LEU:HD12	1:93:A:PHE:HE1	20	0.36
(1,2433)	1:97:A:LEU:HD12	1:93:A:PHE:HE2	20	0.36
(1,2433)	1:97:A:LEU:HD13	1:93:A:PHE:HE1	20	0.36
(1,2433)	1:97:A:LEU:HD13	1:93:A:PHE:HE2	20	0.36
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	13	0.36
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	13	0.36
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	15	0.36
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	15	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	15	0.36
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	15	0.36
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	15	0.36
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	15	0.36
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	15	0.36
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	15	0.36
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	15	0.36
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	18	0.36
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	18	0.36
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	18	0.36
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	18	0.36
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	18	0.36
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	18	0.36
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	18	0.36
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	18	0.36
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	18	0.36
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	8	0.36
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	8	0.36
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	8	0.36
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG21	5	0.36
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG22	5	0.36
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG23	5	0.36
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	16	0.36
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	16	0.36
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	16	0.36
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD11	3	0.36
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD12	3	0.36
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD13	3	0.36
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD11	4	0.36
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD12	4	0.36
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD13	4	0.36
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD11	6	0.36
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD12	6	0.36
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD13	6	0.36
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD11	12	0.36
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD12	12	0.36
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD13	12	0.36
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD11	17	0.36
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD12	17	0.36
(1,1988)	1:118:A:LEU:HA	1:118:A:LEU:HD13	17	0.36
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	19	0.36
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	19	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	19	0.36
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD11	12	0.36
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD12	12	0.36
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD13	12	0.36
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	9	0.36
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD11	12	0.36
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD12	12	0.36
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD13	12	0.36
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD11	12	0.36
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD12	12	0.36
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD13	12	0.36
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD11	12	0.36
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD12	12	0.36
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD13	12	0.36
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD11	19	0.36
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD12	19	0.36
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD13	19	0.36
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD11	19	0.36
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD12	19	0.36
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD13	19	0.36
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD11	19	0.36
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD12	19	0.36
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD13	19	0.36
(1,1709)	1:98:A:GLN:HE22	1:98:A:GLN:HB3	17	0.36
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	11	0.36
(1,1027)	1:27:A:VAL:HG21	1:168:A:ALA:HA	2	0.36
(1,1027)	1:27:A:VAL:HG22	1:168:A:ALA:HA	2	0.36
(1,1027)	1:27:A:VAL:HG23	1:168:A:ALA:HA	2	0.36
(1,1016)	1:183:A:LEU:HD11	1:183:A:LEU:HA	1	0.36
(1,1016)	1:183:A:LEU:HD12	1:183:A:LEU:HA	1	0.36
(1,1016)	1:183:A:LEU:HD13	1:183:A:LEU:HA	1	0.36
(1,934)	1:159:A:VAL:HG11	1:156:A:ARG:HA	11	0.36
(1,934)	1:159:A:VAL:HG12	1:156:A:ARG:HA	11	0.36
(1,934)	1:159:A:VAL:HG13	1:156:A:ARG:HA	11	0.36
(1,934)	1:159:A:VAL:HG11	1:156:A:ARG:HA	19	0.36
(1,934)	1:159:A:VAL:HG12	1:156:A:ARG:HA	19	0.36
(1,934)	1:159:A:VAL:HG13	1:156:A:ARG:HA	19	0.36
(1,896)	1:142:A:VAL:HG21	1:103:A:THR:HA	1	0.36
(1,896)	1:142:A:VAL:HG22	1:103:A:THR:HA	1	0.36
(1,896)	1:142:A:VAL:HG23	1:103:A:THR:HA	1	0.36
(1,648)	1:159:A:VAL:HG21	1:159:A:VAL:HA	5	0.36
(1,648)	1:159:A:VAL:HG22	1:159:A:VAL:HA	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,648)	1:159:A:VAL:HG23	1:159:A:VAL:HA	5	0.36
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	19	0.36
(1,513)	1:150:A:PHE:HA	1:153:A:GLN:HE22	12	0.36
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	7	0.36
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	13	0.36
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	15	0.36
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	15	0.36
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	15	0.36
(1,74)	1:63:A:LEU:HD11	1:65:A:LEU:H	1	0.36
(1,74)	1:63:A:LEU:HD12	1:65:A:LEU:H	1	0.36
(1,74)	1:63:A:LEU:HD13	1:65:A:LEU:H	1	0.36
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	2	0.36
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	2	0.36
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	2	0.36
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	9	0.36
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	9	0.36
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	9	0.36
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	2	0.35
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	4	0.35
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	15	0.35
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	3	0.35
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	6	0.35
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	4	0.35
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	16	0.35
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	17	0.35
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	19	0.35
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	10	0.35
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	11	0.35
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	16	0.35
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	5	0.35
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	8	0.35
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	15	0.35
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	16	0.35
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	18	0.35
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	2	0.35
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	7	0.35
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	10	0.35
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	17	0.35
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	5	0.35
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	8	0.35
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	14	0.35
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	20	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	5	0.35
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	5	0.35
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	5	0.35
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	5	0.35
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE1	20	0.35
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE2	20	0.35
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	8	0.35
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	8	0.35
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	8	0.35
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	8	0.35
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	8	0.35
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	8	0.35
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	8	0.35
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	8	0.35
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	8	0.35
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG11	6	0.35
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG12	6	0.35
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG13	6	0.35
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG21	3	0.35
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG22	3	0.35
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG23	3	0.35
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG21	3	0.35
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG22	3	0.35
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG23	3	0.35
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	9	0.35
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	9	0.35
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	9	0.35
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	9	0.35
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	9	0.35
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	9	0.35
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	9	0.35
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	9	0.35
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	9	0.35
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	16	0.35
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	16	0.35
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	16	0.35
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD21	20	0.35
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD22	20	0.35
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD23	20	0.35
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD11	9	0.35
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD12	9	0.35
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD13	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD11	9	0.35
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD12	9	0.35
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD13	9	0.35
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD11	9	0.35
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD12	9	0.35
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD13	9	0.35
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD11	9	0.35
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD12	9	0.35
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD13	9	0.35
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD11	9	0.35
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD12	9	0.35
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD13	9	0.35
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD11	9	0.35
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD12	9	0.35
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD13	9	0.35
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	11	0.35
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	16	0.35
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	11	0.35
(1,1395)	1:46:A:GLU:H	1:46:A:GLU:HG3	11	0.35
(1,1032)	1:131:A:LEU:HD21	1:115:A:ALA:HA	12	0.35
(1,1032)	1:131:A:LEU:HD22	1:115:A:ALA:HA	12	0.35
(1,1032)	1:131:A:LEU:HD23	1:115:A:ALA:HA	12	0.35
(1,543)	1:181:A:LEU:HD11	1:73:A:GLN:HE21	1	0.35
(1,543)	1:181:A:LEU:HD12	1:73:A:GLN:HE21	1	0.35
(1,543)	1:181:A:LEU:HD13	1:73:A:GLN:HE21	1	0.35
(1,542)	1:172:A:ALA:HB1	1:173:A:GLN:HE22	20	0.35
(1,542)	1:172:A:ALA:HB2	1:173:A:GLN:HE22	20	0.35
(1,542)	1:172:A:ALA:HB3	1:173:A:GLN:HE22	20	0.35
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	7	0.35
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	7	0.35
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	7	0.35
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	8	0.35
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	8	0.35
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	8	0.35
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	17	0.35
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	17	0.35
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	17	0.35
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	18	0.34
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	3	0.34
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	2	0.34
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	11	0.34
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	15	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	19	0.34
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	1	0.34
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	6	0.34
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	9	0.34
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	10	0.34
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	17	0.34
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	19	0.34
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	13	0.34
(2,129)	1:28:A:ALA:O	1:32:A:GLU:N	7	0.34
(1,3011)	1:100:A:LEU:HD21	2:82:B:ILE:HD11	8	0.34
(1,3011)	1:100:A:LEU:HD21	2:82:B:ILE:HD12	8	0.34
(1,3011)	1:100:A:LEU:HD21	2:82:B:ILE:HD13	8	0.34
(1,3011)	1:100:A:LEU:HD22	2:82:B:ILE:HD11	8	0.34
(1,3011)	1:100:A:LEU:HD22	2:82:B:ILE:HD12	8	0.34
(1,3011)	1:100:A:LEU:HD22	2:82:B:ILE:HD13	8	0.34
(1,3011)	1:100:A:LEU:HD23	2:82:B:ILE:HD11	8	0.34
(1,3011)	1:100:A:LEU:HD23	2:82:B:ILE:HD12	8	0.34
(1,3011)	1:100:A:LEU:HD23	2:82:B:ILE:HD13	8	0.34
(1,2593)	1:55:A:PRO:HD3	1:136:A:TYR:HE1	12	0.34
(1,2593)	1:55:A:PRO:HD3	1:136:A:TYR:HE2	12	0.34
(1,2354)	1:76:A:ARG:HB3	1:41:A:TYR:HD1	18	0.34
(1,2354)	1:76:A:ARG:HB3	1:41:A:TYR:HD2	18	0.34
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB1	16	0.34
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB2	16	0.34
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB3	16	0.34
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB1	16	0.34
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB2	16	0.34
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB3	16	0.34
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB1	16	0.34
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB2	16	0.34
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB3	16	0.34
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG21	14	0.34
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG22	14	0.34
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG23	14	0.34
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG21	18	0.34
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG22	18	0.34
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG23	18	0.34
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG11	10	0.34
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG12	10	0.34
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG13	10	0.34
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG11	10	0.34
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG12	10	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG13	10	0.34
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	11	0.34
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	11	0.34
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	11	0.34
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	3	0.34
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	3	0.34
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	3	0.34
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	7	0.34
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	7	0.34
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	7	0.34
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	9	0.34
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	9	0.34
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	9	0.34
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	13	0.34
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	13	0.34
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	13	0.34
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD21	2	0.34
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD22	2	0.34
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD23	2	0.34
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD11	9	0.34
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD12	9	0.34
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD13	9	0.34
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD11	2	0.34
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD12	2	0.34
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD13	2	0.34
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD11	6	0.34
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD12	6	0.34
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD13	6	0.34
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	5	0.34
(1,1764)	1:19:A:LEU:HA	1:19:A:LEU:HG	7	0.34
(1,1750)	1:142:A:VAL:HG21	1:102:A:PRO:HG3	6	0.34
(1,1750)	1:142:A:VAL:HG22	1:102:A:PRO:HG3	6	0.34
(1,1750)	1:142:A:VAL:HG23	1:102:A:PRO:HG3	6	0.34
(1,1740)	1:63:A:LEU:HD11	1:64:A:PRO:HG3	4	0.34
(1,1740)	1:63:A:LEU:HD12	1:64:A:PRO:HG3	4	0.34
(1,1740)	1:63:A:LEU:HD13	1:64:A:PRO:HG3	4	0.34
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	5	0.34
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	5	0.34
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	5	0.34
(1,1050)	1:19:A:LEU:HD21	1:19:A:LEU:HA	7	0.34
(1,1050)	1:19:A:LEU:HD22	1:19:A:LEU:HA	7	0.34
(1,1050)	1:19:A:LEU:HD23	1:19:A:LEU:HA	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1032)	1:131:A:LEU:HD21	1:115:A:ALA:HA	15	0.34
(1,1032)	1:131:A:LEU:HD22	1:115:A:ALA:HA	15	0.34
(1,1032)	1:131:A:LEU:HD23	1:115:A:ALA:HA	15	0.34
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	15	0.34
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	13	0.34
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	13	0.34
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	13	0.34
(1,171)	1:162:A:MET:HB3	1:161:A:PHE:H	10	0.34
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	12	0.34
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	12	0.34
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	12	0.34
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	14	0.34
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	14	0.34
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	14	0.34
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	3	0.33
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	6	0.33
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	17	0.33
(2,159)	1:158:A:VAL:O	1:162:A:MET:N	4	0.33
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	5	0.33
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	10	0.33
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	15	0.33
(2,149)	1:112:A:THR:O	1:116:A:THR:N	3	0.33
(2,149)	1:112:A:THR:O	1:116:A:THR:N	4	0.33
(2,149)	1:112:A:THR:O	1:116:A:THR:N	5	0.33
(2,149)	1:112:A:THR:O	1:116:A:THR:N	14	0.33
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	5	0.33
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	8	0.33
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	14	0.33
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	20	0.33
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	3	0.33
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	6	0.33
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	7	0.33
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	12	0.33
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	13	0.33
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	18	0.33
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	9	0.33
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	15	0.33
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	2	0.33
(1,3011)	1:100:A:LEU:HD21	2:82:B:ILE:HD11	6	0.33
(1,3011)	1:100:A:LEU:HD21	2:82:B:ILE:HD12	6	0.33
(1,3011)	1:100:A:LEU:HD21	2:82:B:ILE:HD13	6	0.33
(1,3011)	1:100:A:LEU:HD22	2:82:B:ILE:HD11	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3011)	1:100:A:LEU:HD22	2:82:B:ILE:HD12	6	0.33
(1,3011)	1:100:A:LEU:HD22	2:82:B:ILE:HD13	6	0.33
(1,3011)	1:100:A:LEU:HD23	2:82:B:ILE:HD11	6	0.33
(1,3011)	1:100:A:LEU:HD23	2:82:B:ILE:HD12	6	0.33
(1,3011)	1:100:A:LEU:HD23	2:82:B:ILE:HD13	6	0.33
(1,3011)	1:100:A:LEU:HD21	2:82:B:ILE:HD11	16	0.33
(1,3011)	1:100:A:LEU:HD21	2:82:B:ILE:HD12	16	0.33
(1,3011)	1:100:A:LEU:HD21	2:82:B:ILE:HD13	16	0.33
(1,3011)	1:100:A:LEU:HD22	2:82:B:ILE:HD11	16	0.33
(1,3011)	1:100:A:LEU:HD22	2:82:B:ILE:HD12	16	0.33
(1,3011)	1:100:A:LEU:HD22	2:82:B:ILE:HD13	16	0.33
(1,3011)	1:100:A:LEU:HD23	2:82:B:ILE:HD11	16	0.33
(1,3011)	1:100:A:LEU:HD23	2:82:B:ILE:HD12	16	0.33
(1,3011)	1:100:A:LEU:HD23	2:82:B:ILE:HD13	16	0.33
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	1	0.33
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	1	0.33
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	11	0.33
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	11	0.33
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	17	0.33
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	17	0.33
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	18	0.33
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	18	0.33
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	7	0.33
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	7	0.33
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	7	0.33
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG11	7	0.33
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG12	7	0.33
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG13	7	0.33
(1,1995)	1:97:A:LEU:HA	1:100:A:LEU:HD21	9	0.33
(1,1995)	1:97:A:LEU:HA	1:100:A:LEU:HD22	9	0.33
(1,1995)	1:97:A:LEU:HA	1:100:A:LEU:HD23	9	0.33
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG21	5	0.33
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG22	5	0.33
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG23	5	0.33
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG21	5	0.33
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG22	5	0.33
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG23	5	0.33
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD21	15	0.33
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD22	15	0.33
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD23	15	0.33
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	7	0.33
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	7	0.33
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	8	0.33
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	8	0.33
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	8	0.33
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	10	0.33
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	10	0.33
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	10	0.33
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD11	15	0.33
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD12	15	0.33
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD13	15	0.33
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD11	15	0.33
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD12	15	0.33
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD13	15	0.33
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD11	15	0.33
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD12	15	0.33
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD13	15	0.33
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD11	15	0.33
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD12	15	0.33
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD13	15	0.33
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD11	15	0.33
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD12	15	0.33
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD13	15	0.33
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD11	15	0.33
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD12	15	0.33
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD13	15	0.33
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD11	18	0.33
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD12	18	0.33
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD13	18	0.33
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD11	17	0.33
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD12	17	0.33
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD13	17	0.33
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	1	0.33
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	2	0.33
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	3	0.33
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	4	0.33
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	19	0.33
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	19	0.33
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	19	0.33
(1,1395)	1:46:A:GLU:H	1:46:A:GLU:HG3	18	0.33
(1,1326)	1:182:A:ASN:H	1:182:A:ASN:HB3	3	0.33
(1,1326)	1:182:A:ASN:H	1:182:A:ASN:HB3	11	0.33
(1,1326)	1:182:A:ASN:H	1:182:A:ASN:HB3	15	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1326)	1:182:A:ASN:H	1:182:A:ASN:HB3	19	0.33
(1,1249)	1:86:A:ASN:HD22	1:42:A:ARG:HD3	2	0.33
(1,934)	1:159:A:VAL:HG11	1:156:A:ARG:HA	14	0.33
(1,934)	1:159:A:VAL:HG12	1:156:A:ARG:HA	14	0.33
(1,934)	1:159:A:VAL:HG13	1:156:A:ARG:HA	14	0.33
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	5	0.33
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	5	0.33
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	5	0.33
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	7	0.32
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	10	0.32
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	11	0.32
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	13	0.32
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	1	0.32
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	7	0.32
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	14	0.32
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	2	0.32
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	20	0.32
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	13	0.32
(2,153)	1:134:A:PHE:O	1:138:A:LEU:N	19	0.32
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	9	0.32
(2,149)	1:112:A:THR:O	1:116:A:THR:N	16	0.32
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	1	0.32
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	9	0.32
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	11	0.32
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	15	0.32
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	19	0.32
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	1	0.32
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	12	0.32
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	8	0.32
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	12	0.32
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	18	0.32
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	7	0.32
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	8	0.32
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	9	0.32
(2,132)	1:32:A:GLU:O	1:36:A:ARG:N	8	0.32
(2,130)	1:30:A:ASP:O	1:34:A:VAL:N	18	0.32
(1,3011)	1:100:A:LEU:HD21	2:82:B:ILE:HD11	11	0.32
(1,3011)	1:100:A:LEU:HD21	2:82:B:ILE:HD12	11	0.32
(1,3011)	1:100:A:LEU:HD21	2:82:B:ILE:HD13	11	0.32
(1,3011)	1:100:A:LEU:HD22	2:82:B:ILE:HD11	11	0.32
(1,3011)	1:100:A:LEU:HD22	2:82:B:ILE:HD12	11	0.32
(1,3011)	1:100:A:LEU:HD22	2:82:B:ILE:HD13	11	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3011)	1:100:A:LEU:HD23	2:82:B:ILE:HD11	11	0.32
(1,3011)	1:100:A:LEU:HD23	2:82:B:ILE:HD12	11	0.32
(1,3011)	1:100:A:LEU:HD23	2:82:B:ILE:HD13	11	0.32
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	1	0.32
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	1	0.32
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	1	0.32
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	4	0.32
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	4	0.32
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	10	0.32
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	10	0.32
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	15	0.32
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	15	0.32
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	19	0.32
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	19	0.32
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	4	0.32
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	4	0.32
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	17	0.32
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	17	0.32
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	17	0.32
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	17	0.32
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB1	9	0.32
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB2	9	0.32
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB3	9	0.32
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB1	9	0.32
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB2	9	0.32
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB3	9	0.32
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB1	9	0.32
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB2	9	0.32
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB3	9	0.32
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG11	18	0.32
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG12	18	0.32
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG13	18	0.32
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG21	5	0.32
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG22	5	0.32
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG23	5	0.32
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG21	5	0.32
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG22	5	0.32
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG23	5	0.32
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG21	20	0.32
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG22	20	0.32
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG23	20	0.32
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG21	20	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG22	20	0.32
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG23	20	0.32
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	8	0.32
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	8	0.32
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	8	0.32
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	2	0.32
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	2	0.32
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	2	0.32
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	12	0.32
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	12	0.32
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	12	0.32
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	20	0.32
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	20	0.32
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	20	0.32
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD11	18	0.32
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD12	18	0.32
(1,1869)	1:181:A:LEU:H	1:181:A:LEU:HD13	18	0.32
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	13	0.32
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	19	0.32
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	1	0.32
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	18	0.32
(1,1326)	1:182:A:ASN:H	1:182:A:ASN:HB3	4	0.32
(1,1326)	1:182:A:ASN:H	1:182:A:ASN:HB3	6	0.32
(1,1326)	1:182:A:ASN:H	1:182:A:ASN:HB3	9	0.32
(1,1071)	1:66:A:GLN:HE22	1:67:A:PRO:HD3	2	0.32
(1,994)	1:50:A:GLU:HG3	1:50:A:GLU:HA	8	0.32
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	20	0.32
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	10	0.32
(1,410)	1:94:A:GLN:HE22	1:95:A:THR:H	14	0.32
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	8	0.32
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	8	0.32
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	8	0.32
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	1	0.32
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	8	0.31
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	12	0.31
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	12	0.31
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	1	0.31
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	7	0.31
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	14	0.31
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	18	0.31
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	19	0.31
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,153)	1:134:A:PHE:O	1:138:A:LEU:N	1	0.31
(2,153)	1:134:A:PHE:O	1:138:A:LEU:N	6	0.31
(2,153)	1:134:A:PHE:O	1:138:A:LEU:N	16	0.31
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	6	0.31
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	14	0.31
(2,149)	1:112:A:THR:O	1:116:A:THR:N	9	0.31
(2,149)	1:112:A:THR:O	1:116:A:THR:N	10	0.31
(2,149)	1:112:A:THR:O	1:116:A:THR:N	11	0.31
(2,149)	1:112:A:THR:O	1:116:A:THR:N	17	0.31
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	16	0.31
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	20	0.31
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	5	0.31
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	13	0.31
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	1	0.31
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	10	0.31
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	11	0.31
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	1	0.31
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	16	0.31
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	19	0.31
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	5	0.31
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	7	0.31
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	12	0.31
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	13	0.31
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	8	0.31
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	8	0.31
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	8	0.31
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	7	0.31
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	7	0.31
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	13	0.31
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	13	0.31
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	14	0.31
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	14	0.31
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE1	13	0.31
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE2	13	0.31
(1,2433)	1:97:A:LEU:HD11	1:93:A:PHE:HE1	7	0.31
(1,2433)	1:97:A:LEU:HD11	1:93:A:PHE:HE2	7	0.31
(1,2433)	1:97:A:LEU:HD12	1:93:A:PHE:HE1	7	0.31
(1,2433)	1:97:A:LEU:HD12	1:93:A:PHE:HE2	7	0.31
(1,2433)	1:97:A:LEU:HD13	1:93:A:PHE:HE1	7	0.31
(1,2433)	1:97:A:LEU:HD13	1:93:A:PHE:HE2	7	0.31
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	1	0.31
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	1	0.31
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	1	0.31
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	1	0.31
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	1	0.31
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	1	0.31
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	1	0.31
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	1	0.31
(1,2223)	1:26:A:GLN:HG3	1:172:A:ALA:HB1	4	0.31
(1,2223)	1:26:A:GLN:HG3	1:172:A:ALA:HB2	4	0.31
(1,2223)	1:26:A:GLN:HG3	1:172:A:ALA:HB3	4	0.31
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB1	6	0.31
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB2	6	0.31
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB3	6	0.31
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB1	6	0.31
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB2	6	0.31
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB3	6	0.31
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB1	6	0.31
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB2	6	0.31
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB3	6	0.31
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	18	0.31
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	18	0.31
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	18	0.31
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	7	0.31
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	7	0.31
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	7	0.31
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG21	3	0.31
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG22	3	0.31
(1,2069)	1:163:A:LEU:HD11	1:159:A:VAL:HG23	3	0.31
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG21	3	0.31
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG22	3	0.31
(1,2069)	1:163:A:LEU:HD12	1:159:A:VAL:HG23	3	0.31
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG21	3	0.31
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG22	3	0.31
(1,2069)	1:163:A:LEU:HD13	1:159:A:VAL:HG23	3	0.31
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG21	3	0.31
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG22	3	0.31
(1,2069)	1:163:A:LEU:HD21	1:159:A:VAL:HG23	3	0.31
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG21	3	0.31
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG22	3	0.31
(1,2069)	1:163:A:LEU:HD22	1:159:A:VAL:HG23	3	0.31
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG21	3	0.31
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG22	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2069)	1:163:A:LEU:HD23	1:159:A:VAL:HG23	3	0.31
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	6	0.31
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	6	0.31
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	6	0.31
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG21	20	0.31
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG22	20	0.31
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG23	20	0.31
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG21	20	0.31
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG22	20	0.31
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG23	20	0.31
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG21	10	0.31
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG22	10	0.31
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG23	10	0.31
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG21	10	0.31
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG22	10	0.31
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG23	10	0.31
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG21	10	0.31
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG22	10	0.31
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG23	10	0.31
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG21	14	0.31
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG22	14	0.31
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG23	14	0.31
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG21	14	0.31
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG22	14	0.31
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG23	14	0.31
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG21	14	0.31
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG22	14	0.31
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG23	14	0.31
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG11	1	0.31
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG12	1	0.31
(1,1911)	1:24:A:GLU:HA	1:27:A:VAL:HG13	1	0.31
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	10	0.31
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	14	0.31
(1,1794)	1:156:A:ARG:H	1:156:A:ARG:HG3	8	0.31
(1,1750)	1:142:A:VAL:HG21	1:102:A:PRO:HG3	8	0.31
(1,1750)	1:142:A:VAL:HG22	1:102:A:PRO:HG3	8	0.31
(1,1750)	1:142:A:VAL:HG23	1:102:A:PRO:HG3	8	0.31
(1,1495)	1:153:A:GLN:H	1:153:A:GLN:HG3	13	0.31
(1,1326)	1:182:A:ASN:H	1:182:A:ASN:HB3	12	0.31
(1,1128)	1:155:A:THR:HB	1:152:A:GLY:HA3	17	0.31
(1,1027)	1:27:A:VAL:HG21	1:168:A:ALA:HA	6	0.31
(1,1027)	1:27:A:VAL:HG22	1:168:A:ALA:HA	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1027)	1:27:A:VAL:HG23	1:168:A:ALA:HA	6	0.31
(1,845)	1:63:A:LEU:HD11	1:37:A:SER:HA	10	0.31
(1,845)	1:63:A:LEU:HD12	1:37:A:SER:HA	10	0.31
(1,845)	1:63:A:LEU:HD13	1:37:A:SER:HA	10	0.31
(1,732)	1:66:A:GLN:HG3	1:69:A:SER:HB3	8	0.31
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	11	0.31
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	14	0.31
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	9	0.31
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	9	0.31
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	9	0.31
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	3	0.31
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	4	0.31
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	17	0.31
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	7	0.31
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	7	0.31
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	7	0.31
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	13	0.31
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	13	0.31
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	13	0.31
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	10	0.3
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	1	0.3
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	14	0.3
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	17	0.3
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	5	0.3
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	11	0.3
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	12	0.3
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	13	0.3
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	4	0.3
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	9	0.3
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	11	0.3
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	16	0.3
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	17	0.3
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	8	0.3
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	11	0.3
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	1	0.3
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	8	0.3
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	17	0.3
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	18	0.3
(2,149)	1:112:A:THR:O	1:116:A:THR:N	19	0.3
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	2	0.3
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	4	0.3
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	13	0.3
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	17	0.3
(2,147)	1:110:A:TYR:O	1:114:A:ILE:N	5	0.3
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	9	0.3
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	6	0.3
(2,139)	1:40:A:PHE:O	1:44:A:GLN:N	20	0.3
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	15	0.3
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	2	0.3
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	14	0.3
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	20	0.3
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	11	0.3
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	13	0.3
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	15	0.3
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	14	0.3
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	3	0.3
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	3	0.3
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	18	0.3
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	18	0.3
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	6	0.3
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	6	0.3
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB1	1	0.3
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB2	1	0.3
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB3	1	0.3
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB1	1	0.3
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB2	1	0.3
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB3	1	0.3
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB1	1	0.3
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB2	1	0.3
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB3	1	0.3
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG21	15	0.3
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG22	15	0.3
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG23	15	0.3
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG11	14	0.3
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG12	14	0.3
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG13	14	0.3
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD11	4	0.3
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD12	4	0.3
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD13	4	0.3
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	15	0.3
(1,1730)	1:144:A:GLN:H	1:145:A:HIS:HB3	4	0.3
(1,1495)	1:153:A:GLN:H	1:153:A:GLN:HG3	11	0.3
(1,1326)	1:182:A:ASN:H	1:182:A:ASN:HB3	16	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1156)	1:156:A:ARG:H	1:156:A:ARG:HD3	8	0.3
(1,1138)	1:52:A:VAL:HG11	1:51:A:GLY:HA3	3	0.3
(1,1138)	1:52:A:VAL:HG12	1:51:A:GLY:HA3	3	0.3
(1,1138)	1:52:A:VAL:HG13	1:51:A:GLY:HA3	3	0.3
(1,1138)	1:52:A:VAL:HG21	1:51:A:GLY:HA3	3	0.3
(1,1138)	1:52:A:VAL:HG22	1:51:A:GLY:HA3	3	0.3
(1,1138)	1:52:A:VAL:HG23	1:51:A:GLY:HA3	3	0.3
(1,1138)	1:52:A:VAL:HG11	1:51:A:GLY:HA3	8	0.3
(1,1138)	1:52:A:VAL:HG12	1:51:A:GLY:HA3	8	0.3
(1,1138)	1:52:A:VAL:HG13	1:51:A:GLY:HA3	8	0.3
(1,1138)	1:52:A:VAL:HG21	1:51:A:GLY:HA3	8	0.3
(1,1138)	1:52:A:VAL:HG22	1:51:A:GLY:HA3	8	0.3
(1,1138)	1:52:A:VAL:HG23	1:51:A:GLY:HA3	8	0.3
(1,1050)	1:19:A:LEU:HD21	1:19:A:LEU:HA	2	0.3
(1,1050)	1:19:A:LEU:HD22	1:19:A:LEU:HA	2	0.3
(1,1050)	1:19:A:LEU:HD23	1:19:A:LEU:HA	2	0.3
(1,1050)	1:19:A:LEU:HD21	1:19:A:LEU:HA	13	0.3
(1,1050)	1:19:A:LEU:HD22	1:19:A:LEU:HA	13	0.3
(1,1050)	1:19:A:LEU:HD23	1:19:A:LEU:HA	13	0.3
(1,390)	1:63:A:LEU:HD11	1:36:A:ARG:H	18	0.3
(1,390)	1:63:A:LEU:HD12	1:36:A:ARG:H	18	0.3
(1,390)	1:63:A:LEU:HD13	1:36:A:ARG:H	18	0.3
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	16	0.3
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	10	0.3
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	10	0.3
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	10	0.3
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	18	0.3
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	18	0.3
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	18	0.3
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	6	0.29
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	16	0.29
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	15	0.29
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	16	0.29
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	8	0.29
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	6	0.29
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	13	0.29
(2,153)	1:134:A:PHE:O	1:138:A:LEU:N	7	0.29
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	16	0.29
(2,149)	1:112:A:THR:O	1:116:A:THR:N	6	0.29
(2,149)	1:112:A:THR:O	1:116:A:THR:N	8	0.29
(2,149)	1:112:A:THR:O	1:116:A:THR:N	13	0.29
(2,149)	1:112:A:THR:O	1:116:A:THR:N	15	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,149)	1:112:A:THR:O	1:116:A:THR:N	20	0.29
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	6	0.29
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	10	0.29
(2,146)	1:107:A:ALA:O	1:111:A:PHE:N	17	0.29
(2,146)	1:107:A:ALA:O	1:111:A:PHE:N	18	0.29
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	2	0.29
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	16	0.29
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	13	0.29
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	14	0.29
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	14	0.29
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	14	0.29
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	14	0.29
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	15	0.29
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	15	0.29
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	15	0.29
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	15	0.29
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	15	0.29
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	15	0.29
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	15	0.29
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	2	0.29
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	2	0.29
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	6	0.29
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	6	0.29
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	12	0.29
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	12	0.29
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	13	0.29
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	13	0.29
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE1	11	0.29
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE2	11	0.29
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	3	0.29
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	3	0.29
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	3	0.29
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG11	14	0.29
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG12	14	0.29
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG13	14	0.29
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD11	2	0.29
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD12	2	0.29
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD13	2	0.29
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD11	3	0.29
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD12	3	0.29
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD13	3	0.29
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	10	0.29
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	10	0.29
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG11	10	0.29
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG12	10	0.29
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG13	10	0.29
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD21	9	0.29
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD22	9	0.29
(1,1895)	1:142:A:VAL:HB	1:147:A:LEU:HD23	9	0.29
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD11	4	0.29
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD12	4	0.29
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD13	4	0.29
(1,1842)	1:165:A:HIS:HA	1:166:A:CYS:HB3	6	0.29
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	8	0.29
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	12	0.29
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	17	0.29
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	20	0.29
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	5	0.29
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	6	0.29
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	8	0.29
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	14	0.29
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	16	0.29
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	19	0.29
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	14	0.29
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	14	0.29
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	14	0.29
(1,1027)	1:27:A:VAL:HG21	1:168:A:ALA:HA	12	0.29
(1,1027)	1:27:A:VAL:HG22	1:168:A:ALA:HA	12	0.29
(1,1027)	1:27:A:VAL:HG23	1:168:A:ALA:HA	12	0.29
(1,874)	1:63:A:LEU:HD21	1:36:A:ARG:HA	4	0.29
(1,874)	1:63:A:LEU:HD22	1:36:A:ARG:HA	4	0.29
(1,874)	1:63:A:LEU:HD23	1:36:A:ARG:HA	4	0.29
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	2	0.29
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	8	0.29
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	11	0.29
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	2	0.29
(1,123)	1:34:A:VAL:HG11	1:74:A:VAL:H	10	0.29
(1,123)	1:34:A:VAL:HG12	1:74:A:VAL:H	10	0.29
(1,123)	1:34:A:VAL:HG13	1:74:A:VAL:H	10	0.29
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	14	0.28
(2,159)	1:158:A:VAL:O	1:162:A:MET:N	6	0.28
(2,157)	1:153:A:GLN:O	1:157:A:PHE:N	13	0.28
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,155)	1:151:A:LEU:O	1:155:A:THR:N	8	0.28
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	3	0.28
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	11	0.28
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	14	0.28
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	17	0.28
(2,149)	1:112:A:THR:O	1:116:A:THR:N	1	0.28
(2,149)	1:112:A:THR:O	1:116:A:THR:N	2	0.28
(2,149)	1:112:A:THR:O	1:116:A:THR:N	7	0.28
(2,149)	1:112:A:THR:O	1:116:A:THR:N	18	0.28
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	20	0.28
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	14	0.28
(2,139)	1:40:A:PHE:O	1:44:A:GLN:N	9	0.28
(2,139)	1:40:A:PHE:O	1:44:A:GLN:N	13	0.28
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	4	0.28
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	7	0.28
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	18	0.28
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	1	0.28
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	4	0.28
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	17	0.28
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	9	0.28
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	15	0.28
(2,9)	1:28:A:ALA:O	1:32:A:GLU:H	20	0.28
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	19	0.28
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	19	0.28
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	19	0.28
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	19	0.28
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	16	0.28
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	16	0.28
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE1	11	0.28
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE2	11	0.28
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE1	11	0.28
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE2	11	0.28
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE1	11	0.28
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE2	11	0.28
(1,2496)	1:158:A:VAL:HG21	1:35:A:PHE:HZ	10	0.28
(1,2496)	1:158:A:VAL:HG22	1:35:A:PHE:HZ	10	0.28
(1,2496)	1:158:A:VAL:HG23	1:35:A:PHE:HZ	10	0.28
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	6	0.28
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	6	0.28
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	6	0.28
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	6	0.28
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	6	0.28
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	6	0.28
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	6	0.28
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	6	0.28
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG11	14	0.28
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG12	14	0.28
(1,2109)	1:147:A:LEU:HD21	1:142:A:VAL:HG13	14	0.28
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG11	14	0.28
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG12	14	0.28
(1,2109)	1:147:A:LEU:HD22	1:142:A:VAL:HG13	14	0.28
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG11	14	0.28
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG12	14	0.28
(1,2109)	1:147:A:LEU:HD23	1:142:A:VAL:HG13	14	0.28
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD11	4	0.28
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD12	4	0.28
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD13	4	0.28
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	8	0.28
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	8	0.28
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	8	0.28
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	19	0.28
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	19	0.28
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	19	0.28
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG11	13	0.28
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG12	13	0.28
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG13	13	0.28
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG11	12	0.28
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG12	12	0.28
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG13	12	0.28
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG21	2	0.28
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG22	2	0.28
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG23	2	0.28
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG21	13	0.28
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG22	13	0.28
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG23	13	0.28
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	12	0.28
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	12	0.28
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	12	0.28
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	12	0.28
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	12	0.28
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	12	0.28
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	12	0.28
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	12	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	12	0.28
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD21	18	0.28
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD22	18	0.28
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD23	18	0.28
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD21	7	0.28
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD22	7	0.28
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD23	7	0.28
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	5	0.28
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	5	0.28
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	5	0.28
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	8	0.28
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	8	0.28
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	8	0.28
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD11	19	0.28
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD12	19	0.28
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD13	19	0.28
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	3	0.28
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	4	0.28
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	9	0.28
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	12	0.28
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	15	0.28
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	17	0.28
(1,1766)	1:20:A:PRO:HD3	1:19:A:LEU:HG	20	0.28
(1,1663)	1:27:A:VAL:HG11	1:24:A:GLU:HB3	6	0.28
(1,1663)	1:27:A:VAL:HG12	1:24:A:GLU:HB3	6	0.28
(1,1663)	1:27:A:VAL:HG13	1:24:A:GLU:HB3	6	0.28
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	1	0.28
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	3	0.28
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	3	0.28
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	3	0.28
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	19	0.28
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	19	0.28
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	19	0.28
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	18	0.27
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	19	0.27
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	19	0.27
(2,159)	1:158:A:VAL:O	1:162:A:MET:N	2	0.27
(2,157)	1:153:A:GLN:O	1:157:A:PHE:N	1	0.27
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	18	0.27
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	3	0.27
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	4	0.27
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	14	0.27
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	18	0.27
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	12	0.27
(2,149)	1:112:A:THR:O	1:116:A:THR:N	12	0.27
(2,146)	1:107:A:ALA:O	1:111:A:PHE:N	15	0.27
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	6	0.27
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	14	0.27
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	3	0.27
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	7	0.27
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	17	0.27
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	10	0.27
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	3	0.27
(2,130)	1:30:A:ASP:O	1:34:A:VAL:N	19	0.27
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	1	0.27
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	2	0.27
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	6	0.27
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	10	0.27
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	16	0.27
(2,9)	1:28:A:ALA:O	1:32:A:GLU:H	6	0.27
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	12	0.27
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	12	0.27
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	12	0.27
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	12	0.27
(1,3097)	1:126:A:GLY:H	2:101:B:ILE:HG13	16	0.27
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG21	19	0.27
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG22	19	0.27
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG23	19	0.27
(1,2922)	2:92:B:MK8:HB1A	2:93:B:VAL:H	8	0.27
(1,2922)	2:92:B:MK8:HB1B	2:93:B:VAL:H	8	0.27
(1,2658)	2:89:B:HIS:HA	2:92:B:MK8:HB	1	0.27
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB1	9	0.27
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB2	9	0.27
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB3	9	0.27
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB1	9	0.27
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB2	9	0.27
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB3	9	0.27
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB1	9	0.27
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB2	9	0.27
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB3	9	0.27
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	17	0.27
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	17	0.27
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG21	2	0.27
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG22	2	0.27
(1,1986)	1:35:A:PHE:HD1	1:39:A:VAL:HG23	2	0.27
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG21	2	0.27
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG22	2	0.27
(1,1986)	1:35:A:PHE:HD2	1:39:A:VAL:HG23	2	0.27
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	11	0.27
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	11	0.27
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	11	0.27
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG21	11	0.27
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG22	11	0.27
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG23	11	0.27
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD21	5	0.27
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD22	5	0.27
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD23	5	0.27
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD21	20	0.27
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD22	20	0.27
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD23	20	0.27
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	6	0.27
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD11	3	0.27
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD12	3	0.27
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD13	3	0.27
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD11	3	0.27
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD12	3	0.27
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD13	3	0.27
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD11	3	0.27
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD12	3	0.27
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD13	3	0.27
(1,1709)	1:98:A:GLN:HE22	1:98:A:GLN:HB3	1	0.27
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	12	0.27
(1,1467)	1:61:A:VAL:HA	1:60:A:MET:HG3	17	0.27
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	6	0.27
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	18	0.27
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	2	0.27
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	13	0.27
(1,1043)	1:182:A:ASN:HB3	1:179:A:ALA:HA	9	0.27
(1,1027)	1:27:A:VAL:HG21	1:168:A:ALA:HA	5	0.27
(1,1027)	1:27:A:VAL:HG22	1:168:A:ALA:HA	5	0.27
(1,1027)	1:27:A:VAL:HG23	1:168:A:ALA:HA	5	0.27
(1,733)	1:26:A:GLN:HG3	1:23:A:SER:HB3	7	0.27
(1,607)	1:105:A:GLU:H	1:103:A:THR:HB	12	0.27
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	15	0.27
(1,190)	1:183:A:LEU:HD21	1:125:A:TRP:H	15	0.27
(1,190)	1:183:A:LEU:HD22	1:125:A:TRP:H	15	0.27
(1,190)	1:183:A:LEU:HD23	1:125:A:TRP:H	15	0.27
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	11	0.27
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	11	0.27
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	11	0.27
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	1	0.26
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	12	0.26
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	13	0.26
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	15	0.26
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	17	0.26
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	20	0.26
(2,158)	1:156:A:ARG:O	1:160:A:ASP:N	10	0.26
(2,157)	1:153:A:GLN:O	1:157:A:PHE:N	4	0.26
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	9	0.26
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	19	0.26
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	4	0.26
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	7	0.26
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	7	0.26
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	19	0.26
(2,139)	1:40:A:PHE:O	1:44:A:GLN:N	15	0.26
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	9	0.26
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	14	0.26
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	6	0.26
(2,130)	1:30:A:ASP:O	1:34:A:VAL:N	4	0.26
(2,130)	1:30:A:ASP:O	1:34:A:VAL:N	17	0.26
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	7	0.26
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	7	0.26
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	7	0.26
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	7	0.26
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	11	0.26
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	11	0.26
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	11	0.26
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	11	0.26
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	17	0.26
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	17	0.26
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	17	0.26
(1,2759)	2:82:B:ILE:H	2:82:B:ILE:HB	17	0.26
(1,2592)	1:55:A:PRO:HA	1:136:A:TYR:HE1	12	0.26
(1,2592)	1:55:A:PRO:HA	1:136:A:TYR:HE2	12	0.26
(1,2483)	1:147:A:LEU:HD21	1:150:A:PHE:HZ	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2483)	1:147:A:LEU:HD22	1:150:A:PHE:HZ	17	0.26
(1,2483)	1:147:A:LEU:HD23	1:150:A:PHE:HZ	17	0.26
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE1	18	0.26
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE2	18	0.26
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE1	18	0.26
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE2	18	0.26
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE1	18	0.26
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE2	18	0.26
(1,2201)	1:97:A:LEU:HA	1:96:A:MET:HE1	17	0.26
(1,2201)	1:97:A:LEU:HA	1:96:A:MET:HE2	17	0.26
(1,2201)	1:97:A:LEU:HA	1:96:A:MET:HE3	17	0.26
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB1	1	0.26
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB2	1	0.26
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB3	1	0.26
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB1	1	0.26
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB2	1	0.26
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB3	1	0.26
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB1	1	0.26
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB2	1	0.26
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB3	1	0.26
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG11	14	0.26
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG12	14	0.26
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG13	14	0.26
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG11	14	0.26
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG12	14	0.26
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG13	14	0.26
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD11	13	0.26
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD12	13	0.26
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD13	13	0.26
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	18	0.26
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	18	0.26
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	18	0.26
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	16	0.26
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	16	0.26
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	16	0.26
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	20	0.26
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	20	0.26
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	20	0.26
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	20	0.26
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	20	0.26
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	20	0.26
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	20	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	20	0.26
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	20	0.26
(1,1860)	1:131:A:LEU:HA	1:118:A:LEU:HD21	19	0.26
(1,1860)	1:131:A:LEU:HA	1:118:A:LEU:HD22	19	0.26
(1,1860)	1:131:A:LEU:HA	1:118:A:LEU:HD23	19	0.26
(1,1730)	1:144:A:GLN:H	1:145:A:HIS:HB3	13	0.26
(1,1663)	1:27:A:VAL:HG11	1:24:A:GLU:HB3	3	0.26
(1,1663)	1:27:A:VAL:HG12	1:24:A:GLU:HB3	3	0.26
(1,1663)	1:27:A:VAL:HG13	1:24:A:GLU:HB3	3	0.26
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	20	0.26
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	20	0.26
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	20	0.26
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	6	0.26
(1,1467)	1:61:A:VAL:HA	1:60:A:MET:HG3	16	0.26
(1,1439)	1:168:A:ALA:HB1	1:24:A:GLU:HG3	11	0.26
(1,1439)	1:168:A:ALA:HB2	1:24:A:GLU:HG3	11	0.26
(1,1439)	1:168:A:ALA:HB3	1:24:A:GLU:HG3	11	0.26
(1,1138)	1:52:A:VAL:HG11	1:51:A:GLY:HA3	5	0.26
(1,1138)	1:52:A:VAL:HG12	1:51:A:GLY:HA3	5	0.26
(1,1138)	1:52:A:VAL:HG13	1:51:A:GLY:HA3	5	0.26
(1,1138)	1:52:A:VAL:HG21	1:51:A:GLY:HA3	5	0.26
(1,1138)	1:52:A:VAL:HG22	1:51:A:GLY:HA3	5	0.26
(1,1138)	1:52:A:VAL:HG23	1:51:A:GLY:HA3	5	0.26
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	4	0.26
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	9	0.26
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	10	0.26
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	14	0.26
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	17	0.26
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	11	0.26
(1,611)	1:63:A:LEU:H	1:62:A:THR:HB	9	0.26
(1,611)	1:63:A:LEU:H	1:62:A:THR:HB	17	0.26
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	6	0.26
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	4	0.26
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	4	0.26
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	4	0.26
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	15	0.26
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	15	0.26
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	15	0.26
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	8	0.25
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	9	0.25
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	18	0.25
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	19	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	20	0.25
(2,159)	1:158:A:VAL:O	1:162:A:MET:N	20	0.25
(2,157)	1:153:A:GLN:O	1:157:A:PHE:N	11	0.25
(2,157)	1:153:A:GLN:O	1:157:A:PHE:N	16	0.25
(2,157)	1:153:A:GLN:O	1:157:A:PHE:N	17	0.25
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	1	0.25
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	3	0.25
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	13	0.25
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	16	0.25
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	17	0.25
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	4	0.25
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	15	0.25
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	2	0.25
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	15	0.25
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	18	0.25
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	3	0.25
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	8	0.25
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	16	0.25
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	8	0.25
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	10	0.25
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	17	0.25
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	18	0.25
(2,140)	1:78:A:LEU:O	1:82:A:GLY:N	19	0.25
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	17	0.25
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	13	0.25
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	15	0.25
(2,136)	1:37:A:SER:O	1:41:A:TYR:N	1	0.25
(2,133)	1:33:A:GLU:O	1:37:A:SER:N	20	0.25
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	3	0.25
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	4	0.25
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	5	0.25
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	12	0.25
(2,109)	1:155:A:THR:O	1:159:A:VAL:H	20	0.25
(2,11)	1:29:A:GLN:O	1:33:A:GLU:H	18	0.25
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	18	0.25
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	18	0.25
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	18	0.25
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD11	19	0.25
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD12	19	0.25
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD13	19	0.25
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD11	19	0.25
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD12	19	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD13	19	0.25
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD11	19	0.25
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD12	19	0.25
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD13	19	0.25
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	2	0.25
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	2	0.25
(1,2753)	2:90:B:LEU:HA	2:90:B:LEU:HD11	9	0.25
(1,2753)	2:90:B:LEU:HA	2:90:B:LEU:HD12	9	0.25
(1,2753)	2:90:B:LEU:HA	2:90:B:LEU:HD13	9	0.25
(1,2443)	1:153:A:GLN:HB3	1:150:A:PHE:HE1	19	0.25
(1,2443)	1:153:A:GLN:HB3	1:150:A:PHE:HE2	19	0.25
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE1	2	0.25
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE2	2	0.25
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE1	2	0.25
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE2	2	0.25
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE1	2	0.25
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE2	2	0.25
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD11	14	0.25
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD12	14	0.25
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD13	14	0.25
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	20	0.25
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	20	0.25
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	20	0.25
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	20	0.25
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	20	0.25
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	20	0.25
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	20	0.25
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	20	0.25
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	20	0.25
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	2	0.25
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	2	0.25
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	2	0.25
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	2	0.25
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	2	0.25
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	2	0.25
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	2	0.25
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	2	0.25
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	2	0.25
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	13	0.25
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	13	0.25
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	13	0.25
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	10	0.25
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	10	0.25
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	17	0.25
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	17	0.25
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	17	0.25
(1,1730)	1:144:A:GLN:H	1:145:A:HIS:HB3	12	0.25
(1,1497)	1:150:A:PHE:HB3	1:153:A:GLN:HG3	14	0.25
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	10	0.25
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	10	0.25
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	10	0.25
(1,1424)	1:163:A:LEU:HD11	1:25:A:GLU:HG3	6	0.25
(1,1424)	1:163:A:LEU:HD12	1:25:A:GLU:HG3	6	0.25
(1,1424)	1:163:A:LEU:HD13	1:25:A:GLU:HG3	6	0.25
(1,1424)	1:163:A:LEU:HD21	1:25:A:GLU:HG3	6	0.25
(1,1424)	1:163:A:LEU:HD22	1:25:A:GLU:HG3	6	0.25
(1,1424)	1:163:A:LEU:HD23	1:25:A:GLU:HG3	6	0.25
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	7	0.25
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	13	0.25
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	16	0.25
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	20	0.25
(1,994)	1:50:A:GLU:HG3	1:50:A:GLU:HA	5	0.25
(1,994)	1:50:A:GLU:HG3	1:50:A:GLU:HA	9	0.25
(1,994)	1:50:A:GLU:HG3	1:50:A:GLU:HA	10	0.25
(1,994)	1:50:A:GLU:HG3	1:50:A:GLU:HA	14	0.25
(1,994)	1:50:A:GLU:HG3	1:50:A:GLU:HA	17	0.25
(1,733)	1:26:A:GLN:HG3	1:23:A:SER:HB3	2	0.25
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	6	0.25
(1,268)	1:50:A:GLU:HB3	1:52:A:VAL:H	19	0.25
(1,190)	1:183:A:LEU:HD21	1:125:A:TRP:H	1	0.25
(1,190)	1:183:A:LEU:HD22	1:125:A:TRP:H	1	0.25
(1,190)	1:183:A:LEU:HD23	1:125:A:TRP:H	1	0.25
(1,65)	1:18:A:ALA:HA	1:19:A:LEU:H	2	0.25
(1,65)	1:18:A:ALA:HA	1:19:A:LEU:H	13	0.25
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	2	0.24
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	11	0.24
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	1	0.24
(2,161)	1:168:A:ALA:O	1:172:A:ALA:N	9	0.24
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	3	0.24
(2,159)	1:158:A:VAL:O	1:162:A:MET:N	15	0.24
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	9	0.24
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	20	0.24
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,146)	1:107:A:ALA:O	1:111:A:PHE:N	1	0.24
(2,146)	1:107:A:ALA:O	1:111:A:PHE:N	13	0.24
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	5	0.24
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	16	0.24
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	12	0.24
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	5	0.24
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	3	0.24
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	7	0.24
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	9	0.24
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	19	0.24
(2,130)	1:30:A:ASP:O	1:34:A:VAL:N	11	0.24
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	13	0.24
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	10	0.24
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	10	0.24
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	10	0.24
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	10	0.24
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	7	0.24
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	7	0.24
(1,2675)	2:82:B:ILE:HG21	2:83:B:ILE:H	7	0.24
(1,2675)	2:82:B:ILE:HG22	2:83:B:ILE:H	7	0.24
(1,2675)	2:82:B:ILE:HG23	2:83:B:ILE:H	7	0.24
(1,2559)	1:145:A:HIS:H	1:145:A:HIS:HD2	2	0.24
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD11	2	0.24
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD12	2	0.24
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD13	2	0.24
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD11	5	0.24
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD12	5	0.24
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD13	5	0.24
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD11	10	0.24
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD12	10	0.24
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD13	10	0.24
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD11	13	0.24
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD12	13	0.24
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD13	13	0.24
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG21	19	0.24
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG22	19	0.24
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG23	19	0.24
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	3	0.24
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	3	0.24
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	3	0.24
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG11	17	0.24
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG12	17	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG13	17	0.24
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG21	2	0.24
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG22	2	0.24
(1,1978)	1:35:A:PHE:HE1	1:39:A:VAL:HG23	2	0.24
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG21	2	0.24
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG22	2	0.24
(1,1978)	1:35:A:PHE:HE2	1:39:A:VAL:HG23	2	0.24
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	3	0.24
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	3	0.24
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	3	0.24
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	13	0.24
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	13	0.24
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	13	0.24
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	18	0.24
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	18	0.24
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	18	0.24
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG21	1	0.24
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG22	1	0.24
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG23	1	0.24
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG21	1	0.24
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG22	1	0.24
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG23	1	0.24
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG21	1	0.24
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG22	1	0.24
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG23	1	0.24
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	2	0.24
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	2	0.24
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	2	0.24
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	2	0.24
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	2	0.24
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	2	0.24
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	2	0.24
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	2	0.24
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	2	0.24
(1,1941)	1:104:A:ALA:H	1:147:A:LEU:HD11	13	0.24
(1,1941)	1:104:A:ALA:H	1:147:A:LEU:HD12	13	0.24
(1,1941)	1:104:A:ALA:H	1:147:A:LEU:HD13	13	0.24
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD21	15	0.24
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD22	15	0.24
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD23	15	0.24
(1,1842)	1:165:A:HIS:HA	1:166:A:CYS:HB3	17	0.24
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	18	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1730)	1:144:A:GLN:H	1:145:A:HIS:HB3	18	0.24
(1,1189)	1:159:A:VAL:HG11	1:156:A:ARG:HD3	15	0.24
(1,1189)	1:159:A:VAL:HG12	1:156:A:ARG:HD3	15	0.24
(1,1189)	1:159:A:VAL:HG13	1:156:A:ARG:HD3	15	0.24
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	2	0.24
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	15	0.24
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	18	0.24
(1,1043)	1:182:A:ASN:HB3	1:179:A:ALA:HA	16	0.24
(1,934)	1:159:A:VAL:HG11	1:156:A:ARG:HA	3	0.24
(1,934)	1:159:A:VAL:HG12	1:156:A:ARG:HA	3	0.24
(1,934)	1:159:A:VAL:HG13	1:156:A:ARG:HA	3	0.24
(1,896)	1:142:A:VAL:HG21	1:103:A:THR:HA	3	0.24
(1,896)	1:142:A:VAL:HG22	1:103:A:THR:HA	3	0.24
(1,896)	1:142:A:VAL:HG23	1:103:A:THR:HA	3	0.24
(1,531)	1:23:A:SER:H	1:26:A:GLN:HE22	7	0.24
(1,252)	1:51:A:GLY:HA3	1:52:A:VAL:H	19	0.24
(1,190)	1:183:A:LEU:HD21	1:125:A:TRP:H	16	0.24
(1,190)	1:183:A:LEU:HD22	1:125:A:TRP:H	16	0.24
(1,190)	1:183:A:LEU:HD23	1:125:A:TRP:H	16	0.24
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	8	0.24
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	3	0.23
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	7	0.23
(2,157)	1:153:A:GLN:O	1:157:A:PHE:N	9	0.23
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	15	0.23
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	17	0.23
(2,153)	1:134:A:PHE:O	1:138:A:LEU:N	20	0.23
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	13	0.23
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	13	0.23
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	20	0.23
(2,148)	1:111:A:PHE:O	1:115:A:ALA:N	7	0.23
(2,146)	1:107:A:ALA:O	1:111:A:PHE:N	9	0.23
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	17	0.23
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	12	0.23
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	2	0.23
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	1	0.23
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	8	0.23
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	9	0.23
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	12	0.23
(2,140)	1:78:A:LEU:O	1:82:A:GLY:N	1	0.23
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	6	0.23
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	11	0.23
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	17	0.23
(2,12)	1:29:A:GLN:O	1:33:A:GLU:N	18	0.23
(2,10)	1:28:A:ALA:O	1:32:A:GLU:N	6	0.23
(2,10)	1:28:A:ALA:O	1:32:A:GLU:N	20	0.23
(2,9)	1:28:A:ALA:O	1:32:A:GLU:H	2	0.23
(2,9)	1:28:A:ALA:O	1:32:A:GLU:H	12	0.23
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	13	0.23
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	13	0.23
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	13	0.23
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	13	0.23
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	7	0.23
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	7	0.23
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	7	0.23
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	19	0.23
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	19	0.23
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	19	0.23
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG21	10	0.23
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG22	10	0.23
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG23	10	0.23
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	6	0.23
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	6	0.23
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE1	15	0.23
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE2	15	0.23
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE1	15	0.23
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE2	15	0.23
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE1	15	0.23
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE2	15	0.23
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB1	12	0.23
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB2	12	0.23
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB3	12	0.23
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB1	12	0.23
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB2	12	0.23
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB3	12	0.23
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB1	12	0.23
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB2	12	0.23
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB3	12	0.23
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	10	0.23
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	10	0.23
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	10	0.23
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	10	0.23
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	10	0.23
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	10	0.23
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	10	0.23
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	10	0.23
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG21	8	0.23
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG22	8	0.23
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG23	8	0.23
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	15	0.23
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	15	0.23
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	15	0.23
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD11	14	0.23
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD12	14	0.23
(1,1872)	1:64:A:PRO:HD3	1:63:A:LEU:HD13	14	0.23
(1,1307)	2:93:B:VAL:HG21	1:89:A:TYR:HB3	6	0.23
(1,1307)	2:93:B:VAL:HG22	1:89:A:TYR:HB3	6	0.23
(1,1307)	2:93:B:VAL:HG23	1:89:A:TYR:HB3	6	0.23
(1,1307)	2:93:B:VAL:HG21	1:89:A:TYR:HB3	10	0.23
(1,1307)	2:93:B:VAL:HG22	1:89:A:TYR:HB3	10	0.23
(1,1307)	2:93:B:VAL:HG23	1:89:A:TYR:HB3	10	0.23
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	1	0.23
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	12	0.23
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	14	0.23
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	19	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	1	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	2	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	3	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	4	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	5	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	6	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	8	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	9	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	12	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	13	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	14	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	15	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	16	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	17	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	18	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	19	0.23
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	20	0.23
(1,1029)	1:147:A:LEU:HD21	1:104:A:ALA:HA	20	0.23
(1,1029)	1:147:A:LEU:HD22	1:104:A:ALA:HA	20	0.23
(1,1029)	1:147:A:LEU:HD23	1:104:A:ALA:HA	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	1	0.23
(1,896)	1:142:A:VAL:HG21	1:103:A:THR:HA	9	0.23
(1,896)	1:142:A:VAL:HG22	1:103:A:THR:HA	9	0.23
(1,896)	1:142:A:VAL:HG23	1:103:A:THR:HA	9	0.23
(1,733)	1:26:A:GLN:HG3	1:23:A:SER:HB3	13	0.23
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	17	0.23
(1,363)	1:86:A:ASN:HD22	1:42:A:ARG:HE	19	0.23
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	16	0.23
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	20	0.23
(2,158)	1:156:A:ARG:O	1:160:A:ASP:N	1	0.22
(2,157)	1:153:A:GLN:O	1:157:A:PHE:N	18	0.22
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	11	0.22
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	9	0.22
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	7	0.22
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	10	0.22
(2,146)	1:107:A:ALA:O	1:111:A:PHE:N	2	0.22
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	15	0.22
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	19	0.22
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	1	0.22
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	20	0.22
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	14	0.22
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	18	0.22
(2,140)	1:78:A:LEU:O	1:82:A:GLY:N	17	0.22
(2,136)	1:37:A:SER:O	1:41:A:TYR:N	2	0.22
(2,136)	1:37:A:SER:O	1:41:A:TYR:N	18	0.22
(2,135)	1:35:A:PHE:O	1:39:A:VAL:N	4	0.22
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	3	0.22
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	3	0.22
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	3	0.22
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	3	0.22
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	4	0.22
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	4	0.22
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	4	0.22
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	4	0.22
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	12	0.22
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	12	0.22
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	12	0.22
(1,2939)	2:99:B:ARG:HG3	2:100:B:SER:H	10	0.22
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	12	0.22
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	12	0.22
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	14	0.22
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2658)	2:89:B:HIS:HA	2:92:B:MK8:HB	10	0.22
(1,2559)	1:145:A:HIS:H	1:145:A:HIS:HD2	3	0.22
(1,2559)	1:145:A:HIS:H	1:145:A:HIS:HD2	6	0.22
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE1	5	0.22
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE2	5	0.22
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE1	5	0.22
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE2	5	0.22
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE1	5	0.22
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE2	5	0.22
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE1	7	0.22
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE2	7	0.22
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE1	7	0.22
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE2	7	0.22
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE1	7	0.22
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE2	7	0.22
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE1	19	0.22
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE2	19	0.22
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE1	19	0.22
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE2	19	0.22
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE1	19	0.22
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE2	19	0.22
(1,2336)	1:145:A:HIS:HA	1:145:A:HIS:HE1	2	0.22
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB1	10	0.22
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB2	10	0.22
(1,2224)	1:27:A:VAL:HG11	1:172:A:ALA:HB3	10	0.22
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB1	10	0.22
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB2	10	0.22
(1,2224)	1:27:A:VAL:HG12	1:172:A:ALA:HB3	10	0.22
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB1	10	0.22
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB2	10	0.22
(1,2224)	1:27:A:VAL:HG13	1:172:A:ALA:HB3	10	0.22
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG11	3	0.22
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG12	3	0.22
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG13	3	0.22
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG11	3	0.22
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG12	3	0.22
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG13	3	0.22
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG11	11	0.22
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG12	11	0.22
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG13	11	0.22
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG11	11	0.22
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG12	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG13	11	0.22
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG11	15	0.22
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG12	15	0.22
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG13	15	0.22
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG11	8	0.22
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG12	8	0.22
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG13	8	0.22
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	7	0.22
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	7	0.22
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	7	0.22
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	14	0.22
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	14	0.22
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	14	0.22
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG21	18	0.22
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG22	18	0.22
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG23	18	0.22
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG21	18	0.22
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG22	18	0.22
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG23	18	0.22
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG21	18	0.22
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG22	18	0.22
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG23	18	0.22
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG21	6	0.22
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG22	6	0.22
(1,1955)	1:159:A:VAL:HG11	1:31:A:THR:HG23	6	0.22
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG21	6	0.22
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG22	6	0.22
(1,1955)	1:159:A:VAL:HG12	1:31:A:THR:HG23	6	0.22
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG21	6	0.22
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG22	6	0.22
(1,1955)	1:159:A:VAL:HG13	1:31:A:THR:HG23	6	0.22
(1,1923)	1:147:A:LEU:HA	1:147:A:LEU:HD11	6	0.22
(1,1923)	1:147:A:LEU:HA	1:147:A:LEU:HD12	6	0.22
(1,1923)	1:147:A:LEU:HA	1:147:A:LEU:HD13	6	0.22
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD11	1	0.22
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD12	1	0.22
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD13	1	0.22
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD11	13	0.22
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD12	13	0.22
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD13	13	0.22
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD11	2	0.22
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD12	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD13	2	0.22
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD11	2	0.22
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD12	2	0.22
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD13	2	0.22
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD11	2	0.22
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD12	2	0.22
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD13	2	0.22
(1,1566)	1:158:A:VAL:H	1:158:A:VAL:HB	10	0.22
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	6	0.22
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	6	0.22
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	6	0.22
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	13	0.22
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	13	0.22
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	13	0.22
(1,1138)	1:52:A:VAL:HG11	1:51:A:GLY:HA3	1	0.22
(1,1138)	1:52:A:VAL:HG12	1:51:A:GLY:HA3	1	0.22
(1,1138)	1:52:A:VAL:HG13	1:51:A:GLY:HA3	1	0.22
(1,1138)	1:52:A:VAL:HG21	1:51:A:GLY:HA3	1	0.22
(1,1138)	1:52:A:VAL:HG22	1:51:A:GLY:HA3	1	0.22
(1,1138)	1:52:A:VAL:HG23	1:51:A:GLY:HA3	1	0.22
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	8	0.22
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	4	0.22
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	9	0.22
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	11	0.22
(1,994)	1:50:A:GLU:HG3	1:50:A:GLU:HA	19	0.22
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	2	0.22
(1,410)	1:94:A:GLN:HE22	1:95:A:THR:H	5	0.22
(1,320)	1:163:A:LEU:HD11	1:29:A:GLN:H	9	0.22
(1,320)	1:163:A:LEU:HD12	1:29:A:GLN:H	9	0.22
(1,320)	1:163:A:LEU:HD13	1:29:A:GLN:H	9	0.22
(1,320)	1:163:A:LEU:HD21	1:29:A:GLN:H	9	0.22
(1,320)	1:163:A:LEU:HD22	1:29:A:GLN:H	9	0.22
(1,320)	1:163:A:LEU:HD23	1:29:A:GLN:H	9	0.22
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	17	0.22
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	14	0.21
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	17	0.21
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	18	0.21
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	2	0.21
(2,157)	1:153:A:GLN:O	1:157:A:PHE:N	15	0.21
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	7	0.21
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	10	0.21
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,146)	1:107:A:ALA:O	1:111:A:PHE:N	4	0.21
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	11	0.21
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	8	0.21
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	16	0.21
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	20	0.21
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	4	0.21
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	7	0.21
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	13	0.21
(2,140)	1:78:A:LEU:O	1:82:A:GLY:N	3	0.21
(2,140)	1:78:A:LEU:O	1:82:A:GLY:N	13	0.21
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	7	0.21
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	8	0.21
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	11	0.21
(2,110)	1:155:A:THR:O	1:159:A:VAL:N	20	0.21
(2,109)	1:155:A:THR:O	1:159:A:VAL:H	2	0.21
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	12	0.21
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	2	0.21
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	2	0.21
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	2	0.21
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	3	0.21
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	3	0.21
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	3	0.21
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	4	0.21
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	4	0.21
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	4	0.21
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	20	0.21
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	20	0.21
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	20	0.21
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG21	8	0.21
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG22	8	0.21
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG23	8	0.21
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD11	1	0.21
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD12	1	0.21
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD13	1	0.21
(1,2728)	2:92:B:MK8:HB1A	2:95:B:ASP:H	9	0.21
(1,2728)	2:92:B:MK8:HB1B	2:95:B:ASP:H	9	0.21
(1,2494)	1:131:A:LEU:HD21	1:119:A:PHE:HZ	6	0.21
(1,2494)	1:131:A:LEU:HD22	1:119:A:PHE:HZ	6	0.21
(1,2494)	1:131:A:LEU:HD23	1:119:A:PHE:HZ	6	0.21
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	10	0.21
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	10	0.21
(1,2336)	1:145:A:HIS:HA	1:145:A:HIS:HE1	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	2	0.21
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	2	0.21
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	2	0.21
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	2	0.21
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	2	0.21
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	2	0.21
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	2	0.21
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	2	0.21
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	2	0.21
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB1	13	0.21
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB2	13	0.21
(1,2107)	1:19:A:LEU:HD11	1:18:A:ALA:HB3	13	0.21
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB1	13	0.21
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB2	13	0.21
(1,2107)	1:19:A:LEU:HD12	1:18:A:ALA:HB3	13	0.21
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB1	13	0.21
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB2	13	0.21
(1,2107)	1:19:A:LEU:HD13	1:18:A:ALA:HB3	13	0.21
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	12	0.21
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	12	0.21
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	12	0.21
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	17	0.21
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	17	0.21
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	17	0.21
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	20	0.21
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	20	0.21
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	20	0.21
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD21	20	0.21
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD22	20	0.21
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD23	20	0.21
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD21	3	0.21
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD22	3	0.21
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD23	3	0.21
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD21	5	0.21
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD22	5	0.21
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD23	5	0.21
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD11	15	0.21
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD12	15	0.21
(1,1870)	1:63:A:LEU:H	1:63:A:LEU:HD13	15	0.21
(1,1851)	1:40:A:PHE:HD1	1:63:A:LEU:HD21	4	0.21
(1,1851)	1:40:A:PHE:HD1	1:63:A:LEU:HD22	4	0.21
(1,1851)	1:40:A:PHE:HD1	1:63:A:LEU:HD23	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1851)	1:40:A:PHE:HD2	1:63:A:LEU:HD21	4	0.21
(1,1851)	1:40:A:PHE:HD2	1:63:A:LEU:HD22	4	0.21
(1,1851)	1:40:A:PHE:HD2	1:63:A:LEU:HD23	4	0.21
(1,1842)	1:165:A:HIS:HA	1:166:A:CYS:HB3	7	0.21
(1,1798)	1:153:A:GLN:H	1:151:A:LEU:HG	3	0.21
(1,1730)	1:144:A:GLN:H	1:145:A:HIS:HB3	10	0.21
(1,1464)	1:101:A:GLN:HA	1:101:A:GLN:HG3	13	0.21
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	11	0.21
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	1	0.21
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	5	0.21
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	7	0.21
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	10	0.21
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	15	0.21
(1,1043)	1:182:A:ASN:HB3	1:179:A:ALA:HA	15	0.21
(1,1027)	1:27:A:VAL:HG21	1:168:A:ALA:HA	10	0.21
(1,1027)	1:27:A:VAL:HG22	1:168:A:ALA:HA	10	0.21
(1,1027)	1:27:A:VAL:HG23	1:168:A:ALA:HA	10	0.21
(1,934)	1:159:A:VAL:HG11	1:156:A:ARG:HA	8	0.21
(1,934)	1:159:A:VAL:HG12	1:156:A:ARG:HA	8	0.21
(1,934)	1:159:A:VAL:HG13	1:156:A:ARG:HA	8	0.21
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	5	0.21
(1,896)	1:142:A:VAL:HG21	1:103:A:THR:HA	11	0.21
(1,896)	1:142:A:VAL:HG22	1:103:A:THR:HA	11	0.21
(1,896)	1:142:A:VAL:HG23	1:103:A:THR:HA	11	0.21
(1,733)	1:26:A:GLN:HG3	1:23:A:SER:HB3	8	0.21
(1,733)	1:26:A:GLN:HG3	1:23:A:SER:HB3	12	0.21
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	10	0.21
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	10	0.21
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	10	0.21
(1,190)	1:183:A:LEU:HD21	1:125:A:TRP:H	11	0.21
(1,190)	1:183:A:LEU:HD22	1:125:A:TRP:H	11	0.21
(1,190)	1:183:A:LEU:HD23	1:125:A:TRP:H	11	0.21
(1,123)	1:34:A:VAL:HG11	1:74:A:VAL:H	18	0.21
(1,123)	1:34:A:VAL:HG12	1:74:A:VAL:H	18	0.21
(1,123)	1:34:A:VAL:HG13	1:74:A:VAL:H	18	0.21
(1,96)	1:29:A:GLN:HB3	1:30:A:ASP:H	6	0.21
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	12	0.21
(1,72)	1:34:A:VAL:HG21	1:38:A:TYR:H	1	0.21
(1,72)	1:34:A:VAL:HG22	1:38:A:TYR:H	1	0.21
(1,72)	1:34:A:VAL:HG23	1:38:A:TYR:H	1	0.21
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	5	0.2
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	9	0.2
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	19	0.2
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	4	0.2
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	6	0.2
(2,159)	1:158:A:VAL:O	1:162:A:MET:N	9	0.2
(2,159)	1:158:A:VAL:O	1:162:A:MET:N	16	0.2
(2,158)	1:156:A:ARG:O	1:160:A:ASP:N	11	0.2
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	19	0.2
(2,153)	1:134:A:PHE:O	1:138:A:LEU:N	13	0.2
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	6	0.2
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	7	0.2
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	19	0.2
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	3	0.2
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	1	0.2
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	5	0.2
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	3	0.2
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	17	0.2
(2,140)	1:78:A:LEU:O	1:82:A:GLY:N	7	0.2
(2,140)	1:78:A:LEU:O	1:82:A:GLY:N	14	0.2
(2,140)	1:78:A:LEU:O	1:82:A:GLY:N	18	0.2
(2,139)	1:40:A:PHE:O	1:44:A:GLN:N	8	0.2
(2,105)	1:153:A:GLN:O	1:157:A:PHE:H	3	0.2
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	19	0.2
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	17	0.2
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	17	0.2
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	17	0.2
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	17	0.2
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	20	0.2
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	20	0.2
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	20	0.2
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	20	0.2
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG21	5	0.2
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG22	5	0.2
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG23	5	0.2
(1,2494)	1:131:A:LEU:HD21	1:119:A:PHE:HZ	14	0.2
(1,2494)	1:131:A:LEU:HD22	1:119:A:PHE:HZ	14	0.2
(1,2494)	1:131:A:LEU:HD23	1:119:A:PHE:HZ	14	0.2
(1,2336)	1:145:A:HIS:HA	1:145:A:HIS:HE1	11	0.2
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD11	11	0.2
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD12	11	0.2
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD13	11	0.2
(1,2248)	1:27:A:VAL:HG21	1:168:A:ALA:HB1	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2248)	1:27:A:VAL:HG21	1:168:A:ALA:HB2	20	0.2
(1,2248)	1:27:A:VAL:HG21	1:168:A:ALA:HB3	20	0.2
(1,2248)	1:27:A:VAL:HG22	1:168:A:ALA:HB1	20	0.2
(1,2248)	1:27:A:VAL:HG22	1:168:A:ALA:HB2	20	0.2
(1,2248)	1:27:A:VAL:HG22	1:168:A:ALA:HB3	20	0.2
(1,2248)	1:27:A:VAL:HG23	1:168:A:ALA:HB1	20	0.2
(1,2248)	1:27:A:VAL:HG23	1:168:A:ALA:HB2	20	0.2
(1,2248)	1:27:A:VAL:HG23	1:168:A:ALA:HB3	20	0.2
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB1	2	0.2
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB2	2	0.2
(1,2185)	1:183:A:LEU:HD21	1:180:A:ALA:HB3	2	0.2
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB1	2	0.2
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB2	2	0.2
(1,2185)	1:183:A:LEU:HD22	1:180:A:ALA:HB3	2	0.2
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB1	2	0.2
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB2	2	0.2
(1,2185)	1:183:A:LEU:HD23	1:180:A:ALA:HB3	2	0.2
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	17	0.2
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	17	0.2
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	17	0.2
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG21	11	0.2
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG22	11	0.2
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG23	11	0.2
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG21	11	0.2
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG22	11	0.2
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG23	11	0.2
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG21	11	0.2
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG22	11	0.2
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG23	11	0.2
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD21	4	0.2
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD22	4	0.2
(1,1904)	1:125:A:TRP:HZ2	1:183:A:LEU:HD23	4	0.2
(1,1893)	1:147:A:LEU:H	1:147:A:LEU:HD21	20	0.2
(1,1893)	1:147:A:LEU:H	1:147:A:LEU:HD22	20	0.2
(1,1893)	1:147:A:LEU:H	1:147:A:LEU:HD23	20	0.2
(1,1730)	1:144:A:GLN:H	1:145:A:HIS:HB3	7	0.2
(1,1660)	1:47:A:GLN:HE21	1:46:A:GLU:HB3	12	0.2
(1,1428)	1:31:A:THR:HB	1:32:A:GLU:HG3	7	0.2
(1,1189)	1:159:A:VAL:HG11	1:156:A:ARG:HD3	9	0.2
(1,1189)	1:159:A:VAL:HG12	1:156:A:ARG:HD3	9	0.2
(1,1189)	1:159:A:VAL:HG13	1:156:A:ARG:HD3	9	0.2
(1,1115)	1:35:A:PHE:HE1	1:135:A:GLY:HA2	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:35:A:PHE:HE2	1:135:A:GLY:HA2	12	0.2
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	3	0.2
(1,1087)	1:47:A:GLN:HE22	1:55:A:PRO:HD3	6	0.2
(1,1029)	1:147:A:LEU:HD21	1:104:A:ALA:HA	6	0.2
(1,1029)	1:147:A:LEU:HD22	1:104:A:ALA:HA	6	0.2
(1,1029)	1:147:A:LEU:HD23	1:104:A:ALA:HA	6	0.2
(1,1027)	1:27:A:VAL:HG21	1:168:A:ALA:HA	14	0.2
(1,1027)	1:27:A:VAL:HG22	1:168:A:ALA:HA	14	0.2
(1,1027)	1:27:A:VAL:HG23	1:168:A:ALA:HA	14	0.2
(1,839)	1:63:A:LEU:HB3	1:62:A:THR:HA	19	0.2
(1,171)	1:162:A:MET:HB3	1:161:A:PHE:H	11	0.2
(1,96)	1:29:A:GLN:HB3	1:30:A:ASP:H	19	0.2
(2,163)	1:170:A:TRP:O	1:174:A:ARG:N	4	0.19
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	2	0.19
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	8	0.19
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	10	0.19
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	16	0.19
(2,158)	1:156:A:ARG:O	1:160:A:ASP:N	17	0.19
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	4	0.19
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	7	0.19
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	14	0.19
(2,153)	1:134:A:PHE:O	1:138:A:LEU:N	15	0.19
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	12	0.19
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	20	0.19
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	4	0.19
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	11	0.19
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	9	0.19
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	13	0.19
(2,139)	1:40:A:PHE:O	1:44:A:GLN:N	11	0.19
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	5	0.19
(2,127)	1:24:A:GLU:O	1:28:A:ALA:N	19	0.19
(2,109)	1:155:A:THR:O	1:159:A:VAL:H	12	0.19
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	3	0.19
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	8	0.19
(2,53)	1:93:A:PHE:O	1:97:A:LEU:H	4	0.19
(2,53)	1:93:A:PHE:O	1:97:A:LEU:H	11	0.19
(2,10)	1:28:A:ALA:O	1:32:A:GLU:N	12	0.19
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB1	5	0.19
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB2	5	0.19
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB3	5	0.19
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	13	0.19
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	13	0.19
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	14	0.19
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	14	0.19
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	14	0.19
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG21	6	0.19
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG22	6	0.19
(1,2967)	1:113:A:LYS:HG3	2:86:B:ILE:HG23	6	0.19
(1,2483)	1:147:A:LEU:HD21	1:150:A:PHE:HZ	3	0.19
(1,2483)	1:147:A:LEU:HD22	1:150:A:PHE:HZ	3	0.19
(1,2483)	1:147:A:LEU:HD23	1:150:A:PHE:HZ	3	0.19
(1,2450)	1:158:A:VAL:HG21	1:111:A:PHE:HE1	10	0.19
(1,2450)	1:158:A:VAL:HG21	1:111:A:PHE:HE2	10	0.19
(1,2450)	1:158:A:VAL:HG22	1:111:A:PHE:HE1	10	0.19
(1,2450)	1:158:A:VAL:HG22	1:111:A:PHE:HE2	10	0.19
(1,2450)	1:158:A:VAL:HG23	1:111:A:PHE:HE1	10	0.19
(1,2450)	1:158:A:VAL:HG23	1:111:A:PHE:HE2	10	0.19
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE1	3	0.19
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE2	3	0.19
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE1	3	0.19
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE2	3	0.19
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE1	3	0.19
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE2	3	0.19
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE1	10	0.19
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE2	10	0.19
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE1	10	0.19
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE2	10	0.19
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE1	10	0.19
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE2	10	0.19
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE1	12	0.19
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE2	12	0.19
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE1	12	0.19
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE2	12	0.19
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE1	12	0.19
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE2	12	0.19
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	11	0.19
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	11	0.19
(1,2336)	1:145:A:HIS:HA	1:145:A:HIS:HE1	6	0.19
(1,2327)	1:162:A:MET:HA	1:167:A:ILE:HD11	4	0.19
(1,2327)	1:162:A:MET:HA	1:167:A:ILE:HD12	4	0.19
(1,2327)	1:162:A:MET:HA	1:167:A:ILE:HD13	4	0.19
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB1	16	0.19
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB2	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB3	16	0.19
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB1	16	0.19
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB2	16	0.19
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB3	16	0.19
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB1	16	0.19
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB2	16	0.19
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB3	16	0.19
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG21	11	0.19
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG22	11	0.19
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG23	11	0.19
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD11	8	0.19
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD12	8	0.19
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD13	8	0.19
(1,1836)	1:175:A:GLY:H	1:174:A:ARG:HG3	7	0.19
(1,1670)	1:137:A:ARG:HD3	1:137:A:ARG:HB3	19	0.19
(1,1428)	1:31:A:THR:HB	1:32:A:GLU:HG3	17	0.19
(1,1427)	1:92:A:GLU:HA	1:92:A:GLU:HG3	10	0.19
(1,1427)	1:92:A:GLU:HA	1:92:A:GLU:HG3	14	0.19
(1,1350)	1:179:A:ALA:HB1	1:182:A:ASN:HB3	15	0.19
(1,1350)	1:179:A:ALA:HB2	1:182:A:ASN:HB3	15	0.19
(1,1350)	1:179:A:ALA:HB3	1:182:A:ASN:HB3	15	0.19
(1,1115)	1:35:A:PHE:HE1	1:135:A:GLY:HA2	4	0.19
(1,1115)	1:35:A:PHE:HE2	1:135:A:GLY:HA2	4	0.19
(1,839)	1:63:A:LEU:HB3	1:62:A:THR:HA	20	0.19
(1,320)	1:163:A:LEU:HD11	1:29:A:GLN:H	16	0.19
(1,320)	1:163:A:LEU:HD12	1:29:A:GLN:H	16	0.19
(1,320)	1:163:A:LEU:HD13	1:29:A:GLN:H	16	0.19
(1,320)	1:163:A:LEU:HD21	1:29:A:GLN:H	16	0.19
(1,320)	1:163:A:LEU:HD22	1:29:A:GLN:H	16	0.19
(1,320)	1:163:A:LEU:HD23	1:29:A:GLN:H	16	0.19
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	14	0.19
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	14	0.19
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	14	0.19
(1,270)	1:23:A:SER:HA	1:25:A:GLU:H	4	0.19
(1,171)	1:162:A:MET:HB3	1:161:A:PHE:H	15	0.19
(1,154)	1:32:A:GLU:HG3	1:32:A:GLU:H	7	0.19
(1,96)	1:29:A:GLN:HB3	1:30:A:ASP:H	17	0.19
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	1	0.19
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	3	0.19
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	5	0.19
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	10	0.19
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	5	0.18
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	12	0.18
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	16	0.18
(2,159)	1:158:A:VAL:O	1:162:A:MET:N	18	0.18
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	8	0.18
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	12	0.18
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	19	0.18
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	15	0.18
(2,143)	1:93:A:PHE:O	1:97:A:LEU:N	19	0.18
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	2	0.18
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	11	0.18
(2,140)	1:78:A:LEU:O	1:82:A:GLY:N	4	0.18
(2,140)	1:78:A:LEU:O	1:82:A:GLY:N	10	0.18
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	16	0.18
(2,110)	1:155:A:THR:O	1:159:A:VAL:N	2	0.18
(2,95)	1:137:A:ARG:O	1:141:A:HIS:H	20	0.18
(2,91)	1:135:A:GLY:O	1:139:A:ALA:H	12	0.18
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	9	0.18
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	17	0.18
(2,77)	1:126:A:GLY:O	1:130:A:ALA:H	1	0.18
(2,53)	1:93:A:PHE:O	1:97:A:LEU:H	9	0.18
(2,10)	1:28:A:ALA:O	1:32:A:GLU:N	2	0.18
(1,3106)	2:93:B:VAL:HG21	1:89:A:TYR:HB3	10	0.18
(1,3106)	2:93:B:VAL:HG22	1:89:A:TYR:HB3	10	0.18
(1,3106)	2:93:B:VAL:HG23	1:89:A:TYR:HB3	10	0.18
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	6	0.18
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	6	0.18
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	6	0.18
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	6	0.18
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	9	0.18
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	9	0.18
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	9	0.18
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	9	0.18
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	18	0.18
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	18	0.18
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	18	0.18
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	18	0.18
(1,3097)	1:126:A:GLY:H	2:101:B:ILE:HG13	19	0.18
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB1	7	0.18
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB2	7	0.18
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB3	7	0.18
(1,3086)	1:129:A:VAL:H	2:97:B:NLE:HD2	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3086)	1:129:A:VAL:H	2:97:B:NLE:HD3	16	0.18
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD11	3	0.18
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD12	3	0.18
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD13	3	0.18
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	6	0.18
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	6	0.18
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	6	0.18
(1,2947)	1:85:A:ILE:HD11	2:97:B:NLE:HD2	5	0.18
(1,2947)	1:85:A:ILE:HD11	2:97:B:NLE:HD3	5	0.18
(1,2947)	1:85:A:ILE:HD12	2:97:B:NLE:HD2	5	0.18
(1,2947)	1:85:A:ILE:HD12	2:97:B:NLE:HD3	5	0.18
(1,2947)	1:85:A:ILE:HD13	2:97:B:NLE:HD2	5	0.18
(1,2947)	1:85:A:ILE:HD13	2:97:B:NLE:HD3	5	0.18
(1,2844)	2:86:B:ILE:HA	2:90:B:LEU:H	1	0.18
(1,2759)	2:82:B:ILE:H	2:82:B:ILE:HB	18	0.18
(1,2730)	2:93:B:VAL:HA	2:96:B:MK8:HB	9	0.18
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE1	2	0.18
(1,2586)	1:100:A:LEU:HD11	1:110:A:TYR:HE2	2	0.18
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE1	2	0.18
(1,2586)	1:100:A:LEU:HD12	1:110:A:TYR:HE2	2	0.18
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE1	2	0.18
(1,2586)	1:100:A:LEU:HD13	1:110:A:TYR:HE2	2	0.18
(1,2559)	1:145:A:HIS:H	1:145:A:HIS:HD2	11	0.18
(1,2556)	1:183:A:LEU:HD21	1:125:A:TRP:HE3	11	0.18
(1,2556)	1:183:A:LEU:HD22	1:125:A:TRP:HE3	11	0.18
(1,2556)	1:183:A:LEU:HD23	1:125:A:TRP:HE3	11	0.18
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE1	17	0.18
(1,2440)	1:131:A:LEU:HD21	1:134:A:PHE:HE2	17	0.18
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE1	17	0.18
(1,2440)	1:131:A:LEU:HD22	1:134:A:PHE:HE2	17	0.18
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE1	17	0.18
(1,2440)	1:131:A:LEU:HD23	1:134:A:PHE:HE2	17	0.18
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG11	8	0.18
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG12	8	0.18
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG13	8	0.18
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG11	3	0.18
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG12	3	0.18
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG13	3	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD11	1	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD12	1	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD13	1	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD11	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD12	2	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD13	2	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD11	5	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD12	5	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD13	5	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD11	7	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD12	7	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD13	7	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD11	10	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD12	10	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD13	10	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD11	11	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD12	11	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD13	11	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD11	13	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD12	13	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD13	13	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD11	15	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD12	15	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD13	15	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD11	16	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD12	16	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD13	16	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD11	18	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD12	18	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD13	18	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD11	20	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD12	20	0.18
(1,1990)	1:118:A:LEU:HB3	1:118:A:LEU:HD13	20	0.18
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG21	2	0.18
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG22	2	0.18
(1,1961)	1:34:A:VAL:HG11	1:74:A:VAL:HG23	2	0.18
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG21	2	0.18
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG22	2	0.18
(1,1961)	1:34:A:VAL:HG12	1:74:A:VAL:HG23	2	0.18
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG21	2	0.18
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG22	2	0.18
(1,1961)	1:34:A:VAL:HG13	1:74:A:VAL:HG23	2	0.18
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG21	19	0.18
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG22	19	0.18
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG23	19	0.18
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD11	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD12	10	0.18
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD13	10	0.18
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD11	10	0.18
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD12	10	0.18
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD13	10	0.18
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD11	10	0.18
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD12	10	0.18
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD13	10	0.18
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD11	15	0.18
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD12	15	0.18
(1,1827)	1:162:A:MET:HE1	1:131:A:LEU:HD13	15	0.18
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD11	15	0.18
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD12	15	0.18
(1,1827)	1:162:A:MET:HE2	1:131:A:LEU:HD13	15	0.18
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD11	15	0.18
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD12	15	0.18
(1,1827)	1:162:A:MET:HE3	1:131:A:LEU:HD13	15	0.18
(1,1777)	1:138:A:LEU:H	1:138:A:LEU:HG	15	0.18
(1,1709)	1:98:A:GLN:HE22	1:98:A:GLN:HB3	15	0.18
(1,1660)	1:47:A:GLN:HE21	1:46:A:GLU:HB3	11	0.18
(1,1549)	1:61:A:VAL:HG11	1:60:A:MET:HB3	4	0.18
(1,1549)	1:61:A:VAL:HG12	1:60:A:MET:HB3	4	0.18
(1,1549)	1:61:A:VAL:HG13	1:60:A:MET:HB3	4	0.18
(1,1537)	1:159:A:VAL:H	1:159:A:VAL:HB	5	0.18
(1,1428)	1:31:A:THR:HB	1:32:A:GLU:HG3	3	0.18
(1,1428)	1:31:A:THR:HB	1:32:A:GLU:HG3	8	0.18
(1,1427)	1:92:A:GLU:HA	1:92:A:GLU:HG3	2	0.18
(1,1427)	1:92:A:GLU:HA	1:92:A:GLU:HG3	13	0.18
(1,1189)	1:159:A:VAL:HG11	1:156:A:ARG:HD3	1	0.18
(1,1189)	1:159:A:VAL:HG12	1:156:A:ARG:HD3	1	0.18
(1,1189)	1:159:A:VAL:HG13	1:156:A:ARG:HD3	1	0.18
(1,1138)	1:52:A:VAL:HG11	1:51:A:GLY:HA3	16	0.18
(1,1138)	1:52:A:VAL:HG12	1:51:A:GLY:HA3	16	0.18
(1,1138)	1:52:A:VAL:HG13	1:51:A:GLY:HA3	16	0.18
(1,1138)	1:52:A:VAL:HG21	1:51:A:GLY:HA3	16	0.18
(1,1138)	1:52:A:VAL:HG22	1:51:A:GLY:HA3	16	0.18
(1,1138)	1:52:A:VAL:HG23	1:51:A:GLY:HA3	16	0.18
(1,1136)	1:50:A:GLU:HB3	1:51:A:GLY:HA3	5	0.18
(1,972)	1:140:A:LEU:HG	1:140:A:LEU:HA	3	0.18
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	13	0.18
(1,743)	1:62:A:THR:HG21	1:58:A:PRO:HA	4	0.18
(1,743)	1:62:A:THR:HG22	1:58:A:PRO:HA	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,743)	1:62:A:THR:HG23	1:58:A:PRO:HA	4	0.18
(1,733)	1:26:A:GLN:HG3	1:23:A:SER:HB3	19	0.18
(1,531)	1:23:A:SER:H	1:26:A:GLN:HE22	1	0.18
(1,531)	1:23:A:SER:H	1:26:A:GLN:HE22	13	0.18
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	5	0.18
(1,123)	1:34:A:VAL:HG11	1:74:A:VAL:H	1	0.18
(1,123)	1:34:A:VAL:HG12	1:74:A:VAL:H	1	0.18
(1,123)	1:34:A:VAL:HG13	1:74:A:VAL:H	1	0.18
(1,123)	1:34:A:VAL:HG11	1:74:A:VAL:H	20	0.18
(1,123)	1:34:A:VAL:HG12	1:74:A:VAL:H	20	0.18
(1,123)	1:34:A:VAL:HG13	1:74:A:VAL:H	20	0.18
(1,96)	1:29:A:GLN:HB3	1:30:A:ASP:H	3	0.18
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	4	0.18
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	7	0.18
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	9	0.18
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	14	0.18
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	19	0.18
(1,74)	1:63:A:LEU:HD11	1:65:A:LEU:H	15	0.18
(1,74)	1:63:A:LEU:HD12	1:65:A:LEU:H	15	0.18
(1,74)	1:63:A:LEU:HD13	1:65:A:LEU:H	15	0.18
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	7	0.17
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	11	0.17
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	15	0.17
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	9	0.17
(2,159)	1:158:A:VAL:O	1:162:A:MET:N	12	0.17
(2,158)	1:156:A:ARG:O	1:160:A:ASP:N	18	0.17
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	16	0.17
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	6	0.17
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	15	0.17
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	2	0.17
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	18	0.17
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	7	0.17
(2,146)	1:107:A:ALA:O	1:111:A:PHE:N	10	0.17
(2,146)	1:107:A:ALA:O	1:111:A:PHE:N	16	0.17
(2,146)	1:107:A:ALA:O	1:111:A:PHE:N	19	0.17
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	1	0.17
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	2	0.17
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	10	0.17
(2,140)	1:78:A:LEU:O	1:82:A:GLY:N	12	0.17
(2,140)	1:78:A:LEU:O	1:82:A:GLY:N	15	0.17
(2,139)	1:40:A:PHE:O	1:44:A:GLN:N	2	0.17
(2,139)	1:40:A:PHE:O	1:44:A:GLN:N	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,130)	1:30:A:ASP:O	1:34:A:VAL:N	5	0.17
(2,110)	1:155:A:THR:O	1:159:A:VAL:N	12	0.17
(2,95)	1:137:A:ARG:O	1:141:A:HIS:H	7	0.17
(2,88)	1:132:A:LEU:O	1:136:A:TYR:N	12	0.17
(2,88)	1:132:A:LEU:O	1:136:A:TYR:N	19	0.17
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	2	0.17
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	5	0.17
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	14	0.17
(2,47)	1:83:A:ASP:O	1:87:A:ARG:N	6	0.17
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	2	0.17
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	2	0.17
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	2	0.17
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	2	0.17
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1A	8	0.17
(1,3103)	1:89:A:TYR:HD1	2:92:B:MK8:HB1B	8	0.17
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1A	8	0.17
(1,3103)	1:89:A:TYR:HD2	2:92:B:MK8:HB1B	8	0.17
(1,3097)	1:126:A:GLY:H	2:101:B:ILE:HG13	14	0.17
(1,3086)	1:129:A:VAL:H	2:97:B:NLE:HD2	14	0.17
(1,3086)	1:129:A:VAL:H	2:97:B:NLE:HD3	14	0.17
(1,2968)	1:113:A:LYS:HD3	2:86:B:ILE:HD11	1	0.17
(1,2968)	1:113:A:LYS:HD3	2:86:B:ILE:HD12	1	0.17
(1,2968)	1:113:A:LYS:HD3	2:86:B:ILE:HD13	1	0.17
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	19	0.17
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	19	0.17
(1,2779)	2:88:B:ARG:HB3	2:88:B:ARG:HD3	15	0.17
(1,2758)	2:82:B:ILE:HB	2:83:B:ILE:H	3	0.17
(1,2758)	2:82:B:ILE:HB	2:83:B:ILE:H	12	0.17
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HD	15	0.17
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HDA	15	0.17
(1,2675)	2:82:B:ILE:HG21	2:83:B:ILE:H	18	0.17
(1,2675)	2:82:B:ILE:HG22	2:83:B:ILE:H	18	0.17
(1,2675)	2:82:B:ILE:HG23	2:83:B:ILE:H	18	0.17
(1,2636)	2:90:B:LEU:HA	2:93:B:VAL:HB	6	0.17
(1,2636)	2:90:B:LEU:HA	2:93:B:VAL:HB	10	0.17
(1,2494)	1:131:A:LEU:HD21	1:119:A:PHE:HZ	16	0.17
(1,2494)	1:131:A:LEU:HD22	1:119:A:PHE:HZ	16	0.17
(1,2494)	1:131:A:LEU:HD23	1:119:A:PHE:HZ	16	0.17
(1,2493)	1:118:A:LEU:HD21	1:119:A:PHE:HZ	9	0.17
(1,2493)	1:118:A:LEU:HD22	1:119:A:PHE:HZ	9	0.17
(1,2493)	1:118:A:LEU:HD23	1:119:A:PHE:HZ	9	0.17
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	14	0.17
(1,2129)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	14	0.17
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG21	11	0.17
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG22	11	0.17
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG23	11	0.17
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG11	3	0.17
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG12	3	0.17
(1,2088)	1:139:A:ALA:HA	1:142:A:VAL:HG13	3	0.17
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG11	9	0.17
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG12	9	0.17
(1,2087)	1:150:A:PHE:HE1	1:142:A:VAL:HG13	9	0.17
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG11	9	0.17
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG12	9	0.17
(1,2087)	1:150:A:PHE:HE2	1:142:A:VAL:HG13	9	0.17
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG11	1	0.17
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG12	1	0.17
(1,2013)	1:31:A:THR:HB	1:159:A:VAL:HG13	1	0.17
(1,1995)	1:97:A:LEU:HA	1:100:A:LEU:HD21	2	0.17
(1,1995)	1:97:A:LEU:HA	1:100:A:LEU:HD22	2	0.17
(1,1995)	1:97:A:LEU:HA	1:100:A:LEU:HD23	2	0.17
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	6	0.17
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	6	0.17
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	6	0.17
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	9	0.17
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	9	0.17
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	9	0.17
(1,1922)	1:115:A:ALA:HB1	1:131:A:LEU:HD21	19	0.17
(1,1922)	1:115:A:ALA:HB1	1:131:A:LEU:HD22	19	0.17
(1,1922)	1:115:A:ALA:HB1	1:131:A:LEU:HD23	19	0.17
(1,1922)	1:115:A:ALA:HB2	1:131:A:LEU:HD21	19	0.17
(1,1922)	1:115:A:ALA:HB2	1:131:A:LEU:HD22	19	0.17
(1,1922)	1:115:A:ALA:HB2	1:131:A:LEU:HD23	19	0.17
(1,1922)	1:115:A:ALA:HB3	1:131:A:LEU:HD21	19	0.17
(1,1922)	1:115:A:ALA:HB3	1:131:A:LEU:HD22	19	0.17
(1,1922)	1:115:A:ALA:HB3	1:131:A:LEU:HD23	19	0.17
(1,1534)	1:160:A:ASP:H	1:159:A:VAL:HB	12	0.17
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	18	0.17
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	18	0.17
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	18	0.17
(1,1428)	1:31:A:THR:HB	1:32:A:GLU:HG3	5	0.17
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	12	0.17
(1,921)	1:98:A:GLN:HE22	1:98:A:GLN:HA	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,839)	1:63:A:LEU:HB3	1:62:A:THR:HA	18	0.17
(1,735)	1:26:A:GLN:H	1:23:A:SER:HB3	17	0.17
(1,653)	1:73:A:GLN:HG3	1:70:A:THR:HA	15	0.17
(1,96)	1:29:A:GLN:HB3	1:30:A:ASP:H	4	0.17
(1,96)	1:29:A:GLN:HB3	1:30:A:ASP:H	5	0.17
(1,96)	1:29:A:GLN:HB3	1:30:A:ASP:H	11	0.17
(1,74)	1:63:A:LEU:HD11	1:65:A:LEU:H	18	0.17
(1,74)	1:63:A:LEU:HD12	1:65:A:LEU:H	18	0.17
(1,74)	1:63:A:LEU:HD13	1:65:A:LEU:H	18	0.17
(2,159)	1:158:A:VAL:O	1:162:A:MET:N	5	0.16
(2,157)	1:153:A:GLN:O	1:157:A:PHE:N	10	0.16
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	5	0.16
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	10	0.16
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	18	0.16
(2,151)	1:127:A:ARG:O	1:131:A:LEU:N	5	0.16
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	6	0.16
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	8	0.16
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	15	0.16
(2,136)	1:37:A:SER:O	1:41:A:TYR:N	10	0.16
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	16	0.16
(2,53)	1:93:A:PHE:O	1:97:A:LEU:H	13	0.16
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB1	6	0.16
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB2	6	0.16
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB3	6	0.16
(1,3086)	1:129:A:VAL:H	2:97:B:NLE:HD2	6	0.16
(1,3086)	1:129:A:VAL:H	2:97:B:NLE:HD3	6	0.16
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD11	4	0.16
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD12	4	0.16
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD13	4	0.16
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD11	4	0.16
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD12	4	0.16
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD13	4	0.16
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD11	4	0.16
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD12	4	0.16
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD13	4	0.16
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD11	12	0.16
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD12	12	0.16
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD13	12	0.16
(1,2779)	2:88:B:ARG:HB3	2:88:B:ARG:HD3	1	0.16
(1,2759)	2:82:B:ILE:H	2:82:B:ILE:HB	7	0.16
(1,2758)	2:82:B:ILE:HB	2:83:B:ILE:H	14	0.16
(1,2636)	2:90:B:LEU:HA	2:93:B:VAL:HB	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2556)	1:183:A:LEU:HD21	1:125:A:TRP:HE3	13	0.16
(1,2556)	1:183:A:LEU:HD22	1:125:A:TRP:HE3	13	0.16
(1,2556)	1:183:A:LEU:HD23	1:125:A:TRP:HE3	13	0.16
(1,2494)	1:131:A:LEU:HD21	1:119:A:PHE:HZ	1	0.16
(1,2494)	1:131:A:LEU:HD22	1:119:A:PHE:HZ	1	0.16
(1,2494)	1:131:A:LEU:HD23	1:119:A:PHE:HZ	1	0.16
(1,2394)	1:107:A:ALA:HB1	1:150:A:PHE:HD1	19	0.16
(1,2394)	1:107:A:ALA:HB1	1:150:A:PHE:HD2	19	0.16
(1,2394)	1:107:A:ALA:HB2	1:150:A:PHE:HD1	19	0.16
(1,2394)	1:107:A:ALA:HB2	1:150:A:PHE:HD2	19	0.16
(1,2394)	1:107:A:ALA:HB3	1:150:A:PHE:HD1	19	0.16
(1,2394)	1:107:A:ALA:HB3	1:150:A:PHE:HD2	19	0.16
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB1	11	0.16
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB2	11	0.16
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB3	11	0.16
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB1	11	0.16
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB2	11	0.16
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB3	11	0.16
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB1	11	0.16
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB2	11	0.16
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB3	11	0.16
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG21	12	0.16
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG22	12	0.16
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG23	12	0.16
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD11	12	0.16
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD12	12	0.16
(1,2051)	1:184:A:GLY:H	1:183:A:LEU:HD13	12	0.16
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD21	8	0.16
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD22	8	0.16
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD23	8	0.16
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD21	8	0.16
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD22	8	0.16
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD23	8	0.16
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD21	8	0.16
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD22	8	0.16
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD23	8	0.16
(1,1890)	1:81:A:ILE:HD11	1:129:A:VAL:HG11	11	0.16
(1,1890)	1:81:A:ILE:HD11	1:129:A:VAL:HG12	11	0.16
(1,1890)	1:81:A:ILE:HD11	1:129:A:VAL:HG13	11	0.16
(1,1890)	1:81:A:ILE:HD12	1:129:A:VAL:HG11	11	0.16
(1,1890)	1:81:A:ILE:HD12	1:129:A:VAL:HG12	11	0.16
(1,1890)	1:81:A:ILE:HD12	1:129:A:VAL:HG13	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1890)	1:81:A:ILE:HD13	1:129:A:VAL:HG11	11	0.16
(1,1890)	1:81:A:ILE:HD13	1:129:A:VAL:HG12	11	0.16
(1,1890)	1:81:A:ILE:HD13	1:129:A:VAL:HG13	11	0.16
(1,1663)	1:27:A:VAL:HG11	1:24:A:GLU:HB3	9	0.16
(1,1663)	1:27:A:VAL:HG12	1:24:A:GLU:HB3	9	0.16
(1,1663)	1:27:A:VAL:HG13	1:24:A:GLU:HB3	9	0.16
(1,1654)	1:159:A:VAL:HG11	1:32:A:GLU:HB3	10	0.16
(1,1654)	1:159:A:VAL:HG12	1:32:A:GLU:HB3	10	0.16
(1,1654)	1:159:A:VAL:HG13	1:32:A:GLU:HB3	10	0.16
(1,1534)	1:160:A:ASP:H	1:159:A:VAL:HB	20	0.16
(1,1428)	1:31:A:THR:HB	1:32:A:GLU:HG3	11	0.16
(1,1428)	1:31:A:THR:HB	1:32:A:GLU:HG3	19	0.16
(1,1424)	1:163:A:LEU:HD11	1:25:A:GLU:HG3	19	0.16
(1,1424)	1:163:A:LEU:HD12	1:25:A:GLU:HG3	19	0.16
(1,1424)	1:163:A:LEU:HD13	1:25:A:GLU:HG3	19	0.16
(1,1424)	1:163:A:LEU:HD21	1:25:A:GLU:HG3	19	0.16
(1,1424)	1:163:A:LEU:HD22	1:25:A:GLU:HG3	19	0.16
(1,1424)	1:163:A:LEU:HD23	1:25:A:GLU:HG3	19	0.16
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	17	0.16
(1,1083)	1:19:A:LEU:HB3	1:20:A:PRO:HD3	10	0.16
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	14	0.16
(1,1032)	1:131:A:LEU:HD21	1:115:A:ALA:HA	2	0.16
(1,1032)	1:131:A:LEU:HD22	1:115:A:ALA:HA	2	0.16
(1,1032)	1:131:A:LEU:HD23	1:115:A:ALA:HA	2	0.16
(1,1032)	1:131:A:LEU:HD21	1:115:A:ALA:HA	10	0.16
(1,1032)	1:131:A:LEU:HD22	1:115:A:ALA:HA	10	0.16
(1,1032)	1:131:A:LEU:HD23	1:115:A:ALA:HA	10	0.16
(1,1032)	1:131:A:LEU:HD21	1:115:A:ALA:HA	17	0.16
(1,1032)	1:131:A:LEU:HD22	1:115:A:ALA:HA	17	0.16
(1,1032)	1:131:A:LEU:HD23	1:115:A:ALA:HA	17	0.16
(1,674)	1:74:A:VAL:HG21	1:34:A:VAL:HA	17	0.16
(1,674)	1:74:A:VAL:HG22	1:34:A:VAL:HA	17	0.16
(1,674)	1:74:A:VAL:HG23	1:34:A:VAL:HA	17	0.16
(1,538)	1:22:A:ALA:HA	1:26:A:GLN:HE22	3	0.16
(1,531)	1:23:A:SER:H	1:26:A:GLN:HE22	2	0.16
(1,531)	1:23:A:SER:H	1:26:A:GLN:HE22	19	0.16
(1,490)	1:164:A:HIS:HB3	1:164:A:HIS:H	12	0.16
(1,442)	1:181:A:LEU:HD11	1:182:A:ASN:H	2	0.16
(1,442)	1:181:A:LEU:HD12	1:182:A:ASN:H	2	0.16
(1,442)	1:181:A:LEU:HD13	1:182:A:ASN:H	2	0.16
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	2	0.16
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	2	0.16
(1,154)	1:32:A:GLU:HG3	1:32:A:GLU:H	8	0.16
(1,154)	1:32:A:GLU:HG3	1:32:A:GLU:H	17	0.16
(1,96)	1:29:A:GLN:HB3	1:30:A:ASP:H	18	0.16
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	18	0.16
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	6	0.15
(2,159)	1:158:A:VAL:O	1:162:A:MET:N	10	0.15
(2,158)	1:156:A:ARG:O	1:160:A:ASP:N	13	0.15
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	2	0.15
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	1	0.15
(2,146)	1:107:A:ALA:O	1:111:A:PHE:N	8	0.15
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	10	0.15
(2,130)	1:30:A:ASP:O	1:34:A:VAL:N	14	0.15
(2,109)	1:155:A:THR:O	1:159:A:VAL:H	6	0.15
(2,97)	1:139:A:ALA:O	1:143:A:TYR:H	7	0.15
(2,91)	1:135:A:GLY:O	1:139:A:ALA:H	19	0.15
(2,88)	1:132:A:LEU:O	1:136:A:TYR:N	3	0.15
(2,88)	1:132:A:LEU:O	1:136:A:TYR:N	8	0.15
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	7	0.15
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	18	0.15
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	20	0.15
(2,77)	1:126:A:GLY:O	1:130:A:ALA:H	10	0.15
(2,75)	1:124:A:ASN:O	1:128:A:VAL:H	17	0.15
(2,47)	1:83:A:ASP:O	1:87:A:ARG:N	19	0.15
(2,11)	1:29:A:GLN:O	1:33:A:GLU:H	2	0.15
(2,11)	1:29:A:GLN:O	1:33:A:GLU:H	16	0.15
(2,11)	1:29:A:GLN:O	1:33:A:GLU:H	20	0.15
(2,9)	1:28:A:ALA:O	1:32:A:GLU:H	10	0.15
(2,5)	1:26:A:GLN:O	1:30:A:ASP:H	4	0.15
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB1	16	0.15
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB2	16	0.15
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB3	16	0.15
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB1	20	0.15
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB2	20	0.15
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB3	20	0.15
(1,2998)	1:81:A:ILE:HD11	2:101:B:ILE:HB	8	0.15
(1,2998)	1:81:A:ILE:HD12	2:101:B:ILE:HB	8	0.15
(1,2998)	1:81:A:ILE:HD13	2:101:B:ILE:HB	8	0.15
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD11	11	0.15
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD12	11	0.15
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD13	11	0.15
(1,2858)	2:80:B:GLU:HA	2:83:B:ILE:HB	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2795)	2:88:B:ARG:HA	2:91:B:ALA:H	15	0.15
(1,2779)	2:88:B:ARG:HB3	2:88:B:ARG:HD3	10	0.15
(1,2779)	2:88:B:ARG:HB3	2:88:B:ARG:HD3	17	0.15
(1,2779)	2:88:B:ARG:HB3	2:88:B:ARG:HD3	20	0.15
(1,2772)	2:83:B:ILE:HB	2:84:B:ARG:H	11	0.15
(1,2683)	2:84:B:ARG:HA	2:84:B:ARG:HD3	12	0.15
(1,2636)	2:90:B:LEU:HA	2:93:B:VAL:HB	13	0.15
(1,2483)	1:147:A:LEU:HD21	1:150:A:PHE:HZ	11	0.15
(1,2483)	1:147:A:LEU:HD22	1:150:A:PHE:HZ	11	0.15
(1,2483)	1:147:A:LEU:HD23	1:150:A:PHE:HZ	11	0.15
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE1	14	0.15
(1,2417)	1:136:A:TYR:HB3	1:35:A:PHE:HE2	14	0.15
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD11	16	0.15
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD12	16	0.15
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD13	16	0.15
(1,2201)	1:97:A:LEU:HA	1:96:A:MET:HE1	1	0.15
(1,2201)	1:97:A:LEU:HA	1:96:A:MET:HE2	1	0.15
(1,2201)	1:97:A:LEU:HA	1:96:A:MET:HE3	1	0.15
(1,2201)	1:97:A:LEU:HA	1:96:A:MET:HE1	19	0.15
(1,2201)	1:97:A:LEU:HA	1:96:A:MET:HE2	19	0.15
(1,2201)	1:97:A:LEU:HA	1:96:A:MET:HE3	19	0.15
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB1	19	0.15
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB2	19	0.15
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB3	19	0.15
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB1	19	0.15
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB2	19	0.15
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB3	19	0.15
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB1	19	0.15
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB2	19	0.15
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB3	19	0.15
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG21	14	0.15
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG22	14	0.15
(1,2095)	1:75:A:GLY:HA2	1:34:A:VAL:HG23	14	0.15
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG21	9	0.15
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG22	9	0.15
(1,2079)	1:102:A:PRO:HD3	1:142:A:VAL:HG23	9	0.15
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	5	0.15
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	5	0.15
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	5	0.15
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	19	0.15
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	19	0.15
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1923)	1:147:A:LEU:HA	1:147:A:LEU:HD11	7	0.15
(1,1923)	1:147:A:LEU:HA	1:147:A:LEU:HD12	7	0.15
(1,1923)	1:147:A:LEU:HA	1:147:A:LEU:HD13	7	0.15
(1,1877)	1:101:A:GLN:H	1:100:A:LEU:HD11	11	0.15
(1,1877)	1:101:A:GLN:H	1:100:A:LEU:HD12	11	0.15
(1,1877)	1:101:A:GLN:H	1:100:A:LEU:HD13	11	0.15
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD11	14	0.15
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD12	14	0.15
(1,1845)	1:178:A:VAL:HA	1:181:A:LEU:HD13	14	0.15
(1,1842)	1:165:A:HIS:HA	1:166:A:CYS:HB3	12	0.15
(1,1663)	1:27:A:VAL:HG11	1:24:A:GLU:HB3	20	0.15
(1,1663)	1:27:A:VAL:HG12	1:24:A:GLU:HB3	20	0.15
(1,1663)	1:27:A:VAL:HG13	1:24:A:GLU:HB3	20	0.15
(1,1494)	1:44:A:GLN:HB3	1:44:A:GLN:HG3	4	0.15
(1,1494)	1:44:A:GLN:HB3	1:44:A:GLN:HG3	5	0.15
(1,1494)	1:44:A:GLN:HB3	1:44:A:GLN:HG3	7	0.15
(1,1494)	1:44:A:GLN:HB3	1:44:A:GLN:HG3	11	0.15
(1,1494)	1:44:A:GLN:HB3	1:44:A:GLN:HG3	12	0.15
(1,1494)	1:44:A:GLN:HB3	1:44:A:GLN:HG3	18	0.15
(1,1428)	1:31:A:THR:HB	1:32:A:GLU:HG3	13	0.15
(1,1320)	1:85:A:ILE:HG21	1:89:A:TYR:HB3	5	0.15
(1,1320)	1:85:A:ILE:HG22	1:89:A:TYR:HB3	5	0.15
(1,1320)	1:85:A:ILE:HG23	1:89:A:TYR:HB3	5	0.15
(1,1117)	1:139:A:ALA:H	1:135:A:GLY:HA3	12	0.15
(1,1111)	2:97:B:NLE:HB2	1:126:A:GLY:HA3	6	0.15
(1,1111)	2:97:B:NLE:HB3	1:126:A:GLY:HA3	6	0.15
(1,1111)	2:97:B:NLE:HB2	1:126:A:GLY:HA3	14	0.15
(1,1111)	2:97:B:NLE:HB3	1:126:A:GLY:HA3	14	0.15
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	3	0.15
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	4	0.15
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	5	0.15
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	6	0.15
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	8	0.15
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	9	0.15
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	12	0.15
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	14	0.15
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	15	0.15
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	16	0.15
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	17	0.15
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	19	0.15
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	20	0.15
(1,1037)	1:65:A:LEU:HD11	1:65:A:LEU:HA	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1037)	1:65:A:LEU:HD12	1:65:A:LEU:HA	8	0.15
(1,1037)	1:65:A:LEU:HD13	1:65:A:LEU:HA	8	0.15
(1,1037)	1:65:A:LEU:HD21	1:65:A:LEU:HA	8	0.15
(1,1037)	1:65:A:LEU:HD22	1:65:A:LEU:HA	8	0.15
(1,1037)	1:65:A:LEU:HD23	1:65:A:LEU:HA	8	0.15
(1,929)	1:150:A:PHE:H	1:151:A:LEU:HA	12	0.15
(1,839)	1:63:A:LEU:HB3	1:62:A:THR:HA	3	0.15
(1,735)	1:26:A:GLN:H	1:23:A:SER:HB3	5	0.15
(1,735)	1:26:A:GLN:H	1:23:A:SER:HB3	14	0.15
(1,543)	1:181:A:LEU:HD11	1:73:A:GLN:HE21	8	0.15
(1,543)	1:181:A:LEU:HD12	1:73:A:GLN:HE21	8	0.15
(1,543)	1:181:A:LEU:HD13	1:73:A:GLN:HE21	8	0.15
(1,510)	1:87:A:ARG:H	1:86:A:ASN:HD21	1	0.15
(1,442)	1:181:A:LEU:HD11	1:182:A:ASN:H	6	0.15
(1,442)	1:181:A:LEU:HD12	1:182:A:ASN:H	6	0.15
(1,442)	1:181:A:LEU:HD13	1:182:A:ASN:H	6	0.15
(1,154)	1:32:A:GLU:HG3	1:32:A:GLU:H	3	0.15
(1,154)	1:32:A:GLU:HG3	1:32:A:GLU:H	5	0.15
(1,106)	1:162:A:MET:HG3	1:168:A:ALA:H	14	0.15
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	11	0.15
(2,162)	1:169:A:ARG:O	1:173:A:GLN:N	13	0.14
(2,158)	1:156:A:ARG:O	1:160:A:ASP:N	7	0.14
(2,156)	1:152:A:GLY:O	1:156:A:ARG:N	10	0.14
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	19	0.14
(2,153)	1:134:A:PHE:O	1:138:A:LEU:N	8	0.14
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	13	0.14
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	17	0.14
(2,139)	1:40:A:PHE:O	1:44:A:GLN:N	14	0.14
(2,138)	1:39:A:VAL:O	1:43:A:HIS:N	20	0.14
(2,119)	1:167:A:ILE:O	1:171:A:ILE:H	10	0.14
(2,107)	1:154:A:VAL:O	1:158:A:VAL:H	20	0.14
(2,91)	1:135:A:GLY:O	1:139:A:ALA:H	3	0.14
(2,88)	1:132:A:LEU:O	1:136:A:TYR:N	9	0.14
(2,88)	1:132:A:LEU:O	1:136:A:TYR:N	17	0.14
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	1	0.14
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	6	0.14
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	10	0.14
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	15	0.14
(2,63)	1:110:A:TYR:O	1:114:A:ILE:H	9	0.14
(2,63)	1:110:A:TYR:O	1:114:A:ILE:H	10	0.14
(2,63)	1:110:A:TYR:O	1:114:A:ILE:H	15	0.14
(2,50)	1:85:A:ILE:O	1:89:A:TYR:H	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,17)	1:32:A:GLU:O	1:36:A:ARG:H	18	0.14
(2,11)	1:29:A:GLN:O	1:33:A:GLU:H	4	0.14
(1,3097)	1:126:A:GLY:H	2:101:B:ILE:HG13	1	0.14
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB1	3	0.14
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB2	3	0.14
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB3	3	0.14
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB1	10	0.14
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB2	10	0.14
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB3	10	0.14
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB1	19	0.14
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB2	19	0.14
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB3	19	0.14
(1,3086)	1:129:A:VAL:H	2:97:B:NLE:HD2	8	0.14
(1,3086)	1:129:A:VAL:H	2:97:B:NLE:HD3	8	0.14
(1,3069)	1:118:A:LEU:HD11	2:91:B:ALA:HA	10	0.14
(1,3069)	1:118:A:LEU:HD12	2:91:B:ALA:HA	10	0.14
(1,3069)	1:118:A:LEU:HD13	2:91:B:ALA:HA	10	0.14
(1,3069)	1:118:A:LEU:HD21	2:91:B:ALA:HA	10	0.14
(1,3069)	1:118:A:LEU:HD22	2:91:B:ALA:HA	10	0.14
(1,3069)	1:118:A:LEU:HD23	2:91:B:ALA:HA	10	0.14
(1,3049)	1:97:A:LEU:HD11	2:86:B:ILE:HG21	18	0.14
(1,3049)	1:97:A:LEU:HD11	2:86:B:ILE:HG22	18	0.14
(1,3049)	1:97:A:LEU:HD11	2:86:B:ILE:HG23	18	0.14
(1,3049)	1:97:A:LEU:HD12	2:86:B:ILE:HG21	18	0.14
(1,3049)	1:97:A:LEU:HD12	2:86:B:ILE:HG22	18	0.14
(1,3049)	1:97:A:LEU:HD12	2:86:B:ILE:HG23	18	0.14
(1,3049)	1:97:A:LEU:HD13	2:86:B:ILE:HG21	18	0.14
(1,3049)	1:97:A:LEU:HD13	2:86:B:ILE:HG22	18	0.14
(1,3049)	1:97:A:LEU:HD13	2:86:B:ILE:HG23	18	0.14
(1,3049)	1:97:A:LEU:HD21	2:86:B:ILE:HG21	18	0.14
(1,3049)	1:97:A:LEU:HD21	2:86:B:ILE:HG22	18	0.14
(1,3049)	1:97:A:LEU:HD21	2:86:B:ILE:HG23	18	0.14
(1,3049)	1:97:A:LEU:HD22	2:86:B:ILE:HG21	18	0.14
(1,3049)	1:97:A:LEU:HD22	2:86:B:ILE:HG22	18	0.14
(1,3049)	1:97:A:LEU:HD22	2:86:B:ILE:HG23	18	0.14
(1,3049)	1:97:A:LEU:HD23	2:86:B:ILE:HG21	18	0.14
(1,3049)	1:97:A:LEU:HD23	2:86:B:ILE:HG22	18	0.14
(1,3049)	1:97:A:LEU:HD23	2:86:B:ILE:HG23	18	0.14
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	5	0.14
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	5	0.14
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	5	0.14
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD11	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD12	3	0.14
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD13	3	0.14
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD11	3	0.14
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD12	3	0.14
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD13	3	0.14
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD11	3	0.14
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD12	3	0.14
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD13	3	0.14
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD11	9	0.14
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD12	9	0.14
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD13	9	0.14
(1,2952)	1:85:A:ILE:HD11	2:97:B:NLE:HE1	1	0.14
(1,2952)	1:85:A:ILE:HD12	2:97:B:NLE:HE1	1	0.14
(1,2952)	1:85:A:ILE:HD13	2:97:B:NLE:HE1	1	0.14
(1,2939)	2:99:B:ARG:HG3	2:100:B:SER:H	11	0.14
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	3	0.14
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	3	0.14
(1,2914)	2:90:B:LEU:HA	2:90:B:LEU:HD11	9	0.14
(1,2914)	2:90:B:LEU:HA	2:90:B:LEU:HD12	9	0.14
(1,2914)	2:90:B:LEU:HA	2:90:B:LEU:HD13	9	0.14
(1,2914)	2:90:B:LEU:HA	2:90:B:LEU:HD21	9	0.14
(1,2914)	2:90:B:LEU:HA	2:90:B:LEU:HD22	9	0.14
(1,2914)	2:90:B:LEU:HA	2:90:B:LEU:HD23	9	0.14
(1,2812)	2:97:B:NLE:HB2	2:101:B:ILE:HG21	9	0.14
(1,2812)	2:97:B:NLE:HB2	2:101:B:ILE:HG22	9	0.14
(1,2812)	2:97:B:NLE:HB2	2:101:B:ILE:HG23	9	0.14
(1,2812)	2:97:B:NLE:HB3	2:101:B:ILE:HG21	9	0.14
(1,2812)	2:97:B:NLE:HB3	2:101:B:ILE:HG22	9	0.14
(1,2812)	2:97:B:NLE:HB3	2:101:B:ILE:HG23	9	0.14
(1,2795)	2:88:B:ARG:HA	2:91:B:ALA:H	17	0.14
(1,2779)	2:88:B:ARG:HB3	2:88:B:ARG:HD3	3	0.14
(1,2772)	2:83:B:ILE:HB	2:84:B:ARG:H	3	0.14
(1,2758)	2:82:B:ILE:HB	2:83:B:ILE:H	2	0.14
(1,2758)	2:82:B:ILE:HB	2:83:B:ILE:H	10	0.14
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HD	9	0.14
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HDA	9	0.14
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HD	10	0.14
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HDA	10	0.14
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HD	17	0.14
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HDA	17	0.14
(1,2494)	1:131:A:LEU:HD21	1:119:A:PHE:HZ	8	0.14
(1,2494)	1:131:A:LEU:HD22	1:119:A:PHE:HZ	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2494)	1:131:A:LEU:HD23	1:119:A:PHE:HZ	8	0.14
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE1	8	0.14
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE2	8	0.14
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE1	16	0.14
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE2	16	0.14
(1,2436)	1:154:A:VAL:HA	1:157:A:PHE:HE1	3	0.14
(1,2436)	1:154:A:VAL:HA	1:157:A:PHE:HE2	3	0.14
(1,2310)	1:27:A:VAL:HG21	1:171:A:ILE:HD11	1	0.14
(1,2310)	1:27:A:VAL:HG21	1:171:A:ILE:HD12	1	0.14
(1,2310)	1:27:A:VAL:HG21	1:171:A:ILE:HD13	1	0.14
(1,2310)	1:27:A:VAL:HG22	1:171:A:ILE:HD11	1	0.14
(1,2310)	1:27:A:VAL:HG22	1:171:A:ILE:HD12	1	0.14
(1,2310)	1:27:A:VAL:HG22	1:171:A:ILE:HD13	1	0.14
(1,2310)	1:27:A:VAL:HG23	1:171:A:ILE:HD11	1	0.14
(1,2310)	1:27:A:VAL:HG23	1:171:A:ILE:HD12	1	0.14
(1,2310)	1:27:A:VAL:HG23	1:171:A:ILE:HD13	1	0.14
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD11	8	0.14
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD12	8	0.14
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD13	8	0.14
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD11	18	0.14
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD12	18	0.14
(1,2300)	1:76:A:ARG:HD3	1:80:A:ILE:HD13	18	0.14
(1,2271)	1:162:A:MET:HE1	1:171:A:ILE:HG21	10	0.14
(1,2271)	1:162:A:MET:HE1	1:171:A:ILE:HG22	10	0.14
(1,2271)	1:162:A:MET:HE1	1:171:A:ILE:HG23	10	0.14
(1,2271)	1:162:A:MET:HE2	1:171:A:ILE:HG21	10	0.14
(1,2271)	1:162:A:MET:HE2	1:171:A:ILE:HG22	10	0.14
(1,2271)	1:162:A:MET:HE2	1:171:A:ILE:HG23	10	0.14
(1,2271)	1:162:A:MET:HE3	1:171:A:ILE:HG21	10	0.14
(1,2271)	1:162:A:MET:HE3	1:171:A:ILE:HG22	10	0.14
(1,2271)	1:162:A:MET:HE3	1:171:A:ILE:HG23	10	0.14
(1,2225)	1:78:A:LEU:H	1:81:A:ILE:HG21	4	0.14
(1,2225)	1:78:A:LEU:H	1:81:A:ILE:HG22	4	0.14
(1,2225)	1:78:A:LEU:H	1:81:A:ILE:HG23	4	0.14
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG11	20	0.14
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG12	20	0.14
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG13	20	0.14
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG21	4	0.14
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG22	4	0.14
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG23	4	0.14
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG21	16	0.14
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG22	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG23	16	0.14
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG21	4	0.14
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG22	4	0.14
(1,2044)	1:177:A:TRP:HE1	1:27:A:VAL:HG23	4	0.14
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG21	1	0.14
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG22	1	0.14
(1,1962)	1:75:A:GLY:H	1:74:A:VAL:HG23	1	0.14
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD21	10	0.14
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD22	10	0.14
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD23	10	0.14
(1,1842)	1:165:A:HIS:HA	1:166:A:CYS:HB3	13	0.14
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	1	0.14
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	4	0.14
(1,1494)	1:44:A:GLN:HB3	1:44:A:GLN:HG3	15	0.14
(1,1483)	1:143:A:TYR:HE1	1:144:A:GLN:HG3	18	0.14
(1,1483)	1:143:A:TYR:HE2	1:144:A:GLN:HG3	18	0.14
(1,1428)	1:31:A:THR:HB	1:32:A:GLU:HG3	4	0.14
(1,1140)	1:81:A:ILE:HG21	1:184:A:GLY:HA2	9	0.14
(1,1140)	1:81:A:ILE:HG22	1:184:A:GLY:HA2	9	0.14
(1,1140)	1:81:A:ILE:HG23	1:184:A:GLY:HA2	9	0.14
(1,1138)	1:52:A:VAL:HG11	1:51:A:GLY:HA3	12	0.14
(1,1138)	1:52:A:VAL:HG12	1:51:A:GLY:HA3	12	0.14
(1,1138)	1:52:A:VAL:HG13	1:51:A:GLY:HA3	12	0.14
(1,1138)	1:52:A:VAL:HG21	1:51:A:GLY:HA3	12	0.14
(1,1138)	1:52:A:VAL:HG22	1:51:A:GLY:HA3	12	0.14
(1,1138)	1:52:A:VAL:HG23	1:51:A:GLY:HA3	12	0.14
(1,1117)	1:139:A:ALA:H	1:135:A:GLY:HA3	19	0.14
(1,1111)	2:97:B:NLE:HB2	1:126:A:GLY:HA3	12	0.14
(1,1111)	2:97:B:NLE:HB3	1:126:A:GLY:HA3	12	0.14
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	20	0.14
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	1	0.14
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	2	0.14
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	13	0.14
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	18	0.14
(1,1032)	1:131:A:LEU:HD21	1:115:A:ALA:HA	3	0.14
(1,1032)	1:131:A:LEU:HD22	1:115:A:ALA:HA	3	0.14
(1,1032)	1:131:A:LEU:HD23	1:115:A:ALA:HA	3	0.14
(1,960)	1:163:A:LEU:HD11	1:164:A:HIS:HA	5	0.14
(1,960)	1:163:A:LEU:HD12	1:164:A:HIS:HA	5	0.14
(1,960)	1:163:A:LEU:HD13	1:164:A:HIS:HA	5	0.14
(1,960)	1:163:A:LEU:HD21	1:164:A:HIS:HA	5	0.14
(1,960)	1:163:A:LEU:HD22	1:164:A:HIS:HA	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,960)	1:163:A:LEU:HD23	1:164:A:HIS:HA	5	0.14
(1,960)	1:163:A:LEU:HD11	1:164:A:HIS:HA	10	0.14
(1,960)	1:163:A:LEU:HD12	1:164:A:HIS:HA	10	0.14
(1,960)	1:163:A:LEU:HD13	1:164:A:HIS:HA	10	0.14
(1,960)	1:163:A:LEU:HD21	1:164:A:HIS:HA	10	0.14
(1,960)	1:163:A:LEU:HD22	1:164:A:HIS:HA	10	0.14
(1,960)	1:163:A:LEU:HD23	1:164:A:HIS:HA	10	0.14
(1,947)	1:144:A:GLN:HE21	1:144:A:GLN:HA	6	0.14
(1,941)	1:68:A:SER:HB3	1:68:A:SER:HA	4	0.14
(1,941)	1:68:A:SER:HB3	1:68:A:SER:HA	8	0.14
(1,941)	1:68:A:SER:HB3	1:68:A:SER:HA	14	0.14
(1,757)	1:41:A:TYR:HE1	1:41:A:TYR:HA	17	0.14
(1,757)	1:41:A:TYR:HE2	1:41:A:TYR:HA	17	0.14
(1,733)	1:26:A:GLN:HG3	1:23:A:SER:HB3	1	0.14
(1,733)	1:26:A:GLN:HG3	1:23:A:SER:HB3	10	0.14
(1,733)	1:26:A:GLN:HG3	1:23:A:SER:HB3	15	0.14
(1,687)	1:24:A:GLU:HA	1:27:A:VAL:HA	4	0.14
(1,531)	1:23:A:SER:H	1:26:A:GLN:HE22	8	0.14
(1,490)	1:164:A:HIS:HB3	1:164:A:HIS:H	19	0.14
(1,442)	1:181:A:LEU:HD11	1:182:A:ASN:H	12	0.14
(1,442)	1:181:A:LEU:HD12	1:182:A:ASN:H	12	0.14
(1,442)	1:181:A:LEU:HD13	1:182:A:ASN:H	12	0.14
(1,424)	1:163:A:LEU:HD11	1:165:A:HIS:H	4	0.14
(1,424)	1:163:A:LEU:HD12	1:165:A:HIS:H	4	0.14
(1,424)	1:163:A:LEU:HD13	1:165:A:HIS:H	4	0.14
(1,424)	1:163:A:LEU:HD21	1:165:A:HIS:H	4	0.14
(1,424)	1:163:A:LEU:HD22	1:165:A:HIS:H	4	0.14
(1,424)	1:163:A:LEU:HD23	1:165:A:HIS:H	4	0.14
(1,154)	1:32:A:GLU:HG3	1:32:A:GLU:H	9	0.14
(1,154)	1:32:A:GLU:HG3	1:32:A:GLU:H	19	0.14
(1,123)	1:34:A:VAL:HG11	1:74:A:VAL:H	2	0.14
(1,123)	1:34:A:VAL:HG12	1:74:A:VAL:H	2	0.14
(1,123)	1:34:A:VAL:HG13	1:74:A:VAL:H	2	0.14
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	2	0.14
(1,78)	1:64:A:PRO:HB3	1:65:A:LEU:H	13	0.14
(2,159)	1:158:A:VAL:O	1:162:A:MET:N	3	0.13
(2,154)	1:150:A:PHE:O	1:154:A:VAL:N	1	0.13
(2,153)	1:134:A:PHE:O	1:138:A:LEU:N	5	0.13
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	11	0.13
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	20	0.13
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	5	0.13
(2,136)	1:37:A:SER:O	1:41:A:TYR:N	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,128)	1:27:A:VAL:O	1:31:A:THR:N	6	0.13
(2,125)	1:170:A:TRP:O	1:174:A:ARG:H	10	0.13
(2,113)	1:157:A:PHE:O	1:161:A:PHE:H	5	0.13
(2,110)	1:155:A:THR:O	1:159:A:VAL:N	6	0.13
(2,109)	1:155:A:THR:O	1:159:A:VAL:H	10	0.13
(2,91)	1:135:A:GLY:O	1:139:A:ALA:H	4	0.13
(2,88)	1:132:A:LEU:O	1:136:A:TYR:N	2	0.13
(2,88)	1:132:A:LEU:O	1:136:A:TYR:N	5	0.13
(2,88)	1:132:A:LEU:O	1:136:A:TYR:N	14	0.13
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	11	0.13
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	13	0.13
(2,75)	1:124:A:ASN:O	1:128:A:VAL:H	4	0.13
(2,75)	1:124:A:ASN:O	1:128:A:VAL:H	16	0.13
(2,71)	1:114:A:ILE:O	1:118:A:LEU:H	14	0.13
(2,63)	1:110:A:TYR:O	1:114:A:ILE:H	4	0.13
(2,63)	1:110:A:TYR:O	1:114:A:ILE:H	8	0.13
(2,63)	1:110:A:TYR:O	1:114:A:ILE:H	18	0.13
(2,53)	1:93:A:PHE:O	1:97:A:LEU:H	15	0.13
(2,17)	1:32:A:GLU:O	1:36:A:ARG:H	4	0.13
(2,13)	1:30:A:ASP:O	1:34:A:VAL:H	18	0.13
(2,11)	1:29:A:GLN:O	1:33:A:GLU:H	10	0.13
(2,11)	1:29:A:GLN:O	1:33:A:GLU:H	12	0.13
(2,11)	1:29:A:GLN:O	1:33:A:GLU:H	15	0.13
(2,9)	1:28:A:ALA:O	1:32:A:GLU:H	3	0.13
(1,3097)	1:126:A:GLY:H	2:101:B:ILE:HG13	5	0.13
(1,3097)	1:126:A:GLY:H	2:101:B:ILE:HG13	11	0.13
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB1	2	0.13
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB2	2	0.13
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB3	2	0.13
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB1	8	0.13
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB2	8	0.13
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB3	8	0.13
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB1	9	0.13
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB2	9	0.13
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB3	9	0.13
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB1	11	0.13
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB2	11	0.13
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB3	11	0.13
(1,3086)	1:129:A:VAL:H	2:97:B:NLE:HD2	3	0.13
(1,3086)	1:129:A:VAL:H	2:97:B:NLE:HD3	3	0.13
(1,3086)	1:129:A:VAL:H	2:97:B:NLE:HD2	12	0.13
(1,3086)	1:129:A:VAL:H	2:97:B:NLE:HD3	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3069)	1:118:A:LEU:HD11	2:91:B:ALA:HA	5	0.13
(1,3069)	1:118:A:LEU:HD12	2:91:B:ALA:HA	5	0.13
(1,3069)	1:118:A:LEU:HD13	2:91:B:ALA:HA	5	0.13
(1,3069)	1:118:A:LEU:HD21	2:91:B:ALA:HA	5	0.13
(1,3069)	1:118:A:LEU:HD22	2:91:B:ALA:HA	5	0.13
(1,3069)	1:118:A:LEU:HD23	2:91:B:ALA:HA	5	0.13
(1,3069)	1:118:A:LEU:HD11	2:91:B:ALA:HA	11	0.13
(1,3069)	1:118:A:LEU:HD12	2:91:B:ALA:HA	11	0.13
(1,3069)	1:118:A:LEU:HD13	2:91:B:ALA:HA	11	0.13
(1,3069)	1:118:A:LEU:HD21	2:91:B:ALA:HA	11	0.13
(1,3069)	1:118:A:LEU:HD22	2:91:B:ALA:HA	11	0.13
(1,3069)	1:118:A:LEU:HD23	2:91:B:ALA:HA	11	0.13
(1,3055)	1:100:A:LEU:HD11	2:82:B:ILE:HG21	17	0.13
(1,3055)	1:100:A:LEU:HD11	2:82:B:ILE:HG22	17	0.13
(1,3055)	1:100:A:LEU:HD11	2:82:B:ILE:HG23	17	0.13
(1,3055)	1:100:A:LEU:HD12	2:82:B:ILE:HG21	17	0.13
(1,3055)	1:100:A:LEU:HD12	2:82:B:ILE:HG22	17	0.13
(1,3055)	1:100:A:LEU:HD12	2:82:B:ILE:HG23	17	0.13
(1,3055)	1:100:A:LEU:HD13	2:82:B:ILE:HG21	17	0.13
(1,3055)	1:100:A:LEU:HD13	2:82:B:ILE:HG22	17	0.13
(1,3055)	1:100:A:LEU:HD13	2:82:B:ILE:HG23	17	0.13
(1,3055)	1:100:A:LEU:HD21	2:82:B:ILE:HG21	17	0.13
(1,3055)	1:100:A:LEU:HD21	2:82:B:ILE:HG22	17	0.13
(1,3055)	1:100:A:LEU:HD21	2:82:B:ILE:HG23	17	0.13
(1,3055)	1:100:A:LEU:HD22	2:82:B:ILE:HG21	17	0.13
(1,3055)	1:100:A:LEU:HD22	2:82:B:ILE:HG22	17	0.13
(1,3055)	1:100:A:LEU:HD22	2:82:B:ILE:HG23	17	0.13
(1,3055)	1:100:A:LEU:HD23	2:82:B:ILE:HG21	17	0.13
(1,3055)	1:100:A:LEU:HD23	2:82:B:ILE:HG22	17	0.13
(1,3055)	1:100:A:LEU:HD23	2:82:B:ILE:HG23	17	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD11	2	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD12	2	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD13	2	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD11	4	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD12	4	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD13	4	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD11	9	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD12	9	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD13	9	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD11	12	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD12	12	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD13	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD11	14	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD12	14	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD13	14	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD11	17	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD12	17	0.13
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD13	17	0.13
(1,2983)	1:85:A:ILE:HG21	2:93:B:VAL:HB	15	0.13
(1,2983)	1:85:A:ILE:HG22	2:93:B:VAL:HB	15	0.13
(1,2983)	1:85:A:ILE:HG23	2:93:B:VAL:HB	15	0.13
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD11	1	0.13
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD12	1	0.13
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD13	1	0.13
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD11	1	0.13
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD12	1	0.13
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD13	1	0.13
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD11	1	0.13
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD12	1	0.13
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD13	1	0.13
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD11	5	0.13
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD12	5	0.13
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD13	5	0.13
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD11	5	0.13
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD12	5	0.13
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD13	5	0.13
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD11	5	0.13
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD12	5	0.13
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD13	5	0.13
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD11	13	0.13
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD12	13	0.13
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD13	13	0.13
(1,2795)	2:88:B:ARG:HA	2:91:B:ALA:H	10	0.13
(1,2772)	2:83:B:ILE:HB	2:84:B:ARG:H	19	0.13
(1,2758)	2:82:B:ILE:HB	2:83:B:ILE:H	1	0.13
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HD	1	0.13
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HDA	1	0.13
(1,2658)	2:89:B:HIS:HA	2:92:B:MK8:HB	15	0.13
(1,2636)	2:90:B:LEU:HA	2:93:B:VAL:HB	2	0.13
(1,2394)	1:107:A:ALA:HB1	1:150:A:PHE:HD1	3	0.13
(1,2394)	1:107:A:ALA:HB1	1:150:A:PHE:HD2	3	0.13
(1,2394)	1:107:A:ALA:HB2	1:150:A:PHE:HD1	3	0.13
(1,2394)	1:107:A:ALA:HB2	1:150:A:PHE:HD2	3	0.13
(1,2394)	1:107:A:ALA:HB3	1:150:A:PHE:HD1	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2394)	1:107:A:ALA:HB3	1:150:A:PHE:HD2	3	0.13
(1,2394)	1:107:A:ALA:HB1	1:150:A:PHE:HD1	7	0.13
(1,2394)	1:107:A:ALA:HB1	1:150:A:PHE:HD2	7	0.13
(1,2394)	1:107:A:ALA:HB2	1:150:A:PHE:HD1	7	0.13
(1,2394)	1:107:A:ALA:HB2	1:150:A:PHE:HD2	7	0.13
(1,2394)	1:107:A:ALA:HB3	1:150:A:PHE:HD1	7	0.13
(1,2394)	1:107:A:ALA:HB3	1:150:A:PHE:HD2	7	0.13
(1,2241)	1:28:A:ALA:H	1:168:A:ALA:HB1	2	0.13
(1,2241)	1:28:A:ALA:H	1:168:A:ALA:HB2	2	0.13
(1,2241)	1:28:A:ALA:H	1:168:A:ALA:HB3	2	0.13
(1,2206)	1:129:A:VAL:HB	1:130:A:ALA:HB1	12	0.13
(1,2206)	1:129:A:VAL:HB	1:130:A:ALA:HB2	12	0.13
(1,2206)	1:129:A:VAL:HB	1:130:A:ALA:HB3	12	0.13
(1,2114)	1:46:A:GLU:HA	1:49:A:ALA:HB1	3	0.13
(1,2114)	1:46:A:GLU:HA	1:49:A:ALA:HB2	3	0.13
(1,2114)	1:46:A:GLU:HA	1:49:A:ALA:HB3	3	0.13
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG11	1	0.13
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG12	1	0.13
(1,2108)	1:150:A:PHE:HB3	1:142:A:VAL:HG13	1	0.13
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG21	7	0.13
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG22	7	0.13
(1,2094)	1:177:A:TRP:HZ3	1:34:A:VAL:HG23	7	0.13
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG21	1	0.13
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG22	1	0.13
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG23	1	0.13
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG21	20	0.13
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG22	20	0.13
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG23	20	0.13
(1,2014)	1:159:A:VAL:HA	1:159:A:VAL:HG11	2	0.13
(1,2014)	1:159:A:VAL:HA	1:159:A:VAL:HG12	2	0.13
(1,2014)	1:159:A:VAL:HA	1:159:A:VAL:HG13	2	0.13
(1,2014)	1:159:A:VAL:HA	1:159:A:VAL:HG11	6	0.13
(1,2014)	1:159:A:VAL:HA	1:159:A:VAL:HG12	6	0.13
(1,2014)	1:159:A:VAL:HA	1:159:A:VAL:HG13	6	0.13
(1,2014)	1:159:A:VAL:HA	1:159:A:VAL:HG11	12	0.13
(1,2014)	1:159:A:VAL:HA	1:159:A:VAL:HG12	12	0.13
(1,2014)	1:159:A:VAL:HA	1:159:A:VAL:HG13	12	0.13
(1,2014)	1:159:A:VAL:HA	1:159:A:VAL:HG11	20	0.13
(1,2014)	1:159:A:VAL:HA	1:159:A:VAL:HG12	20	0.13
(1,2014)	1:159:A:VAL:HA	1:159:A:VAL:HG13	20	0.13
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD21	17	0.13
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD22	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1946)	1:110:A:TYR:HA	1:100:A:LEU:HD23	17	0.13
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG11	12	0.13
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG12	12	0.13
(1,1931)	1:71:A:MET:HA	1:74:A:VAL:HG13	12	0.13
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD21	6	0.13
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD22	6	0.13
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD23	6	0.13
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD21	6	0.13
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD22	6	0.13
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD23	6	0.13
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD21	6	0.13
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD22	6	0.13
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD23	6	0.13
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD21	10	0.13
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD22	10	0.13
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD23	10	0.13
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD21	10	0.13
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD22	10	0.13
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD23	10	0.13
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD21	10	0.13
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD22	10	0.13
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD23	10	0.13
(1,1893)	1:147:A:LEU:H	1:147:A:LEU:HD21	11	0.13
(1,1893)	1:147:A:LEU:H	1:147:A:LEU:HD22	11	0.13
(1,1893)	1:147:A:LEU:H	1:147:A:LEU:HD23	11	0.13
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD11	10	0.13
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD12	10	0.13
(1,1871)	1:63:A:LEU:HA	1:63:A:LEU:HD13	10	0.13
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD21	1	0.13
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD22	1	0.13
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD23	1	0.13
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD21	1	0.13
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD22	1	0.13
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD23	1	0.13
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD21	1	0.13
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD22	1	0.13
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD23	1	0.13
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD21	1	0.13
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD22	1	0.13
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD23	1	0.13
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD21	1	0.13
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD22	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD23	1	0.13
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD21	1	0.13
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD22	1	0.13
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD23	1	0.13
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	3	0.13
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	14	0.13
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	19	0.13
(1,1709)	1:98:A:GLN:HE22	1:98:A:GLN:HB3	11	0.13
(1,1707)	1:94:A:GLN:HE22	1:94:A:GLN:HB3	4	0.13
(1,1534)	1:160:A:ASP:H	1:159:A:VAL:HB	2	0.13
(1,1494)	1:44:A:GLN:HB3	1:44:A:GLN:HG3	13	0.13
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	20	0.13
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	16	0.13
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	10	0.13
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	11	0.13
(1,1037)	1:65:A:LEU:HD11	1:65:A:LEU:HA	1	0.13
(1,1037)	1:65:A:LEU:HD12	1:65:A:LEU:HA	1	0.13
(1,1037)	1:65:A:LEU:HD13	1:65:A:LEU:HA	1	0.13
(1,1037)	1:65:A:LEU:HD21	1:65:A:LEU:HA	1	0.13
(1,1037)	1:65:A:LEU:HD22	1:65:A:LEU:HA	1	0.13
(1,1037)	1:65:A:LEU:HD23	1:65:A:LEU:HA	1	0.13
(1,941)	1:68:A:SER:HB3	1:68:A:SER:HA	6	0.13
(1,941)	1:68:A:SER:HB3	1:68:A:SER:HA	10	0.13
(1,941)	1:68:A:SER:HB3	1:68:A:SER:HA	18	0.13
(1,923)	1:76:A:ARG:HG3	1:77:A:GLN:HA	14	0.13
(1,901)	1:94:A:GLN:H	1:92:A:GLU:HA	4	0.13
(1,901)	1:94:A:GLN:H	1:92:A:GLU:HA	5	0.13
(1,757)	1:41:A:TYR:HE1	1:41:A:TYR:HA	4	0.13
(1,757)	1:41:A:TYR:HE2	1:41:A:TYR:HA	4	0.13
(1,757)	1:41:A:TYR:HE1	1:41:A:TYR:HA	11	0.13
(1,757)	1:41:A:TYR:HE2	1:41:A:TYR:HA	11	0.13
(1,531)	1:23:A:SER:H	1:26:A:GLN:HE22	10	0.13
(1,490)	1:164:A:HIS:HB3	1:164:A:HIS:H	15	0.13
(1,442)	1:181:A:LEU:HD11	1:182:A:ASN:H	4	0.13
(1,442)	1:181:A:LEU:HD12	1:182:A:ASN:H	4	0.13
(1,442)	1:181:A:LEU:HD13	1:182:A:ASN:H	4	0.13
(1,368)	1:119:A:PHE:HA	1:123:A:ILE:H	1	0.13
(1,320)	1:163:A:LEU:HD11	1:29:A:GLN:H	10	0.13
(1,320)	1:163:A:LEU:HD12	1:29:A:GLN:H	10	0.13
(1,320)	1:163:A:LEU:HD13	1:29:A:GLN:H	10	0.13
(1,320)	1:163:A:LEU:HD21	1:29:A:GLN:H	10	0.13
(1,320)	1:163:A:LEU:HD22	1:29:A:GLN:H	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:163:A:LEU:HD23	1:29:A:GLN:H	10	0.13
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	1	0.13
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	1	0.13
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	1	0.13
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	12	0.13
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	12	0.13
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	12	0.13
(1,318)	1:27:A:VAL:HG11	1:177:A:TRP:H	20	0.13
(1,318)	1:27:A:VAL:HG12	1:177:A:TRP:H	20	0.13
(1,318)	1:27:A:VAL:HG13	1:177:A:TRP:H	20	0.13
(1,283)	1:42:A:ARG:HB3	1:41:A:TYR:H	20	0.13
(1,175)	1:118:A:LEU:HD11	1:131:A:LEU:H	11	0.13
(1,175)	1:118:A:LEU:HD12	1:131:A:LEU:H	11	0.13
(1,175)	1:118:A:LEU:HD13	1:131:A:LEU:H	11	0.13
(1,154)	1:32:A:GLU:HG3	1:32:A:GLU:H	11	0.13
(1,154)	1:32:A:GLU:HG3	1:32:A:GLU:H	13	0.13
(1,9)	1:174:A:ARG:HA	1:125:A:TRP:HE1	4	0.13
(2,157)	1:153:A:GLN:O	1:157:A:PHE:N	19	0.12
(2,153)	1:134:A:PHE:O	1:138:A:LEU:N	4	0.12
(2,153)	1:134:A:PHE:O	1:138:A:LEU:N	10	0.12
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	1	0.12
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	9	0.12
(2,150)	1:113:A:LYS:O	1:117:A:SER:N	5	0.12
(2,146)	1:107:A:ALA:O	1:111:A:PHE:N	3	0.12
(2,145)	1:106:A:ASN:O	1:110:A:TYR:N	11	0.12
(2,142)	1:84:A:ASP:O	1:88:A:ARG:N	18	0.12
(2,140)	1:78:A:LEU:O	1:82:A:GLY:N	6	0.12
(2,136)	1:37:A:SER:O	1:41:A:TYR:N	6	0.12
(2,123)	1:169:A:ARG:O	1:173:A:GLN:H	20	0.12
(2,115)	1:158:A:VAL:O	1:162:A:MET:H	4	0.12
(2,98)	1:139:A:ALA:O	1:143:A:TYR:N	7	0.12
(2,95)	1:137:A:ARG:O	1:141:A:HIS:H	2	0.12
(2,88)	1:132:A:LEU:O	1:136:A:TYR:N	7	0.12
(2,88)	1:132:A:LEU:O	1:136:A:TYR:N	16	0.12
(2,88)	1:132:A:LEU:O	1:136:A:TYR:N	20	0.12
(2,87)	1:132:A:LEU:O	1:136:A:TYR:H	4	0.12
(2,75)	1:124:A:ASN:O	1:128:A:VAL:H	3	0.12
(2,75)	1:124:A:ASN:O	1:128:A:VAL:H	6	0.12
(2,75)	1:124:A:ASN:O	1:128:A:VAL:H	8	0.12
(2,75)	1:124:A:ASN:O	1:128:A:VAL:H	14	0.12
(2,71)	1:114:A:ILE:O	1:118:A:LEU:H	19	0.12
(2,63)	1:110:A:TYR:O	1:114:A:ILE:H	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,57)	1:106:A:ASN:O	1:110:A:TYR:H	5	0.12
(2,57)	1:106:A:ASN:O	1:110:A:TYR:H	10	0.12
(2,50)	1:85:A:ILE:O	1:89:A:TYR:H	1	0.12
(2,50)	1:85:A:ILE:O	1:89:A:TYR:H	7	0.12
(2,47)	1:83:A:ASP:O	1:87:A:ARG:N	10	0.12
(2,47)	1:83:A:ASP:O	1:87:A:ARG:N	20	0.12
(2,31)	1:39:A:VAL:O	1:43:A:HIS:H	13	0.12
(2,31)	1:39:A:VAL:O	1:43:A:HIS:H	15	0.12
(2,19)	1:33:A:GLU:O	1:37:A:SER:H	14	0.12
(2,17)	1:32:A:GLU:O	1:36:A:ARG:H	12	0.12
(2,17)	1:32:A:GLU:O	1:36:A:ARG:H	19	0.12
(2,11)	1:29:A:GLN:O	1:33:A:GLU:H	1	0.12
(2,11)	1:29:A:GLN:O	1:33:A:GLU:H	8	0.12
(2,11)	1:29:A:GLN:O	1:33:A:GLU:H	9	0.12
(2,11)	1:29:A:GLN:O	1:33:A:GLU:H	14	0.12
(2,10)	1:28:A:ALA:O	1:32:A:GLU:N	10	0.12
(2,9)	1:28:A:ALA:O	1:32:A:GLU:H	1	0.12
(2,5)	1:26:A:GLN:O	1:30:A:ASP:H	6	0.12
(1,3097)	1:126:A:GLY:H	2:101:B:ILE:HG13	12	0.12
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB1	4	0.12
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB2	4	0.12
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB3	4	0.12
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB1	12	0.12
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB2	12	0.12
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB3	12	0.12
(1,3086)	1:129:A:VAL:H	2:97:B:NLE:HD2	17	0.12
(1,3086)	1:129:A:VAL:H	2:97:B:NLE:HD3	17	0.12
(1,3045)	1:81:A:ILE:HG13	2:101:B:ILE:HG21	16	0.12
(1,3045)	1:81:A:ILE:HG13	2:101:B:ILE:HG22	16	0.12
(1,3045)	1:81:A:ILE:HG13	2:101:B:ILE:HG23	16	0.12
(1,3044)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	1	0.12
(1,3044)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	1	0.12
(1,3044)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	1	0.12
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD11	11	0.12
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD12	11	0.12
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD13	11	0.12
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD11	18	0.12
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD12	18	0.12
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD13	18	0.12
(1,2983)	1:85:A:ILE:HG21	2:93:B:VAL:HB	14	0.12
(1,2983)	1:85:A:ILE:HG22	2:93:B:VAL:HB	14	0.12
(1,2983)	1:85:A:ILE:HG23	2:93:B:VAL:HB	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD11	12	0.12
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD12	12	0.12
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD13	12	0.12
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD11	12	0.12
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD12	12	0.12
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD13	12	0.12
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD11	12	0.12
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD12	12	0.12
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD13	12	0.12
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD11	18	0.12
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD12	18	0.12
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD13	18	0.12
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD11	18	0.12
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD12	18	0.12
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD13	18	0.12
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD11	18	0.12
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD12	18	0.12
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD13	18	0.12
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD11	3	0.12
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD12	3	0.12
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD13	3	0.12
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD11	16	0.12
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD12	16	0.12
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD13	16	0.12
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	20	0.12
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	20	0.12
(1,2888)	2:83:B:ILE:H	2:83:B:ILE:HG13	19	0.12
(1,2751)	2:86:B:ILE:H	2:87:B:ALA:H	8	0.12
(1,2701)	2:97:B:NLE:H	2:97:B:NLE:HD2	5	0.12
(1,2701)	2:97:B:NLE:H	2:97:B:NLE:HD3	5	0.12
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HD	18	0.12
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HDA	18	0.12
(1,2636)	2:90:B:LEU:HA	2:93:B:VAL:HB	20	0.12
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE1	14	0.12
(1,2447)	1:131:A:LEU:HB3	1:119:A:PHE:HE2	14	0.12
(1,2365)	2:93:B:VAL:HG21	1:89:A:TYR:HD1	17	0.12
(1,2365)	2:93:B:VAL:HG21	1:89:A:TYR:HD2	17	0.12
(1,2365)	2:93:B:VAL:HG22	1:89:A:TYR:HD1	17	0.12
(1,2365)	2:93:B:VAL:HG22	1:89:A:TYR:HD2	17	0.12
(1,2365)	2:93:B:VAL:HG23	1:89:A:TYR:HD1	17	0.12
(1,2365)	2:93:B:VAL:HG23	1:89:A:TYR:HD2	17	0.12
(1,2352)	1:44:A:GLN:HB3	1:41:A:TYR:HD1	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2352)	1:44:A:GLN:HB3	1:41:A:TYR:HD2	9	0.12
(1,2241)	1:28:A:ALA:H	1:168:A:ALA:HB1	20	0.12
(1,2241)	1:28:A:ALA:H	1:168:A:ALA:HB2	20	0.12
(1,2241)	1:28:A:ALA:H	1:168:A:ALA:HB3	20	0.12
(1,2206)	1:129:A:VAL:HB	1:130:A:ALA:HB1	3	0.12
(1,2206)	1:129:A:VAL:HB	1:130:A:ALA:HB2	3	0.12
(1,2206)	1:129:A:VAL:HB	1:130:A:ALA:HB3	3	0.12
(1,2206)	1:129:A:VAL:HB	1:130:A:ALA:HB1	10	0.12
(1,2206)	1:129:A:VAL:HB	1:130:A:ALA:HB2	10	0.12
(1,2206)	1:129:A:VAL:HB	1:130:A:ALA:HB3	10	0.12
(1,2206)	1:129:A:VAL:HB	1:130:A:ALA:HB1	17	0.12
(1,2206)	1:129:A:VAL:HB	1:130:A:ALA:HB2	17	0.12
(1,2206)	1:129:A:VAL:HB	1:130:A:ALA:HB3	17	0.12
(1,2201)	1:97:A:LEU:HA	1:96:A:MET:HE1	6	0.12
(1,2201)	1:97:A:LEU:HA	1:96:A:MET:HE2	6	0.12
(1,2201)	1:97:A:LEU:HA	1:96:A:MET:HE3	6	0.12
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG21	17	0.12
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG22	17	0.12
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG23	17	0.12
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG11	16	0.12
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG12	16	0.12
(1,2016)	1:32:A:GLU:H	1:159:A:VAL:HG13	16	0.12
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG21	20	0.12
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG22	20	0.12
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG23	20	0.12
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD21	9	0.12
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD22	9	0.12
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD23	9	0.12
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD21	9	0.12
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD22	9	0.12
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD23	9	0.12
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD21	9	0.12
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD22	9	0.12
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD23	9	0.12
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD21	11	0.12
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD22	11	0.12
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD23	11	0.12
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD21	11	0.12
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD22	11	0.12
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD23	11	0.12
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD21	11	0.12
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD22	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD23	11	0.12
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD21	16	0.12
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD22	16	0.12
(1,1899)	2:101:B:ILE:HD11	1:183:A:LEU:HD23	16	0.12
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD21	16	0.12
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD22	16	0.12
(1,1899)	2:101:B:ILE:HD12	1:183:A:LEU:HD23	16	0.12
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD21	16	0.12
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD22	16	0.12
(1,1899)	2:101:B:ILE:HD13	1:183:A:LEU:HD23	16	0.12
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD11	13	0.12
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD12	13	0.12
(1,1874)	1:65:A:LEU:HD11	1:63:A:LEU:HD13	13	0.12
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD11	13	0.12
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD12	13	0.12
(1,1874)	1:65:A:LEU:HD12	1:63:A:LEU:HD13	13	0.12
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD11	13	0.12
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD12	13	0.12
(1,1874)	1:65:A:LEU:HD13	1:63:A:LEU:HD13	13	0.12
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD11	13	0.12
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD12	13	0.12
(1,1874)	1:65:A:LEU:HD21	1:63:A:LEU:HD13	13	0.12
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD11	13	0.12
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD12	13	0.12
(1,1874)	1:65:A:LEU:HD22	1:63:A:LEU:HD13	13	0.12
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD11	13	0.12
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD12	13	0.12
(1,1874)	1:65:A:LEU:HD23	1:63:A:LEU:HD13	13	0.12
(1,1768)	1:97:A:LEU:H	1:97:A:LEU:HG	16	0.12
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	2	0.12
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	6	0.12
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	7	0.12
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	9	0.12
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	10	0.12
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	13	0.12
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	15	0.12
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	16	0.12
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	17	0.12
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	20	0.12
(1,1660)	1:47:A:GLN:HE21	1:46:A:GLU:HB3	1	0.12
(1,1660)	1:47:A:GLN:HE21	1:46:A:GLU:HB3	5	0.12
(1,1534)	1:160:A:ASP:H	1:159:A:VAL:HB	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1494)	1:44:A:GLN:HB3	1:44:A:GLN:HG3	9	0.12
(1,1428)	1:31:A:THR:HB	1:32:A:GLU:HG3	10	0.12
(1,1424)	1:163:A:LEU:HD11	1:25:A:GLU:HG3	4	0.12
(1,1424)	1:163:A:LEU:HD12	1:25:A:GLU:HG3	4	0.12
(1,1424)	1:163:A:LEU:HD13	1:25:A:GLU:HG3	4	0.12
(1,1424)	1:163:A:LEU:HD21	1:25:A:GLU:HG3	4	0.12
(1,1424)	1:163:A:LEU:HD22	1:25:A:GLU:HG3	4	0.12
(1,1424)	1:163:A:LEU:HD23	1:25:A:GLU:HG3	4	0.12
(1,1315)	1:39:A:VAL:HG11	1:40:A:PHE:HB3	1	0.12
(1,1315)	1:39:A:VAL:HG12	1:40:A:PHE:HB3	1	0.12
(1,1315)	1:39:A:VAL:HG13	1:40:A:PHE:HB3	1	0.12
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	4	0.12
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	6	0.12
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	8	0.12
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	12	0.12
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	17	0.12
(1,1108)	1:38:A:TYR:H	1:75:A:GLY:HA2	6	0.12
(1,1088)	1:65:A:LEU:H	1:64:A:PRO:HD3	8	0.12
(1,1003)	1:182:A:ASN:HA	1:181:A:LEU:HA	13	0.12
(1,879)	1:28:A:ALA:H	1:25:A:GLU:HA	2	0.12
(1,868)	1:25:A:GLU:HG3	1:25:A:GLU:HA	11	0.12
(1,868)	1:25:A:GLU:HG3	1:25:A:GLU:HA	14	0.12
(1,757)	1:41:A:TYR:HE1	1:41:A:TYR:HA	3	0.12
(1,757)	1:41:A:TYR:HE2	1:41:A:TYR:HA	3	0.12
(1,674)	1:74:A:VAL:HG21	1:34:A:VAL:HA	14	0.12
(1,674)	1:74:A:VAL:HG22	1:34:A:VAL:HA	14	0.12
(1,674)	1:74:A:VAL:HG23	1:34:A:VAL:HA	14	0.12
(1,657)	1:35:A:PHE:H	1:31:A:THR:HA	19	0.12
(1,531)	1:23:A:SER:H	1:26:A:GLN:HE22	6	0.12
(1,499)	1:119:A:PHE:HD1	1:116:A:THR:H	14	0.12
(1,499)	1:119:A:PHE:HD2	1:116:A:THR:H	14	0.12
(1,490)	1:164:A:HIS:HB3	1:164:A:HIS:H	20	0.12
(1,410)	1:94:A:GLN:HE22	1:95:A:THR:H	10	0.12
(1,154)	1:32:A:GLU:HG3	1:32:A:GLU:H	1	0.12
(1,154)	1:32:A:GLU:HG3	1:32:A:GLU:H	14	0.12
(1,26)	1:23:A:SER:HB3	1:24:A:GLU:H	5	0.12
(1,17)	1:52:A:VAL:HB	1:53:A:ALA:H	3	0.12
(2,160)	1:159:A:VAL:O	1:163:A:LEU:N	20	0.11
(2,153)	1:134:A:PHE:O	1:138:A:LEU:N	18	0.11
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	3	0.11
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	4	0.11
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	13	0.11
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	16	0.11
(2,146)	1:107:A:ALA:O	1:111:A:PHE:N	11	0.11
(2,144)	1:94:A:GLN:O	1:98:A:GLN:N	18	0.11
(2,142)	1:84:A:ASP:O	1:88:A:ARG:N	3	0.11
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	10	0.11
(2,140)	1:78:A:LEU:O	1:82:A:GLY:N	11	0.11
(2,139)	1:40:A:PHE:O	1:44:A:GLN:N	10	0.11
(2,139)	1:40:A:PHE:O	1:44:A:GLN:N	12	0.11
(2,137)	1:38:A:TYR:O	1:42:A:ARG:N	8	0.11
(2,136)	1:37:A:SER:O	1:41:A:TYR:N	17	0.11
(2,134)	1:34:A:VAL:O	1:38:A:TYR:N	18	0.11
(2,131)	1:31:A:THR:O	1:35:A:PHE:N	20	0.11
(2,130)	1:30:A:ASP:O	1:34:A:VAL:N	15	0.11
(2,125)	1:170:A:TRP:O	1:174:A:ARG:H	6	0.11
(2,125)	1:170:A:TRP:O	1:174:A:ARG:H	16	0.11
(2,121)	1:168:A:ALA:O	1:172:A:ALA:H	5	0.11
(2,117)	1:159:A:VAL:O	1:163:A:LEU:H	10	0.11
(2,113)	1:157:A:PHE:O	1:161:A:PHE:H	8	0.11
(2,106)	1:153:A:GLN:O	1:157:A:PHE:N	3	0.11
(2,99)	1:150:A:PHE:O	1:154:A:VAL:H	3	0.11
(2,97)	1:139:A:ALA:O	1:143:A:TYR:H	6	0.11
(2,97)	1:139:A:ALA:O	1:143:A:TYR:H	20	0.11
(2,95)	1:137:A:ARG:O	1:141:A:HIS:H	12	0.11
(2,92)	1:135:A:GLY:O	1:139:A:ALA:N	12	0.11
(2,92)	1:135:A:GLY:O	1:139:A:ALA:N	19	0.11
(2,91)	1:135:A:GLY:O	1:139:A:ALA:H	2	0.11
(2,91)	1:135:A:GLY:O	1:139:A:ALA:H	20	0.11
(2,88)	1:132:A:LEU:O	1:136:A:TYR:N	1	0.11
(2,88)	1:132:A:LEU:O	1:136:A:TYR:N	18	0.11
(2,85)	1:131:A:LEU:O	1:135:A:GLY:H	4	0.11
(2,85)	1:131:A:LEU:O	1:135:A:GLY:H	12	0.11
(2,83)	1:130:A:ALA:O	1:134:A:PHE:H	1	0.11
(2,81)	1:129:A:VAL:O	1:133:A:GLY:H	9	0.11
(2,81)	1:129:A:VAL:O	1:133:A:GLY:H	16	0.11
(2,81)	1:129:A:VAL:O	1:133:A:GLY:H	20	0.11
(2,79)	1:127:A:ARG:O	1:131:A:LEU:H	6	0.11
(2,79)	1:127:A:ARG:O	1:131:A:LEU:H	8	0.11
(2,79)	1:127:A:ARG:O	1:131:A:LEU:H	14	0.11
(2,78)	1:126:A:GLY:O	1:130:A:ALA:N	1	0.11
(2,77)	1:126:A:GLY:O	1:130:A:ALA:H	8	0.11
(2,77)	1:126:A:GLY:O	1:130:A:ALA:H	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,77)	1:126:A:GLY:O	1:130:A:ALA:H	19	0.11
(2,75)	1:124:A:ASN:O	1:128:A:VAL:H	1	0.11
(2,63)	1:110:A:TYR:O	1:114:A:ILE:H	3	0.11
(2,63)	1:110:A:TYR:O	1:114:A:ILE:H	11	0.11
(2,63)	1:110:A:TYR:O	1:114:A:ILE:H	14	0.11
(2,63)	1:110:A:TYR:O	1:114:A:ILE:H	16	0.11
(2,63)	1:110:A:TYR:O	1:114:A:ILE:H	19	0.11
(2,57)	1:106:A:ASN:O	1:110:A:TYR:H	18	0.11
(2,57)	1:106:A:ASN:O	1:110:A:TYR:H	20	0.11
(2,54)	1:93:A:PHE:O	1:97:A:LEU:N	4	0.11
(2,53)	1:93:A:PHE:O	1:97:A:LEU:H	14	0.11
(2,50)	1:85:A:ILE:O	1:89:A:TYR:H	12	0.11
(2,47)	1:83:A:ASP:O	1:87:A:ARG:N	4	0.11
(2,47)	1:83:A:ASP:O	1:87:A:ARG:N	13	0.11
(2,43)	1:78:A:LEU:O	1:82:A:GLY:H	1	0.11
(2,31)	1:39:A:VAL:O	1:43:A:HIS:H	9	0.11
(2,25)	1:36:A:ARG:O	1:40:A:PHE:H	18	0.11
(2,19)	1:33:A:GLU:O	1:37:A:SER:H	4	0.11
(2,17)	1:32:A:GLU:O	1:36:A:ARG:H	6	0.11
(2,17)	1:32:A:GLU:O	1:36:A:ARG:H	8	0.11
(2,17)	1:32:A:GLU:O	1:36:A:ARG:H	9	0.11
(2,17)	1:32:A:GLU:O	1:36:A:ARG:H	11	0.11
(2,17)	1:32:A:GLU:O	1:36:A:ARG:H	16	0.11
(2,12)	1:29:A:GLN:O	1:33:A:GLU:N	16	0.11
(2,11)	1:29:A:GLN:O	1:33:A:GLU:H	6	0.11
(2,11)	1:29:A:GLN:O	1:33:A:GLU:H	13	0.11
(2,11)	1:29:A:GLN:O	1:33:A:GLU:H	19	0.11
(2,10)	1:28:A:ALA:O	1:32:A:GLU:N	3	0.11
(2,9)	1:28:A:ALA:O	1:32:A:GLU:H	4	0.11
(2,9)	1:28:A:ALA:O	1:32:A:GLU:H	9	0.11
(2,9)	1:28:A:ALA:O	1:32:A:GLU:H	16	0.11
(2,9)	1:28:A:ALA:O	1:32:A:GLU:H	19	0.11
(2,5)	1:26:A:GLN:O	1:30:A:ASP:H	17	0.11
(2,5)	1:26:A:GLN:O	1:30:A:ASP:H	19	0.11
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB1	1	0.11
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB2	1	0.11
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB3	1	0.11
(1,3094)	1:184:A:GLY:H	2:101:B:ILE:HB	9	0.11
(1,3083)	1:126:A:GLY:H	2:101:B:ILE:HG21	8	0.11
(1,3083)	1:126:A:GLY:H	2:101:B:ILE:HG22	8	0.11
(1,3083)	1:126:A:GLY:H	2:101:B:ILE:HG23	8	0.11
(1,3078)	1:114:A:ILE:H	2:86:B:ILE:HD11	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3078)	1:114:A:ILE:H	2:86:B:ILE:HD12	5	0.11
(1,3078)	1:114:A:ILE:H	2:86:B:ILE:HD13	5	0.11
(1,3049)	1:97:A:LEU:HD11	2:86:B:ILE:HG21	11	0.11
(1,3049)	1:97:A:LEU:HD11	2:86:B:ILE:HG22	11	0.11
(1,3049)	1:97:A:LEU:HD11	2:86:B:ILE:HG23	11	0.11
(1,3049)	1:97:A:LEU:HD12	2:86:B:ILE:HG21	11	0.11
(1,3049)	1:97:A:LEU:HD12	2:86:B:ILE:HG22	11	0.11
(1,3049)	1:97:A:LEU:HD12	2:86:B:ILE:HG23	11	0.11
(1,3049)	1:97:A:LEU:HD13	2:86:B:ILE:HG21	11	0.11
(1,3049)	1:97:A:LEU:HD13	2:86:B:ILE:HG22	11	0.11
(1,3049)	1:97:A:LEU:HD13	2:86:B:ILE:HG23	11	0.11
(1,3049)	1:97:A:LEU:HD21	2:86:B:ILE:HG21	11	0.11
(1,3049)	1:97:A:LEU:HD21	2:86:B:ILE:HG22	11	0.11
(1,3049)	1:97:A:LEU:HD21	2:86:B:ILE:HG23	11	0.11
(1,3049)	1:97:A:LEU:HD22	2:86:B:ILE:HG21	11	0.11
(1,3049)	1:97:A:LEU:HD22	2:86:B:ILE:HG22	11	0.11
(1,3049)	1:97:A:LEU:HD22	2:86:B:ILE:HG23	11	0.11
(1,3049)	1:97:A:LEU:HD23	2:86:B:ILE:HG21	11	0.11
(1,3049)	1:97:A:LEU:HD23	2:86:B:ILE:HG22	11	0.11
(1,3049)	1:97:A:LEU:HD23	2:86:B:ILE:HG23	11	0.11
(1,3044)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	15	0.11
(1,3044)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	15	0.11
(1,3044)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	15	0.11
(1,3044)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	17	0.11
(1,3044)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	17	0.11
(1,3044)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	17	0.11
(1,3019)	1:114:A:ILE:HG21	2:87:B:ALA:H	13	0.11
(1,3019)	1:114:A:ILE:HG22	2:87:B:ALA:H	13	0.11
(1,3019)	1:114:A:ILE:HG23	2:87:B:ALA:H	13	0.11
(1,3010)	1:100:A:LEU:HD21	2:82:B:ILE:HB	1	0.11
(1,3010)	1:100:A:LEU:HD22	2:82:B:ILE:HB	1	0.11
(1,3010)	1:100:A:LEU:HD23	2:82:B:ILE:HB	1	0.11
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD11	16	0.11
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD12	16	0.11
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD13	16	0.11
(1,2983)	1:85:A:ILE:HG21	2:93:B:VAL:HB	1	0.11
(1,2983)	1:85:A:ILE:HG22	2:93:B:VAL:HB	1	0.11
(1,2983)	1:85:A:ILE:HG23	2:93:B:VAL:HB	1	0.11
(1,2983)	1:85:A:ILE:HG21	2:93:B:VAL:HB	11	0.11
(1,2983)	1:85:A:ILE:HG22	2:93:B:VAL:HB	11	0.11
(1,2983)	1:85:A:ILE:HG23	2:93:B:VAL:HB	11	0.11
(1,2979)	1:81:A:ILE:HG21	2:101:B:ILE:HG13	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2979)	1:81:A:ILE:HG22	2:101:B:ILE:HG13	9	0.11
(1,2979)	1:81:A:ILE:HG23	2:101:B:ILE:HG13	9	0.11
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD11	13	0.11
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD12	13	0.11
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD13	13	0.11
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD11	13	0.11
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD12	13	0.11
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD13	13	0.11
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD11	13	0.11
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD12	13	0.11
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD13	13	0.11
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD11	14	0.11
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD12	14	0.11
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD13	14	0.11
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD11	14	0.11
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD12	14	0.11
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD13	14	0.11
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD11	14	0.11
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD12	14	0.11
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD13	14	0.11
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD11	15	0.11
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD12	15	0.11
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD13	15	0.11
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD11	15	0.11
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD12	15	0.11
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD13	15	0.11
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD11	15	0.11
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD12	15	0.11
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD13	15	0.11
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD11	4	0.11
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD12	4	0.11
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD13	4	0.11
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD11	14	0.11
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD12	14	0.11
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD13	14	0.11
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD11	18	0.11
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD12	18	0.11
(1,2965)	1:113:A:LYS:HB3	2:86:B:ILE:HD13	18	0.11
(1,2964)	1:129:A:VAL:HG11	2:97:B:NLE:HE1	1	0.11
(1,2964)	1:129:A:VAL:HG12	2:97:B:NLE:HE1	1	0.11
(1,2964)	1:129:A:VAL:HG13	2:97:B:NLE:HE1	1	0.11
(1,2894)	2:84:B:ARG:HG3	2:85:B:ASN:H	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2875)	2:81:B:ASP:HA	2:84:B:ARG:H	7	0.11
(1,2871)	2:97:B:NLE:HG2	2:98:B:ASP:H	19	0.11
(1,2871)	2:97:B:NLE:HG3	2:98:B:ASP:H	19	0.11
(1,2858)	2:80:B:GLU:HA	2:83:B:ILE:HB	13	0.11
(1,2847)	2:95:B:ASP:HA	2:99:B:ARG:H	10	0.11
(1,2847)	2:95:B:ASP:HA	2:99:B:ARG:H	17	0.11
(1,2812)	2:97:B:NLE:HB2	2:101:B:ILE:HG21	8	0.11
(1,2812)	2:97:B:NLE:HB2	2:101:B:ILE:HG22	8	0.11
(1,2812)	2:97:B:NLE:HB2	2:101:B:ILE:HG23	8	0.11
(1,2812)	2:97:B:NLE:HB3	2:101:B:ILE:HG21	8	0.11
(1,2812)	2:97:B:NLE:HB3	2:101:B:ILE:HG22	8	0.11
(1,2812)	2:97:B:NLE:HB3	2:101:B:ILE:HG23	8	0.11
(1,2805)	2:81:B:ASP:HA	2:84:B:ARG:HB3	8	0.11
(1,2795)	2:88:B:ARG:HA	2:91:B:ALA:H	8	0.11
(1,2794)	2:91:B:ALA:H	2:92:B:MK8:H	9	0.11
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HD	11	0.11
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HDA	11	0.11
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HD	13	0.11
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HDA	13	0.11
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HD	19	0.11
(1,2690)	2:92:B:MK8:HE	2:96:B:MK8:HDA	19	0.11
(1,2495)	1:128:A:VAL:HG21	1:119:A:PHE:HZ	6	0.11
(1,2495)	1:128:A:VAL:HG22	1:119:A:PHE:HZ	6	0.11
(1,2495)	1:128:A:VAL:HG23	1:119:A:PHE:HZ	6	0.11
(1,2495)	1:128:A:VAL:HG21	1:119:A:PHE:HZ	8	0.11
(1,2495)	1:128:A:VAL:HG22	1:119:A:PHE:HZ	8	0.11
(1,2495)	1:128:A:VAL:HG23	1:119:A:PHE:HZ	8	0.11
(1,2407)	1:143:A:TYR:H	1:143:A:TYR:HD1	4	0.11
(1,2407)	1:143:A:TYR:H	1:143:A:TYR:HD2	4	0.11
(1,2383)	1:104:A:ALA:HA	1:150:A:PHE:HD1	5	0.11
(1,2383)	1:104:A:ALA:HA	1:150:A:PHE:HD2	5	0.11
(1,2382)	1:147:A:LEU:HD21	1:150:A:PHE:HD1	13	0.11
(1,2382)	1:147:A:LEU:HD21	1:150:A:PHE:HD2	13	0.11
(1,2382)	1:147:A:LEU:HD22	1:150:A:PHE:HD1	13	0.11
(1,2382)	1:147:A:LEU:HD22	1:150:A:PHE:HD2	13	0.11
(1,2382)	1:147:A:LEU:HD23	1:150:A:PHE:HD1	13	0.11
(1,2382)	1:147:A:LEU:HD23	1:150:A:PHE:HD2	13	0.11
(1,2324)	2:98:B:ASP:H	1:85:A:ILE:HD11	10	0.11
(1,2324)	2:98:B:ASP:H	1:85:A:ILE:HD12	10	0.11
(1,2324)	2:98:B:ASP:H	1:85:A:ILE:HD13	10	0.11
(1,2318)	1:84:A:ASP:HB3	1:85:A:ILE:HD11	1	0.11
(1,2318)	1:84:A:ASP:HB3	1:85:A:ILE:HD12	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2318)	1:84:A:ASP:HB3	1:85:A:ILE:HD13	1	0.11
(1,2318)	1:84:A:ASP:HB3	1:85:A:ILE:HD11	19	0.11
(1,2318)	1:84:A:ASP:HB3	1:85:A:ILE:HD12	19	0.11
(1,2318)	1:84:A:ASP:HB3	1:85:A:ILE:HD13	19	0.11
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB1	7	0.11
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB2	7	0.11
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB3	7	0.11
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB1	7	0.11
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB2	7	0.11
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB3	7	0.11
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB1	7	0.11
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB2	7	0.11
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB3	7	0.11
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG21	14	0.11
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG22	14	0.11
(1,2056)	1:160:A:ASP:H	1:158:A:VAL:HG23	14	0.11
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG21	6	0.11
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG22	6	0.11
(1,1960)	1:177:A:TRP:HE3	1:74:A:VAL:HG23	6	0.11
(1,1923)	1:147:A:LEU:HA	1:147:A:LEU:HD11	4	0.11
(1,1923)	1:147:A:LEU:HA	1:147:A:LEU:HD12	4	0.11
(1,1923)	1:147:A:LEU:HA	1:147:A:LEU:HD13	4	0.11
(1,1893)	1:147:A:LEU:H	1:147:A:LEU:HD21	5	0.11
(1,1893)	1:147:A:LEU:H	1:147:A:LEU:HD22	5	0.11
(1,1893)	1:147:A:LEU:H	1:147:A:LEU:HD23	5	0.11
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD21	13	0.11
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD22	13	0.11
(1,1857)	1:138:A:LEU:HD11	1:97:A:LEU:HD23	13	0.11
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD21	13	0.11
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD22	13	0.11
(1,1857)	1:138:A:LEU:HD12	1:97:A:LEU:HD23	13	0.11
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD21	13	0.11
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD22	13	0.11
(1,1857)	1:138:A:LEU:HD13	1:97:A:LEU:HD23	13	0.11
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD21	13	0.11
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD22	13	0.11
(1,1857)	1:138:A:LEU:HD21	1:97:A:LEU:HD23	13	0.11
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD21	13	0.11
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD22	13	0.11
(1,1857)	1:138:A:LEU:HD22	1:97:A:LEU:HD23	13	0.11
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD21	13	0.11
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD22	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1857)	1:138:A:LEU:HD23	1:97:A:LEU:HD23	13	0.11
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	8	0.11
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	11	0.11
(1,1760)	1:68:A:SER:H	1:67:A:PRO:HG3	12	0.11
(1,1663)	1:27:A:VAL:HG11	1:24:A:GLU:HB3	10	0.11
(1,1663)	1:27:A:VAL:HG12	1:24:A:GLU:HB3	10	0.11
(1,1663)	1:27:A:VAL:HG13	1:24:A:GLU:HB3	10	0.11
(1,1479)	1:34:A:VAL:HG11	1:71:A:MET:HG3	9	0.11
(1,1479)	1:34:A:VAL:HG12	1:71:A:MET:HG3	9	0.11
(1,1479)	1:34:A:VAL:HG13	1:71:A:MET:HG3	9	0.11
(1,1428)	1:31:A:THR:HB	1:32:A:GLU:HG3	1	0.11
(1,1428)	1:31:A:THR:HB	1:32:A:GLU:HG3	14	0.11
(1,1320)	1:85:A:ILE:HG21	1:89:A:TYR:HB3	7	0.11
(1,1320)	1:85:A:ILE:HG22	1:89:A:TYR:HB3	7	0.11
(1,1320)	1:85:A:ILE:HG23	1:89:A:TYR:HB3	7	0.11
(1,1315)	1:39:A:VAL:HG11	1:40:A:PHE:HB3	4	0.11
(1,1315)	1:39:A:VAL:HG12	1:40:A:PHE:HB3	4	0.11
(1,1315)	1:39:A:VAL:HG13	1:40:A:PHE:HB3	4	0.11
(1,1194)	1:85:A:ILE:HA	1:88:A:ARG:HD3	18	0.11
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	1	0.11
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	2	0.11
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	3	0.11
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	5	0.11
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	7	0.11
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	10	0.11
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	13	0.11
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	14	0.11
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	15	0.11
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	16	0.11
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	19	0.11
(1,1123)	1:35:A:PHE:HZ	1:135:A:GLY:HA2	14	0.11
(1,1111)	2:97:B:NLE:HB2	1:126:A:GLY:HA3	3	0.11
(1,1111)	2:97:B:NLE:HB3	1:126:A:GLY:HA3	3	0.11
(1,1098)	2:97:B:NLE:HB2	1:126:A:GLY:HA2	4	0.11
(1,1098)	2:97:B:NLE:HB3	1:126:A:GLY:HA2	4	0.11
(1,1098)	2:97:B:NLE:HB2	1:126:A:GLY:HA2	18	0.11
(1,1098)	2:97:B:NLE:HB3	1:126:A:GLY:HA2	18	0.11
(1,1084)	1:19:A:LEU:H	1:20:A:PRO:HD3	7	0.11
(1,1062)	1:23:A:SER:HB3	1:22:A:ALA:HA	17	0.11
(1,941)	1:68:A:SER:HB3	1:68:A:SER:HA	11	0.11
(1,901)	1:94:A:GLN:H	1:92:A:GLU:HA	1	0.11
(1,901)	1:94:A:GLN:H	1:92:A:GLU:HA	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,896)	1:142:A:VAL:HG21	1:103:A:THR:HA	6	0.11
(1,896)	1:142:A:VAL:HG22	1:103:A:THR:HA	6	0.11
(1,896)	1:142:A:VAL:HG23	1:103:A:THR:HA	6	0.11
(1,868)	1:25:A:GLU:HG3	1:25:A:GLU:HA	7	0.11
(1,868)	1:25:A:GLU:HG3	1:25:A:GLU:HA	13	0.11
(1,868)	1:25:A:GLU:HG3	1:25:A:GLU:HA	15	0.11
(1,784)	1:56:A:ALA:H	1:55:A:PRO:HA	1	0.11
(1,757)	1:41:A:TYR:HE1	1:41:A:TYR:HA	5	0.11
(1,757)	1:41:A:TYR:HE2	1:41:A:TYR:HA	5	0.11
(1,757)	1:41:A:TYR:HE1	1:41:A:TYR:HA	9	0.11
(1,757)	1:41:A:TYR:HE2	1:41:A:TYR:HA	9	0.11
(1,757)	1:41:A:TYR:HE1	1:41:A:TYR:HA	13	0.11
(1,757)	1:41:A:TYR:HE2	1:41:A:TYR:HA	13	0.11
(1,757)	1:41:A:TYR:HE1	1:41:A:TYR:HA	15	0.11
(1,757)	1:41:A:TYR:HE2	1:41:A:TYR:HA	15	0.11
(1,757)	1:41:A:TYR:HE1	1:41:A:TYR:HA	19	0.11
(1,757)	1:41:A:TYR:HE2	1:41:A:TYR:HA	19	0.11
(1,757)	1:41:A:TYR:HE1	1:41:A:TYR:HA	20	0.11
(1,757)	1:41:A:TYR:HE2	1:41:A:TYR:HA	20	0.11
(1,579)	1:124:A:ASN:HB3	1:126:A:GLY:H	5	0.11
(1,527)	1:176:A:GLY:HA2	1:26:A:GLN:HE21	4	0.11
(1,499)	1:119:A:PHE:HD1	1:116:A:THR:H	16	0.11
(1,499)	1:119:A:PHE:HD2	1:116:A:THR:H	16	0.11
(1,475)	1:152:A:GLY:HA3	1:155:A:THR:H	3	0.11
(1,394)	1:161:A:PHE:HB3	1:162:A:MET:H	12	0.11
(1,268)	1:50:A:GLU:HB3	1:52:A:VAL:H	8	0.11
(1,154)	1:32:A:GLU:HG3	1:32:A:GLU:H	4	0.11
(1,154)	1:32:A:GLU:HG3	1:32:A:GLU:H	10	0.11
(1,106)	1:162:A:MET:HG3	1:168:A:ALA:H	17	0.11
(1,16)	1:54:A:ALA:H	1:53:A:ALA:H	19	0.11
(2,157)	1:153:A:GLN:O	1:157:A:PHE:N	8	0.1
(2,153)	1:134:A:PHE:O	1:138:A:LEU:N	12	0.1
(2,152)	1:131:A:LEU:O	1:135:A:GLY:N	17	0.1
(2,141)	1:82:A:GLY:O	1:86:A:ASN:N	20	0.1
(2,140)	1:78:A:LEU:O	1:82:A:GLY:N	2	0.1
(2,117)	1:159:A:VAL:O	1:163:A:LEU:H	4	0.1
(2,101)	1:151:A:LEU:O	1:155:A:THR:H	20	0.1
(2,95)	1:137:A:ARG:O	1:141:A:HIS:H	16	0.1
(2,91)	1:135:A:GLY:O	1:139:A:ALA:H	7	0.1
(2,88)	1:132:A:LEU:O	1:136:A:TYR:N	10	0.1
(2,88)	1:132:A:LEU:O	1:136:A:TYR:N	15	0.1
(2,85)	1:131:A:LEU:O	1:135:A:GLY:H	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,81)	1:129:A:VAL:O	1:133:A:GLY:H	13	0.1
(2,75)	1:124:A:ASN:O	1:128:A:VAL:H	9	0.1
(2,75)	1:124:A:ASN:O	1:128:A:VAL:H	11	0.1
(2,75)	1:124:A:ASN:O	1:128:A:VAL:H	13	0.1
(2,71)	1:114:A:ILE:O	1:118:A:LEU:H	2	0.1
(2,71)	1:114:A:ILE:O	1:118:A:LEU:H	11	0.1
(2,71)	1:114:A:ILE:O	1:118:A:LEU:H	17	0.1
(2,63)	1:110:A:TYR:O	1:114:A:ILE:H	13	0.1
(2,53)	1:93:A:PHE:O	1:97:A:LEU:H	3	0.1
(2,51)	1:85:A:ILE:O	1:89:A:TYR:N	5	0.1
(2,50)	1:85:A:ILE:O	1:89:A:TYR:H	4	0.1
(2,31)	1:39:A:VAL:O	1:43:A:HIS:H	16	0.1
(2,25)	1:36:A:ARG:O	1:40:A:PHE:H	1	0.1
(2,18)	1:32:A:GLU:O	1:36:A:ARG:N	12	0.1
(2,17)	1:32:A:GLU:O	1:36:A:ARG:H	1	0.1
(2,17)	1:32:A:GLU:O	1:36:A:ARG:H	17	0.1
(2,17)	1:32:A:GLU:O	1:36:A:ARG:H	20	0.1
(2,12)	1:29:A:GLN:O	1:33:A:GLU:N	4	0.1
(2,12)	1:29:A:GLN:O	1:33:A:GLU:N	20	0.1
(2,9)	1:28:A:ALA:O	1:32:A:GLU:H	11	0.1
(2,3)	1:24:A:GLU:O	1:28:A:ALA:H	20	0.1
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB1	13	0.1
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB2	13	0.1
(1,3095)	1:117:A:SER:H	2:87:B:ALA:HB3	13	0.1
(1,3049)	1:97:A:LEU:HD11	2:86:B:ILE:HG21	9	0.1
(1,3049)	1:97:A:LEU:HD11	2:86:B:ILE:HG22	9	0.1
(1,3049)	1:97:A:LEU:HD11	2:86:B:ILE:HG23	9	0.1
(1,3049)	1:97:A:LEU:HD12	2:86:B:ILE:HG21	9	0.1
(1,3049)	1:97:A:LEU:HD12	2:86:B:ILE:HG22	9	0.1
(1,3049)	1:97:A:LEU:HD12	2:86:B:ILE:HG23	9	0.1
(1,3049)	1:97:A:LEU:HD13	2:86:B:ILE:HG21	9	0.1
(1,3049)	1:97:A:LEU:HD13	2:86:B:ILE:HG22	9	0.1
(1,3049)	1:97:A:LEU:HD13	2:86:B:ILE:HG23	9	0.1
(1,3049)	1:97:A:LEU:HD21	2:86:B:ILE:HG21	9	0.1
(1,3049)	1:97:A:LEU:HD21	2:86:B:ILE:HG22	9	0.1
(1,3049)	1:97:A:LEU:HD21	2:86:B:ILE:HG23	9	0.1
(1,3049)	1:97:A:LEU:HD22	2:86:B:ILE:HG21	9	0.1
(1,3049)	1:97:A:LEU:HD22	2:86:B:ILE:HG22	9	0.1
(1,3049)	1:97:A:LEU:HD22	2:86:B:ILE:HG23	9	0.1
(1,3049)	1:97:A:LEU:HD23	2:86:B:ILE:HG21	9	0.1
(1,3049)	1:97:A:LEU:HD23	2:86:B:ILE:HG22	9	0.1
(1,3049)	1:97:A:LEU:HD23	2:86:B:ILE:HG23	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB1	11	0.1
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB2	11	0.1
(1,3032)	1:118:A:LEU:HD11	2:91:B:ALA:HB3	11	0.1
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB1	11	0.1
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB2	11	0.1
(1,3032)	1:118:A:LEU:HD12	2:91:B:ALA:HB3	11	0.1
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB1	11	0.1
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB2	11	0.1
(1,3032)	1:118:A:LEU:HD13	2:91:B:ALA:HB3	11	0.1
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD11	15	0.1
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD12	15	0.1
(1,3007)	1:113:A:LYS:HE3	2:86:B:ILE:HD13	15	0.1
(1,2993)	1:130:A:ALA:HB1	2:97:B:NLE:HE1	14	0.1
(1,2993)	1:130:A:ALA:HB2	2:97:B:NLE:HE1	14	0.1
(1,2993)	1:130:A:ALA:HB3	2:97:B:NLE:HE1	14	0.1
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD11	7	0.1
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD12	7	0.1
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD13	7	0.1
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD11	7	0.1
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD12	7	0.1
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD13	7	0.1
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD11	7	0.1
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD12	7	0.1
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD13	7	0.1
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD11	20	0.1
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD12	20	0.1
(1,2975)	1:81:A:ILE:HG21	2:101:B:ILE:HD13	20	0.1
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD11	20	0.1
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD12	20	0.1
(1,2975)	1:81:A:ILE:HG22	2:101:B:ILE:HD13	20	0.1
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD11	20	0.1
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD12	20	0.1
(1,2975)	1:81:A:ILE:HG23	2:101:B:ILE:HD13	20	0.1
(1,2921)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	8	0.1
(1,2921)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	8	0.1
(1,2846)	2:93:B:VAL:HA	2:97:B:NLE:H	12	0.1
(1,2812)	2:97:B:NLE:HB2	2:101:B:ILE:HG21	6	0.1
(1,2812)	2:97:B:NLE:HB2	2:101:B:ILE:HG22	6	0.1
(1,2812)	2:97:B:NLE:HB2	2:101:B:ILE:HG23	6	0.1
(1,2812)	2:97:B:NLE:HB3	2:101:B:ILE:HG21	6	0.1
(1,2812)	2:97:B:NLE:HB3	2:101:B:ILE:HG22	6	0.1
(1,2812)	2:97:B:NLE:HB3	2:101:B:ILE:HG23	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2795)	2:88:B:ARG:HA	2:91:B:ALA:H	18	0.1
(1,2719)	2:90:B:LEU:H	2:91:B:ALA:H	1	0.1
(1,2667)	2:92:B:MK8:HB1A	2:95:B:ASP:HB3	17	0.1
(1,2667)	2:92:B:MK8:HB1B	2:95:B:ASP:HB3	17	0.1
(1,2666)	2:98:B:ASP:HA	2:101:B:ILE:HB	1	0.1
(1,2599)	1:108:A:TYR:HB3	1:108:A:TYR:HE1	7	0.1
(1,2599)	1:108:A:TYR:HB3	1:108:A:TYR:HE2	7	0.1
(1,2599)	1:108:A:TYR:HB3	1:108:A:TYR:HE1	12	0.1
(1,2599)	1:108:A:TYR:HB3	1:108:A:TYR:HE2	12	0.1
(1,2495)	1:128:A:VAL:HG21	1:119:A:PHE:HZ	16	0.1
(1,2495)	1:128:A:VAL:HG22	1:119:A:PHE:HZ	16	0.1
(1,2495)	1:128:A:VAL:HG23	1:119:A:PHE:HZ	16	0.1
(1,2241)	1:28:A:ALA:H	1:168:A:ALA:HB1	5	0.1
(1,2241)	1:28:A:ALA:H	1:168:A:ALA:HB2	5	0.1
(1,2241)	1:28:A:ALA:H	1:168:A:ALA:HB3	5	0.1
(1,2176)	1:138:A:LEU:H	1:139:A:ALA:HB1	7	0.1
(1,2176)	1:138:A:LEU:H	1:139:A:ALA:HB2	7	0.1
(1,2176)	1:138:A:LEU:H	1:139:A:ALA:HB3	7	0.1
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB1	17	0.1
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB2	17	0.1
(1,2133)	1:159:A:VAL:HG21	1:28:A:ALA:HB3	17	0.1
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB1	17	0.1
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB2	17	0.1
(1,2133)	1:159:A:VAL:HG22	1:28:A:ALA:HB3	17	0.1
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB1	17	0.1
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB2	17	0.1
(1,2133)	1:159:A:VAL:HG23	1:28:A:ALA:HB3	17	0.1
(1,1981)	1:136:A:TYR:HD1	1:39:A:VAL:HG21	11	0.1
(1,1981)	1:136:A:TYR:HD1	1:39:A:VAL:HG22	11	0.1
(1,1981)	1:136:A:TYR:HD1	1:39:A:VAL:HG23	11	0.1
(1,1981)	1:136:A:TYR:HD2	1:39:A:VAL:HG21	11	0.1
(1,1981)	1:136:A:TYR:HD2	1:39:A:VAL:HG22	11	0.1
(1,1981)	1:136:A:TYR:HD2	1:39:A:VAL:HG23	11	0.1
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD21	8	0.1
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD22	8	0.1
(1,1924)	1:180:A:ALA:HA	1:183:A:LEU:HD23	8	0.1
(1,1755)	1:56:A:ALA:H	1:55:A:PRO:HG3	8	0.1
(1,1708)	1:30:A:ASP:HA	1:29:A:GLN:HB3	3	0.1
(1,1707)	1:94:A:GLN:HE22	1:94:A:GLN:HB3	7	0.1
(1,1428)	1:31:A:THR:HB	1:32:A:GLU:HG3	9	0.1
(1,1346)	1:157:A:PHE:HD1	1:111:A:PHE:HB3	20	0.1
(1,1346)	1:157:A:PHE:HD2	1:111:A:PHE:HB3	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1189)	1:159:A:VAL:HG11	1:156:A:ARG:HD3	13	0.1
(1,1189)	1:159:A:VAL:HG12	1:156:A:ARG:HD3	13	0.1
(1,1189)	1:159:A:VAL:HG13	1:156:A:ARG:HD3	13	0.1
(1,1189)	1:159:A:VAL:HG11	1:156:A:ARG:HD3	16	0.1
(1,1189)	1:159:A:VAL:HG12	1:156:A:ARG:HD3	16	0.1
(1,1189)	1:159:A:VAL:HG13	1:156:A:ARG:HD3	16	0.1
(1,1145)	1:174:A:ARG:H	1:175:A:GLY:HA3	11	0.1
(1,1111)	2:97:B:NLE:HB2	1:126:A:GLY:HA3	17	0.1
(1,1111)	2:97:B:NLE:HB3	1:126:A:GLY:HA3	17	0.1
(1,1087)	1:47:A:GLN:HE22	1:55:A:PRO:HD3	8	0.1
(1,1063)	1:19:A:LEU:HB3	1:18:A:ALA:HA	2	0.1
(1,1063)	1:19:A:LEU:HB3	1:18:A:ALA:HA	13	0.1
(1,1027)	1:27:A:VAL:HG21	1:168:A:ALA:HA	3	0.1
(1,1027)	1:27:A:VAL:HG22	1:168:A:ALA:HA	3	0.1
(1,1027)	1:27:A:VAL:HG23	1:168:A:ALA:HA	3	0.1
(1,1003)	1:182:A:ASN:HA	1:181:A:LEU:HA	14	0.1
(1,1003)	1:182:A:ASN:HA	1:181:A:LEU:HA	20	0.1
(1,959)	2:82:B:ILE:HD11	1:99:A:HIS:HA	1	0.1
(1,959)	2:82:B:ILE:HD12	1:99:A:HIS:HA	1	0.1
(1,959)	2:82:B:ILE:HD13	1:99:A:HIS:HA	1	0.1
(1,901)	1:94:A:GLN:H	1:92:A:GLU:HA	7	0.1
(1,868)	1:25:A:GLU:HG3	1:25:A:GLU:HA	8	0.1
(1,868)	1:25:A:GLU:HG3	1:25:A:GLU:HA	17	0.1
(1,757)	1:41:A:TYR:HE1	1:41:A:TYR:HA	7	0.1
(1,757)	1:41:A:TYR:HE2	1:41:A:TYR:HA	7	0.1
(1,542)	1:172:A:ALA:HB1	1:173:A:GLN:HE22	15	0.1
(1,542)	1:172:A:ALA:HB2	1:173:A:GLN:HE22	15	0.1
(1,542)	1:172:A:ALA:HB3	1:173:A:GLN:HE22	15	0.1
(1,499)	1:119:A:PHE:HD1	1:116:A:THR:H	1	0.1
(1,499)	1:119:A:PHE:HD2	1:116:A:THR:H	1	0.1
(1,410)	1:94:A:GLN:HE22	1:95:A:THR:H	8	0.1
(1,410)	1:94:A:GLN:HE22	1:95:A:THR:H	17	0.1
(1,368)	1:119:A:PHE:HA	1:123:A:ILE:H	10	0.1
(1,175)	1:118:A:LEU:HD11	1:131:A:LEU:H	5	0.1
(1,175)	1:118:A:LEU:HD12	1:131:A:LEU:H	5	0.1
(1,175)	1:118:A:LEU:HD13	1:131:A:LEU:H	5	0.1
(1,123)	1:34:A:VAL:HG11	1:74:A:VAL:H	11	0.1
(1,123)	1:34:A:VAL:HG12	1:74:A:VAL:H	11	0.1
(1,123)	1:34:A:VAL:HG13	1:74:A:VAL:H	11	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found